

A GUIDE TO THE DIVIMP CODE

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This Guide is supplemented by the
DIVIMP User Manual
which describes how to run the code itself. This Guide describes the purpose,
basic ideas and physics assumptions of DIVIMP.

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Note: This Guide is being updated regularly. Before using it
check with P. C. Stangeby that you have the current version.

The DIVIMP Code was developed at JET and at the University of Toronto with support by JET and by the Canadian Fusion Fuels Technology Project.

The basic documentation of the DIVIMP Code is a set of numbered “Notes” in three series:

- (a) notes designated by an “N” originated with P. C. Stangeby and were sent to colleagues at JET.
- (b) notes designated by a “TN” originated with P. C. Stangeby and were sent to colleagues in Toronto.
- (c) notes designated by an “A” originated with L. D. Horton and were sent to P. C. Stangeby and other colleagues.

In this Guide, and in the DIVIMP User Manual these Notes are frequently referenced. Copies of any specific Note can be obtained from P. C. Stangeby.

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Overview

DIVIMP (Divertor Impurities) is a Monte Carlo code which follows the trajectories of individual impurity particles in the edge plasma of a divertor tokamak. In the simplest version of the code, the plasma, “background plasma,” typically hydrogenic, is *specified*, e.g., the spatial variations of n_e , T_e , T_i are specified. The DIVIMP code then launches impurity ions or neutrals, e.g., from sputtering of the divertor target, into this fixed plasma background and follows the particle through successive stages of ionization (or recombination) as it moves through the plasma — taking both the cross-field and parallel-to-field motion into account. The parallel motion is taken to be described by classical physics (Spitzer collision times). The cross-field motion is assumed to be anomalous with prescribed cross-field diffusion coefficients (and possibly a pinch).

Usually toroidal symmetry is assumed and the particle motion can then be considered to be 2-D and to occur in the poloidal plane.

The particle is followed until it deposits out on a solid surface — the divertor targets or the vessel walls. Self-sputtering can then be included and the self-sputtering “cascade” is followed until the statistical weight of the particle (which is equal to the product of all the sputtering yields of the sputtering steps in the cascade) falls below some specified number, say 0.1. That particle is then taken to have finally deposited out and a new particle is launched. The launch location, for the initial sputtering event, the launch velocity and the launch angle are chosen in a Monte Carlo way and are weighted by the calculated sputtering yield (based on the specified plasma background) and known velocity and angular variations for sputtered particles.

Impurities can also be launched as from a gas puff or from a wall source.

When a large number of particles have been launched, typically 10^3 - 10^4 , the 2-D spatial distributions of the successive charge states are computed. Since the particles have been followed in time, it is possible to model a time-dependent impurity source. Usually, however, steady-state is assumed and the standard DIVIMP output involves a time integration which assumes that the source has been on at a steady rate for a time which is long compared with the average dwell-time of particles in the plasma.

From the spatial distribution of all the charge states of the impurity it is possible to then calculate such observables as the integrated line-of-sight intensities of specific spectroscopic lines, which can then be compared directly with measurements. Other calculated quantities which can be compared with measurements are 2-D impurity temperature patterns, 2-D Z_{eff} , 2-D total radiation power, erosion and deposition patterns, and several other experimental observables.

The calculations are performed on a 2-D grid, typically generated from the magnetics measurements for a specific shot on a specific tokamak at a specific time in the shot. The grids may be orthogonal or non-orthogonal. Such grids are widely available, having been generated for the application of 2-D edge fluid codes, such as EDGE2D, B2, LEDGE, etc., and hydrogenic neutral codes, such as NIMBUS, EIRENE, DEGAS, etc. It is therefore convenient and most useful to couple DIVIMP to these other codes — for either interpretive or predictive work.

The original, and still most basic, purpose of the DIVIMP code is the interpretation of experiments. In this situation one will often have experimental measurements of the plasma density and temperature variations across the divertor targets. One can then use such measurements as boundary conditions to construct one-dimensional models (along \bar{B}) of the background plasma, thereby creating a two-dimensional description of the plasma edge which is a mixture of experiment and theory. Such models are termed Onion-Skin Models, and a number of these, incorporating various

degrees of sophistication in the physics, are available internally to the DIVIMP code as “SOL Options.”

Also available as an option for specifying the plasma background are the 2-D solutions of the 2-D edge fluid codes, such as EDGE2D and B2, which can be directly coupled to DIVIMP.

Under development are feedback modes of operating DIVIMP where the impurity radiation, densities, and other quantities, are fed back in an iterative way to either the internal Onion Skin Model, or to the coupled, external 2-D edge fluid code. The objective with the first type of coupling is to have a better interpretive tool, and for the second, a better predictive tool.

Whether based on an internal Onion-Skin Model for the plasma background, or an external fluid code, it is very advantageous to calculate the neutral hydrogenic 2-D ionization pattern, etc., from a code such as NIMBUS or EIRENE. The spatial location of the hydrogenic ionization controls the drift speed of the plasma along \bar{B} , and thus the critically important frictional force on the impurities. It is therefore important to have as realistic a description of the neutral hydrogen behaviour as possible.

The code requires atomic data for ionization and recombination rates, and for excitation of radiating levels. A number of atomic data base options are available within DIVIMP, but the preferred one is the ADAS, Atomic Data and Analysis Structure, code of H. P. Summers, to which DIVIMP is coupled. ADAS assumes that the excited levels for each state of ionization of the impurity are “instantly” in equilibrium with the local electron distribution (n_e and T_e), and so calculates the radiation intensity for each spectroscopic line of interest as of a function of n_e , T_e and the local impurity density of the charge state n_q^{imp} (charge q) — allowing for many excited levels in each atomic level system. The local (2D) values of n_q^{imp} are provided by the DIVIMP calculation.

1.0 Introduction and General Philosophy

1.1 The Problem of Interpreting Edge Measurements

It is evident that the edge plasma is rather complicated. Spatial variations are generally at least two-dimensional (toroidal symmetry may hold which allows one to eliminate three-dimensional variation). By contrast the core plasma often exhibits only one-dimensional variation. In addition, this two-dimensional region has a contorted *shape*, making measurements such as line-of-sight ones difficult to interpret. In addition, it is also a very *thin* region, which causes problems in making spatially resolved measurements reliably.

There never seem to be enough experimental measurements of important edge quantities. Some important quantities, such as T_i , are typically not measured at all. The electron density and temperature will often be available — but only at a few locations. The reliability of such basic edge measurements as T_e from Langmuir probes may also be in question; typically Langmuir probe analysis is based on the I-V characteristic using data only above floating potential, and so only the high energy tail of the electron distribution is sampled; fast (epithermal) electrons may be present and so the measured value of T_e may not be representative of most of the electrons.

Uncertainties of every sort are present — see Sec. 1.2. Even if there was no error on the edge measurements and even if the atomic and other data bases needed to interpret the results were complete and error-free — what *sense* can one make of the measurements? What *use* can one put them to? How can one make up a *physics story*, based on the measurements? What can one *learn* from the measurements about the processes going on in the edge? What, for example, do we learn from some particular 2-D line-of-

sight survey of some CIV line in the edge? What sense can we make of it? The answer is not immediately obvious.

Clearly, in general, we cannot make anything very useful from an *individual* measurement in the edge. Sometimes a “local story” can be constructed from one or two local measurements that do not involve problems of line-of-sight deconvolution or other problems which distort or modify the interpretation of the measurement. But generally, *it seems likely that the best way to understand what is going on in the edge is to interpret all of the available experimental data simultaneously*. In this way the effect of the uncertainties — error bars on the measurements, uncertainties in the data bases, etc. — can be reduced through the *redundancy* and expected *self-consistency* of experimental information. The same argument applies regarding the key quantities about which there is, usually, no experimental information at all (e.g. T_i , the plasma parallel drift velocity v_B , the parallel electric field, cross-field drifts and other quantities). In addition, line-of-sight information which may not be *directly* useable to resolve these characteristics at positions along the line-of-sight can add greatly to the confidence that one has modeled the basic situation correctly, if the line-of-sight measurements match the model calculations. On the other hand, if they do not match, one may not know immediately just what is wrong but may have some indications of what effects might be contributing to the experimental observations.

The fact that processes throughout the edge are generally strongly coupled is also addressed in such an all-inclusive approach; in the edge we are generally interested in variations *along* the \bar{B} -field, which is not usually the case in the core plasma. Parallel transport is extremely fast and parallel characteristic times are milli-seconds or less. Since the cross-field extent of the edge plasma is governed by a balance between parallel and perpendicular transport, these same short characteristic times typify edge radial variations also.

The edge plasma then is a tightly-knit two-dimensional complex. Interpreting edge measurements so as to learn something useful about edge behaviour generally requires an ambitious undertaking in data

interpretation — and one which should confront one’s model with *all* of the available experimental data simultaneously. This can generally only be done using sophisticated codes to do the “bookkeeping”. One’s model may not be very sophisticated in it’s essential components, but its results, in the complex environment and geometry of the edge, can manifest itself in such complicated ways (even if trivially so, as in line-of-sight integrals), that one has little hope of keeping track of things by hand, or by analytic methods. One such code-based approach is through the DIVIMP (Divertor Impurity) code, as described here.

1.2 Uncertainties About the Edge

The present level of understanding about edge processes presumably reflects the fact that (a) the edge plasma is more complex than the core plasma, and (b) the edge has received only a small fraction of the research effort expended on the core. It should thus be no surprise that we are uncertain about almost all aspects of the edge — not just about the processes which may be important, but even the edge plasma parameters. While our *theoretical* ideas about the edge have become extremely sophisticated — driven primarily by predictive code design efforts for INTOR and ITER — we should not let this mislead us - *We have, at best, only weak experimental confirmation of even the simplest theoretical ideas, concerning edge behaviour.*

One may take the existence of parallel temperature gradients as an illustration of this point. There is scarcely a more important idea regarding the edge plasma in divertor experiments. Such gradients are essential if one is to have a reasonably low plasma density and thus fairly high temperature, in the Scrape-Off-Layer (SOL) at the “upstream” end of the SOL (i.e. at the mid-plane or generally at the edge of the confined plasma) — while simultaneously having a low temperature (and high density, if pressure is constant along \bar{B}) at the target. The latter is essential for the control of plasma impurity and target erosion. Considerable effort has gone into experimentally confirming the simple theoretical predictions of parallel temperature gradients based on parallel electron thermal conduction. Unfortunately this is very difficult to do. Radial temperature gradients are

very steep and one must achieve great accuracy, radially, when making the temperature measurements. In addition, very fine spatial resolution, on the order of millimeters, is also required. It may be that only Langmuir probes can meet these requirements. One must not only be extremely accurate as to the probe location in terms of the machine (R, Z) coordinates — but it is essential to know what magnetic flux surface one is sampling. This introduces further substantial uncertainties. In addition, there are the uncertainties about measuring T_e using a Langmuir probe referred to in the last section. Taking all these uncertainties together, it has to be acknowledged that the experimental evidence confirming the existence of parallel T_e -gradients is less than overwhelming. And — it should be noted — there has probably been no-more-studied an edge phenomenon than this.

The following is a partial listing of things we are uncertain about in the edge. A separation has been made into aspects involving the “background” plasma (e- D^+ , say) and impurities.

1.2.1 The Plasma Background

1. *Measurements of Basic Quantities.* As already discussed n_e and T_e may only be measured at a few points; location in terms of the magnetic flux surface may not be known to better than ~ 1 cm, which can be the order of the radial characteristic length; Langmuir probes have interpretation uncertainties; other diagnostic methods typically have poorer spatial resolution. Typically there is no experimental information on such critical quantities as T_i , the parallel drift velocity or the parallel electric field. Radial electric fields are poorly known. Thus radial and poloidal $\vec{E} \times \vec{B}$ drifts are poorly known. The parallel flow may involve flow reversal, but if it does then very fine spatial resolution is required to detect it. Langmuir “Mach” probes only measure flow direction, not flow magnitude (since we do not know the relation between perpendicular particle and momentum diffusivities).
2. *Modeling Uncertainties*

- (a) Cross-field transport coefficients. Little is known about edge values of the particle, heat, momentum diffusivities, D_{\perp} , $\chi_{\perp}^{e,i}$, η_{\perp} or how they depend on density, temperature, poloidal magnetic field, toroidal magnetic field, etc. The common assumption of spatially constant coefficients has little justification.
- (b) Power outflow from the core to the SOL. One can deduce the total power into the SOL from measurements of P_{in} and P_{rad}^{core} ; however, for purposes of a complete modeling of the edge (as per 2-D fluid codes) one needs to know the split between the two channels $P_{SOL}^{e,i}$. Little is known about this split.
- (c) Parallel transport uncertainties. If the edge plasma were strongly collisional then the fluid approximation would be excellent, and one would have little concern about modeling parallel transport. Unfortunately, edge collisionality is marginal. Much work has been invested in making kinetic corrections, involving “flux limits” to parallel viscosity, heat conduction, etc. Great complexity is encountered and confidence cannot be high given the lack of experimental confirmation of the effects. The plasma flow can be sonic or supersonic and so the ion velocity distributions can be highly non-Maxwellian, making linearizing assumptions uncertain.
- (d) Extreme volatility when modeling the SOL “top-down”. For *predictive* work one has little choice but to model the edge using a 2-D fluid code, such as B2, EDGE2D, LEDGE, etc., “top down”, that is, assuming boundary conditions at the top end (e.g., mid-plane) of the SOL, specifically $P_{SOL}^{e,i}$, n_{top} — and computing “downstream” to the targets. As discussed in Sec. 3.1.1, for the “high recycling regime”, this results in very volatile predictions for n , T , etc., at the target: small changes/uncertainties in virtually any quantity of interest causes n_t , T_t , etc., to vary greatly. For *interpretive* work, fortunately, one can start from

measured n_t , T_t and calculate “upstream”. This enjoys the inverse effect: predictions of the upstream conditions are highly robust; see Sec. 3.1.1. Such “Onion-Skin Modeling”, however, has its own problems and limitations, Sec. 3.1.1.

1.2.2 Impurity Behaviour

1. *Experimental measurements.* Actually this is the bright spot of the problem, and getting brighter. Fortunately, impurities are very visible and readily identifiable (as to species and charge state) in a hot plasma. Two-dimensionally, absolutely-calibrated surveys are available for more and more lines-of-sight, and different spectroscopic lines, at visible and other wavelengths, on more and more machines. Doppler temperatures and drift velocities are becoming available, with 2-D resolution. The multiplicity of impurities and charge states make impurities an ideal diagnostic opportunity and if impurities were not produced naturally in tokamaks, they would be injected simply because of the diagnostic potential, as is indeed done.
2. *Impurity modeling.* Modeling the impurity behaviour is still more uncertain than modeling the plasma background: since the impurity behaviour is highly sensitive to the background, all the uncertainties associated with the latter carry over; in addition, there are the uncertainties specific to the impurity production and transport:
 - (a) Production. The simplest case, perhaps, is physical sputtering and laboratory data on sputtering yields, and on the velocity and angular distribution of sputtered particles have been measured for many cases of interest. Laboratory studies show that the angle of incidence of the impacting particle and the degree of surface roughness can strongly influence the yields, velocity and angular distributions. Our knowledge about angles of incidence and surface roughness is generally poor, for the actual tokamak environment. Therefore, *in effect*, the parameters needed to model physical sputtering are *not* well known.

For chemical and Radiation Enhanced Sputtering (RES) of carbon, the tokamak situation is still less clear, and the applicability of the laboratory data still more uncertain.

The sputtering of the *walls* may be more important than the target sputtering, since such impurity sources may be able to contaminate the core plasma more efficiently. Wall sputtering may be due to the impact of charge-exchange neutrals — which can be calculated, in principle, using a neutral hydrogen code such as NIMBUS, EIRENE or DEGAS — albeit with further uncertainties. It may also be that some type of ion loss to the walls may be involved (“loss orbits”, “stray field effects”, etc.). Also, release of impurities may be due to thermal or photon effects. The cause of wall release of impurities then, involves uncertainties as to mechanism, spatial distribution, yields, and many other factors.

- (b) Impurity transport. The same uncertainties involved in the perpendicular and parallel transport of the background plasma apply to the impurities. It is also not known if the anomalous cross-field transport coefficients differ among impurities, their different charge states or between impurities and the hydrogenic species.

1.3 Given Such Uncertainty: How to Proceed to Interpret Edge Measurements?

One sometimes hears the statement from a modeler: “I have put in all the physics that is known.” Unfortunately, in the case of modeling the edge, this is very little! It is certainly worth having *options*, in one’s modeling approach, where one puts in all the physics that one *thinks* might apply. It would, however, be imprudent to have this as one’s only option in interpreting the tokamak edge. This is also a rather inflexible approach, given all the uncertainties.

Thus one also needs to have options in the modeling which are more like *prescriptions*, than models as normally understood (i.e. models based on the conservation of mass, momentum and energy). For example, it is useful to have simple (or not-so-simple) prescriptions for:

- (a) How n_e , T_e , T_i , drift velocity (including flow reversal), etc., vary along each field line — based, ideally, on measured conditions, at least for n_e and T_e , along the targets, i.e., for each flux tube.
- (b) Impurity production — both as to spatial distribution and intensity, from targets and walls,
- (c) $\vec{E} \times \vec{B}$ drifts,
- (d) Cross-field diffusion transport coefficients.
- (e) Etc

Thus, it is useful to have “models” with many “adjustable knobs”, one for each of the many quantities that we do not know. Provided that one can confront the model predictions of observables (e.g. particular line-of-sight measurements and such) with a sufficiently large number of measurements — then the “adjustable knobs” become constrained and ideally, over-constrained, thus providing consistency checks on the modeling process.

Of course, one is also interested to see if the experimental data can be matched using a model based on the physics that one thinks may hold. Thus models based on the conservation equations are also wanted — although, keeping in mind that we are unsure about many of the terms that should be used in these equations; one should therefore also leave as much flexibility in these models as possible (i.e. more knobs).

1.4 The Advantage of Interpreting In The Upstream Direction Starting from the Target Region

It is particularly useful to have measurements of plasma conditions across the target plates. One can then proceed to use an *extremely* simple prescription for the plasma background. Thus one can model the lowest charge states of the impurities released at the plate (e.g. C^0 (CI), C^+ (CII) for carbon targets) by assuming conditions remain constant, at the local target values, along each flux tube. Such a simple prescription should usually be adequate for at least a first order estimate since, in the case of the lowest charge states, their spatial distribution, intensity and Doppler-temperatures are usually only sensitive to plasma conditions very near the targets.

Thus one can bring to bear a relatively extensive set of experimental data to sort out what the conditions near the target *really* are - after all:

- (a) one does not necessarily trust the target Langmuir probe measurements of n_e and T_e ; epithermal electrons and other effects may be present.
- (b) in any case the critical quantity, T_i , is not measured by the Langmuir probes; one must try to “back its value out” from the overall set of measurements.
- (c) the plasma flow to the target may be supersonic.
- (d) we do not know, *a priori*, what the impurity production mechanism is, nor how to characterize it quantitatively.

One hopes to be able to sort out all these *boundary* conditions at the target first, by just focusing on the lowest impurity charge states. This does not yet get one entangled in questions about *transport* of the impurities, cross-field transport coefficients, the presence of drifts or flow reversal, and the questions of how to correctly model the plasma as one moves upstream from the targets.

Assuming that the boundary conditions have been well sorted out, one can then move on to the next charge state, e.g., C^{2+} (CIII), which will now start to provide information at some distance — but still rather short — from the targets. This will provide information to discriminate between and to test different models/prescriptions for how n_e , T_e , T_i , etc., vary along the field lines.

And so one can proceed a step at a time through the charge states to build up a model of the edge plasma, pushing upstream further and further.

Thus, impurities released at the target provide a valuable opportunity for *incrementally* developing a picture of the edge processes. One is not forced to simply calculate the “whole thing” and then confront model with experiment — which is clearly a less flexible, less informative approach. Of course, one is free to *also* use such options, and *should* do so. After all, who knows? Perhaps all the relevant physics really is *already* in the model for some situations? In any case, the “Onion-Skin Modeling” approach, which calculates in the upstream direction, has its own problems and limitations, see 3.1.1.

1.5 The Approach Taken in DIVIMP

For *predictive* work one has no choice but to calculate “the whole thing” — the hydrogenic plasma together with the impurities. Confidence in our ability to model even a pure edge plasma cannot be great for the reasons discussed earlier, and so confidence in modeling the impure edge must be still less. For the impurities one is unfortunately compounding uncertainty on top of uncertainty.

For *interpretive* work one has an opportunity to reduce uncertainty regarding the interpretation of the impurity behaviour. One can try to take the “plasma background”, principally the hydrogenic 2-D distributions, from *experimental* measurements. Ideally one would have complete experimental - 2-D distributions of n_e , T_e , T_i and flow velocity throughout the edge. Of course, we are very far from such an ideal situation. Nevertheless, in principle, it remains an attractive alternative to attempt to *separate* the problem into (a) the “plasma background” model/prescription, and (b) the impurity modeling.

For the plasma background one is obliged to use a mixture of experimental measurement and model/prescription in order to come up with

a *complete* 2-D spatial specification of n_e , T_e , T_i , plasma drift velocity, electric field and the other required background quantities.

Into this *specified* plasma background one can then launch the impurities and see how they behave according to the model. One then confronts the experimental measurements with the calculated values and adjusts *both* the plasma background, as well as the impurity, “adjustable knobs” to get agreement. Given sufficient measurements the exercise is constrained and one is involved in a physics-learning exercise. On the other hand, with too little experimental data, relative to the number of “adjustable knobs”, the exercise is merely one of data-fitting, teaching one little physics. It is also important that *critical judgment* be exercised in the use of the fitting “knobs”. It may be possible to match a specific set of experimental observables but then one must consider critically the particular modeling options chosen to obtain that result. If, for example, a good match was obtained, but it involved using a cross-field diffusion coefficient of $100 \text{ m}^2/\text{s}$, then it might be worthwhile to investigate other alternatives or to conjecture about some missing physics to account for the observations.

A most natural way to model the impurities in a situation where the plasma background is thus *given*, is a Monte Carlo one, as used in DIVIMP:

1. Monte Carlo modeling involves straightforward mathematics with no convergence or stability problems (in the most basic approach), and thus one can concentrate fully on physics issues, not troubling about mathematical ones.
2. It incurs negligible computational penalty to allow the impurities - each charge state followed individually - to have their own temperature, different from the background plasma ions (to which they are, however (imperfectly) coupled). Indeed, in the Monte Carlo approach one does not even assume that the impurity ions have a Maxwellian velocity distribution, and one follows the actual velocity distribution; the approach is thus a quasi-kinetic one, an advantage given the marginal collisionality of the edge plasma. Since experimental measurements are becoming available of impurity

Doppler-temperatures, one wishes to be able to model T_i , and to not simply assume $T_i = T_{iB}$, the background ion temperature (which is the usual assumption in 2-D fluid modeling, where the use of separate energy equations for each impurity, and each charge state, is impractical).

3. The approach is also quasi-kinetic in that no assumptions or constraints are placed on the collisional mean free paths of the impurity ions. Any and all values, relative to the system scale lengths, are automatically handled.
4. The “plasma background” can be generated at various levels of sophistication:
 - (a) options are available for direct coupling to the 2-D fluid codes, EDGE2D and B2, in order to use their output as input to DIVIMP; see Sec. 3.2.
 - (b) internal to DIVIMP are a number of “SOL Options”, which are “Onion-Skin Models” (1-D for each flux tube, starting from boundary conditions at the target) — ranging from simple prescriptions to models incorporating many physical processes; see Sec. 3.1.

This, then, constitutes the basic method of applying DIVIMP to the interpretation of experimental edge data.

In reality, the “background plasma” and the impurities are coupled in more complex ways than the one-way link implicit in the basic method of using DIVIMP, as just outlined. Probably the most important way that the impurities *feed back* on the background plasma, is via the cooling of the electrons due to impurity radiation. This, however, can be allowed for even in the most basic DIVIMP approach since a number of the “SOL Options” allow for a 2-D electron radiative cooling term, P_{rad} , to be *specified*, e.g., from *experimental* measurements; alternatively, one can simply specify P_{rad} arbitrarily, or one can be guided by the DIVIMP output itself, i.e., in a crude,

“by-hand”, feedback mode. Currently under development are true feedback modes:

- (a) At Toronto this is being done using the internal SOL Option Onion-Skin Models, Sec. 3.1, which DIVIMP will iterate to convergence. Initially only the 2-D P_{rad} is fed back, but feedback of the 2-D spatial densities of each charge state will also be made in order to correct the frictional force term, the electron and ion temperature gradient force coefficients and others, following the formulations of Yu. Igitkhanov, Contrib. Plasma Phys. 28 (1988) 477.
- (b) At Jülich, DIVIMP is being coupled to the B2 hydrogenic fluid ion code and the EIRENE hydrogenic neutral Monte Carlo code. The code outputs will be iterated to convergence. This coupled code system will thus also be useable for predictive work.

2.0 Grids

2.1 Introduction

The DIVIMP code uses a set of grids derived from the measurements of the magnetic field on a certain machine for a certain shot at a certain time, as the basis for tracking and accounting for the injected particles. These grids form the underpinning of DIVIMP operation and their characteristics are crucial to obtaining meaningful results from DIVIMP simulations. DIVIMP does not generate these grids itself - they are instead generated by independent codes GRID2D (at JET) and Sonnet (for CMOD and AUG). These are the same grids that are used by the corresponding fluid codes in use at JET and AUG. Essentially these grids map the plasma space of a poloidal cross-section of the tokamak onto a series of connected polygons that extend from a distance radially into the Scrape-off layer and to some distance into the main plasma. The spatial variation and coverage of these grids is one of the characteristics controlled by the grid generation programs. Furthermore, the index numbers of the cells, their order, and their sizes and shapes are all other specifiable characteristics for the grid generation programs. Included in this is whether or not the grids themselves are orthogonal. Orthogonality is defined by several factors. First, if one joins the midpoints of opposite sides of the polygon (assuming 4 sides) then the angle at which these lines cross will be 90 degrees for an orthogonal cell. Furthermore, the sides of the polygon lying along the field lines will be parallel to the field line and the other two sides of the polygon will be perpendicular to the field lines (see fig 2.1 and fig 2.2).

In some cases it is necessary to make the grids non-orthogonal to match the spatial placement of the targets relative to the grid configuration. This is done by moving the corners of the polygons along the field lines so that the center-line and sides that started parallel to the field lines remain parallel. However, the polygon sides and center-line that were perpendicular

to the magnetic field are not necessarily perpendicular after the adjustments. DIVIMP simply uses the grids that result from these grid programs. This section will describe the grids and primary DIVIMP options related to the interpretation of these grids.

The grids consist of a listing of (R,Z) coordinates of the center point and each of the corners of the polygons (sometimes referred to as cells) indexed in a variety of ways. Typically there will be four corners though this is not strictly required for determining which cell a particle is in. The corners determine if the cell is orthogonal or not. With knowledge of the center and corner points it is possible to determine whether any R,Z position in space lies within the grided region and if it does, exactly which cell it lies in. This method is used to track both neutrals and ions in DIVIMP. A previous version of DIVIMP (DIVIMP2) made use of the cell center points only and had no knowledge of the cell corners. In this configuration DIVIMP used a finely resolved underlying rectangular grid and calculated the closest grid center point to each of these before injecting any particles - these XY grids were used in accumulating the neutral particle statistics. This method is no longer in use because it is less precise than using the exact cell structure information. However, it is still supported in the case of grids for which only the center points are available. Furthermore, there are a variety of code sections in DIVIMP that still calculate quantities based solely on cell centers, this is in part to maintain compatibility with older grids, however the code is being updated when the time is available. A still older version of DIVIMP (DIVIMP1) utilized a grid generated internally by assuming a magnetic field generated by two straight parallel conductors carrying the same current. This version is no longer in use and will not be discussed further. (references N306, N309, N315).

One key characteristic of grids is their orthogonality/non-orthogonality. Orthogonal grids are easier to work with because one can then simplify the ion transport process by assuming that transport parallel to the magnetic field lies along the axis of the cell and transport cross-field can be obtained by simply moving the particle out to a corresponding point on the next field line. When grids are not orthogonal - the assumption for parallel transport is still valid (due to the design of the grid calculation programs) but the cross-field transport is not. The particle position and indexing on each field line needs to be recalculated in a complex way as the particle moves cross-field on a non-

orthogonal mesh. This calculation is supported for JET grids which supply ancillary information to facilitate the calculations. This ancillary information is in the form of a metric coefficient, calculated when the grids are dilated from orthogonal to non-orthogonal, that remains constant when particles move perpendicularly from one field line to the next. It is not currently supported for other grid configurations. Non-orthogonal JET grids are discussed in Sec. 2.4.

2.2 Orthogonal Grids - General

Orthogonal grids cover the poloidal extent of the plasma with a series of polygons. Volumetrically speaking each polygon is assumed to have a toroidal extent of 1 meter in order to facilitate the calculation of densities and other quantities. The following is based directly on J. Wesson's "Tokamaks" pg 289.

The elemental volume is therefore:

$$V = h_1 \times h_2 \times h_3 \times du_1 \times du_2 \times du_3 \quad (2.1)$$

Thus for example one can evaluate the divergence of a vector quantity \vec{A} ($\nabla \cdot \vec{A}$), which is the rate of change of \vec{A} -flux per unit volume. Thus we would expect the first contribution to $\nabla \cdot \vec{A}$ to be:

$$\nabla \cdot \vec{A}_1 = \frac{\Delta(A_1 h_2 h_3 du_2 du_3)}{h_1 h_2 h_3 du_1 du_2 du_3} \quad (2.2)$$

where delta indicates the change of the bracketed quantity in moving a distance $h_1 du_1$ in the u_1 -direction. One notes that the h 's may themselves change with position. Thus the above quantity equals:

$$= \frac{1}{h_1 h_2 h_3} \times \frac{\partial}{\partial u_1} (A_1 h_2 h_3) \quad (2.3)$$

A proper derivation of these relations is quite involved (see “Advanced Calculus” W. Kaplan, Addison-Wesley, p 212) . If one is carrying out a fluid model analysis, one then has to express the conservation equations appropriately. This is also quite involved. (see PhD thesis of M. Baelmans, Jülich Rept. 2891, 1994).

In the case of a tokamak the grid coordinates are:

- a) u_1 is measured along a magnetic flux surface in the poloidal plane.
- b) u_2 is measured “radially” (i.e. cross-field) in the poloidal plane.
- c) u_3 is measured toroidally.

The distance Δs_{tor} (the displacement along direction u_3) is not equal to the distance Δs_{para} measured parallel to the magnetic field line.

An additional characteristic of all of the grids in use is that there is a layer of “buffer” polygons surrounding the entire grided area on the outside of the SOL, the targets, the trapped or private plasma region and on the inner edge of the core region. These polygons have a specific use in the fluid codes. They are used to impose the boundary conditions of the fluid solutions. Their existence is common to all the following grids, however they do not have the same characteristics. In the case of ASDEX Upgrade, these buffer cells are negligibly small. In the case of JET they can be substantial. In addition, for some of these geometries only the center points of these boundary cells are defined. In some cases there are no defined polygons for these boundary cells. Typically, the location of the target is midway between the first two cells on the SOL rings. The details of how this is interpreted and how the rings are designated will be found in the section describing the DIVIMP interpretation of the grids.

2.2.1 JET Grids

JET grids consist of a series of polygons covering the plasma volume. In addition, for JET grids, there is a set of polygons that connects the outermost ring to the location of the vessel wall. These polygons are unusual in that they will have a non-uniform shape and will not-necessarily follow the field lines. Their key characteristic is that one surface of these polygons

defines the wall of the plasma vessel. We will discuss the regular polygons first. (see fig 2.3 and table 2.1)

In the case of JET grids, the individual polygons are characterized by the quantities H_θ and H_ρ which are related to the dimensions of the cell as follows. One notes that the values of H_θ and H_ρ represent the average values for the two opposing sides of the cell.

$$\Delta s_{\text{pol}} = H_\theta \times \Delta\theta \quad (2.4)$$

$$\Delta s_{\text{rad}} = H_\rho \times \Delta\rho \quad (2.5)$$

$$\text{One also defines } h_\theta = B_{\text{pol}} / B \quad (2.6)$$

$$\text{Thus } \Delta s_{\text{para}} = \Delta s_{\text{pol}} / h_\theta \quad (2.7)$$

This also leads to a formula for the cell volume $\Delta V = H_\rho \times H_\theta \times \Delta\theta \times \Delta\rho$ since a distance of 1 cm or 1 m, depending on the units of the other quantities, is understood for the cell extent in the toroidal direction. DIVIMP actually uses a different expression for calculating cell volumes (see sec 2.3.4) because these quantities H_ρ and H_θ are not available for grids other than JET's.

Based on the measurements of magnetic pick-up coils, the shape of the magnetic flux surfaces in the poloidal plane is calculated for each JET shot at each time of interest.

These grids (both orthogonal and non-orthogonal) are generated by the GRID2D program which then outputs the values of H_ρ , H_θ , $\Delta\theta$, $\Delta\rho$, h_θ and the coordinates of the cell centers and corner points.

The values of $\Delta\theta$ and $\Delta\rho$ are typically set to an arbitrary value of 100 and are used for indexing. However, it is possible to modify the value of θ along the field line to reflect the degree of non-orthogonality in the particular cell. By keeping the θ coordinate constant when moving between field lines it is possible to ensure proper perpendicular particle transport. It is this additional information provided by JET grids that makes following non-orthogonal cross-field transport relatively straight forward. (see sec 2.4)

The NIMBUS hydrogen neutral code at JET also supplies it's own listing of polygons that supplement the original grid. These polygons contain two additional pieces of information. First, the inner surface of the far field polygons defines the wall of the plasma vessel. These far field polygons extend out to some far, physically unimportant surface. The next inward set of polygons fills the space between the vessel wall and the outer ring of the properly grided plasma volume. These pieces of information are not read in

from the standard JET grids but are only used in conjunction with NIMBUS results. The polygon indexing scheme used by NIMBUS is also used to index NIMBUS results for such effects as CX-recombination sputtering of impurities from the vessel walls. Thus, it is possible to use a NIMBUS run to generate a supplementary source of impurity neutrals.

Figure 2.3 and Table 2.1 are an example of a selection of cells at the outer target of JET on rings 8, 9 and 10, for shot G50501. The G designation indicates a non-orthogonal grid and by examining the cell examples in this case one can see that the angle at which lines drawn through the mid-points of the sides of each polygon cross at, is not equal to 90 degrees, which is part of the definition of orthogonality. The target position in this case is across the top of the diagram. This plot does not include the “virtual” or “buffer” cells that are initially found across the target - these are removed prior to DIVIMP running. The line across the top represents the position of the target as calculated by DIVIMP based on cell center point positions. It does not exactly match the position that is defined by the polygon boundaries, because, as was previously indicated, certain sections of the code still operate primarily on the basis of cell centers. A new option that could be implemented would use the polygon boundaries to define the targets.

2.2.2 Sonnet Based Grids

The second major class of grids currently supported by DIVIMP are those generated by Sonnet for both ASDEX Upgrade at Garching and CMOD at MIT. These contain less information and are formatted very differently from JET grids. The only information contained in these grid files are the coordinates of the cell vertices (corners) and the cell centers as well as the magnetic field ratio B_{pol}/B in each of the cells. There is no ancillary information describing the nature or degree of orthogonality of the grid. See table 2.2 for a sample listing. These grids arrange the polygons using an ix,iy indexing system where each row has the same number of polygons. Rows represent either a field line in the main SOL connecting opposing targets or two field line segments, one in the Private Plasma and the second in the core. If, for example, the separatrix field line in the main SOL has 120 elements

then the sum of elements in the first core field line and the first field line in the Private Plasma - both of which are adjacent to the main SOL ring - will be 120. Thus there will be a one to one mapping of cells between these regions. DIVIMP is organized somewhat differently, it treats the Private Plasma and core as distinct rings. The sonnet grids are exactly the same as those used by the Braams fluid modeling code and the EIRENE Monte Carlo neutral hydrogen transport code. Although the structure of the grid is not the same as that used internally by DIVIMP - it is straightforward to convert the input to the DIVIMP format if certain characteristic quantities of the grid are known. These quantities are the total number of nodes along each field line, the total number of lines, the number of lines in the core plasma (this is also equal to the number in the Private Plasma region) and the indices of the “cut points” or “cut lines” that define the places where polygons adjacent in the indexing array are not physically adjacent because one lies in the trapped or Private Plasma region and the other lies in the core. This structure is a technique used in some grids in order to generate a grid with a regular structure with the same number of nodes on each indexing line, which is useful for fluid code implementations.

Table 2.2 contains a sample listing of some Sonnet grid formatted output for an ASDEX Upgrade geometry. As can be seen, with the exception of the ρ and θ data, the grids contain basically the same information.

2.3 DIVIMP Grid Representations

DIVIMP reads in the grids in their normal format and converts them into an internal representation compatible with the way DIVIMP has been implemented. Briefly, DIVIMP organizes the polygon indices into rings, with each polygon being a knot on a ring. There are three regions of rings - the core plasma, the main SOL, and the trapped or Private Plasma. The numbering scheme for the rings is as follows.

Innermost core plasma ring (ring #1) to the last closed plasma ring (index number = IRSEP -1)). The rings number outward from the center of the main plasma region.

Separatrix ring to Outer Wall ring: The Separatrix ring (IRSEP) is defined as the first open ring (the first that strikes both targets) that goes around the main plasma. The numbering then marches across the main SOL to the last defined ring before the vessel wall - this is known as the Outer Wall Ring (IRWALL).

Lastly, in the Private Plasma region, the outermost ring of polygons joins the inner corners of the targets. It also is the last ring before the vessel wall but it does not go around the core plasma from one target to the other. This ring is given an index number ($IRTRAP = IRWALL + 1$) one greater than the Outer Wall Ring and is known as the Trap Wall Ring. The indexing counts inward from this ring to the last Private Plasma ring - which is adjacent to the first segments of the separatrix ring at both targets. This is the last ring and is given the index number (NRS) and equals the total number of rings in the system.

Besides separating the space into rings - each polygon is a “knot” on one of the rings. Each polygon is defined by its center and corner points. Adjacent cells have common sides - the sides of cells at the ends of the open rings can be used to define the target positions (see Target Options, sec. 2.3.1).

The key difference between DIVIMP and Sonnet or JET representations is that DIVIMP adjusts the indexing of the polygons to fit the potentially more intuitive representation of the grid. However, it is important to note that the information itself is exactly the same.

There is an additional piece of information available from NIMBUS for JET grids. This extra information provides data on the location of the actual (“true”) vessel wall and can be used to interpret the results of a NIMBUS run in DIVIMP context. In NIMBUS though, there is also the option to use the outer wall ring as the vessel wall (“false” wall) which corresponds to the standard usage in DIVIMP. The index numbers of these polygons and the vessel wall segment coordinates represented by these, have been hard-coded into DIVIMP for a few specific JET grids. This data can also be entered manually in the input data file.

DIVIMP has a number of input options that are used to interpret the grid information. These options have to do with the exact placement and nature of the targets and the walls. Walls need to be considered

independently for both neutrals and ions because the nature of their transport and interaction with wall surfaces are different.

The following sections cover some details about the different Target and Wall Options - for more information - refer to the DIVIMP User Manual.

2.3.1 Specifying the Target Location

As mentioned previously, the fluid codes locate the target on the polygon boundary midway between the first cell on the SOL rings (which is used for boundary conditions only and is actually located outside the plasma region) and the first real polygon inside the plasma. The boundary cell is sometimes referred to as a virtual cell in the DIVIMP documentation because it does not contain real values of the plasma parameters and because a particle cannot occupy the space represented by this polygon. Currently, these cells may be removed from the grid for DIVIMP processing. How these points are interpreted is controlled by the *Target Options*. A number of possibilities exist for specifying the target location. The target location is important since it defines the source of sputtered neutral impurity atoms. In addition, for events that occur on a small scale the precise location of the targets may be important to obtaining meaningful results. However, quite often, the grid resolution is so poor that the precise location of the targets is not crucial. In addition, because the boundary cells on Sonnet grids for ASDEX Upgrade are negligibly small (1.0×10^{-6} m in size), the difference caused in target position due to the different options is not significant. For JET grids, on the other hand, the boundary cell may be of the same size as the first cell, which in some cases can be on the order of a centimeter and thus the target can be moved somewhat by the different Target Options.

DIVIMP typically records cells based on the cell center coordinates. For this reason, the Target Options specify points that lie along the center of each ring of polygons to define the target, whereas the fluid codes base their definition on the polygon boundaries that extend to vertices that do not line up with the polygon centers. Thus DIVIMP targets are not located in exactly the same place as the fluid codes at this time (Feb 1995), however it would be

straightforward to add an additional option that uses the polygon edges to define the target.

Target Position Option 0: The target is located at the first polygon center point on the SOL and Private Plasma rings. The boundary cells are discarded. This Option corresponds to the original DIVIMP implementation when only a grid without boundary cells was made available to DIVIMP and only the cell centers were passed - no polygon vertex information was available. Thus the target was defined by joining all of the cell centers of the first real polygons.

Target Position Option 1: The target is located midway between the centers of the boundary cell and the first plasma polygon. The set of these points for each SOL and Private Plasma ring will define the target position. This is very close to the target used by the fluid codes and approximates to using the polygon boundary of the first real cell. The target points are calculated by taking the mean of the positions of the polygon centers. Thus, if R_{pc}, Z_{pc} are the coordinates of the plasma cell center at one end of the ring and R_{bc}, Z_{bc} are the coordinates for the center of the corresponding boundary cell, then the coordinates of the target point for this end of this ring will be $R_t = (R_{bc} + R_{pc}) / 2$, $Z_t = (Z_{bc} + Z_{pc}) / 2$. These will be calculated for both ends of the rings in the SOL and Private Plasma. Connecting the coordinates for each end of the rings defines the Inner and Outer targets. The boundary cells are discarded after this calculation is made. The reason for discarding the boundary cells is to maintain the compatibility with the ion-following code in DIVIMP which was not designed to deal with cells at the targets which could not be entered by particles. This implementation will be changing to accommodate some features of Sonnet grids used for CMOD.

The rest of the Target Position Options are effectively variations on the above. The target is defined either at or between two grid points or as a set of R,Z coordinates included in the input data file with one point specified for each end of each ring - where these points then form the targets.

Target Position Option 2: The target is specified by a set of data points entered in the input. These are then linked to the coordinates of the first real plasma cell. These data points could be anywhere - but would typically lie between the boundary cell and the plasma cell at the end of the ring. This allows an arbitrary placement of the target at the end ring. The boundary polygons are discarded (this means that they are removed from the DIVIMP internal representation of the grid and all grid characteristics are adjusted to account for it.)

Target Position Option 3: This Option is tied to the Geometry option (see DIVIMP User Manual) - it is possible to have the wall and target characteristics for specific shots loaded into DIVIMP by hand. These will then be available for use with these specific grids only. In addition, this Option also makes available to the program a corresponding set of polygon numbers for these grids, so that NIMBUS results run on the same grid can be automatically read and interpreted correctly. In particular it allows wall sputtering sources to be automatically mapped into DIVIMP structures and used for DIVIMP launch options. It is not commonly used at the moment and in the future DIVIMP may be more fully automated to utilize the neutral code results. Other than the fact that the specific numbers are pre-loaded, this Option otherwise behaves exactly as Option 2 mentioned above.

Target Position Option 4: This Option operates identically to Option Zero except that the cell center coordinates of the boundary cells themselves form the target. The boundary cells are not discarded and are in fact treated as regular plasma cells. This is possible because, since DIVIMP is a Monte Carlo code, the usual fluid boundary conditions are not required.

Target Position Option 5: This is identical to Option Two except that the data points which have been input are connected to the boundary cells at the ends of the ring and the boundary cells are treated as if they were regular plasma cells. This allows one to push the target away from the grid somewhat. Although there is no resolution of the background plasma conditions in this region it might prove useful to adjust the treatment of the target in this portion of the grid.

Now that the R_t, Z_t coordinates of the target have been defined - it is necessary to actually construct the target. The target is created by joining each of the R_t, Z_t as calculated above. A particular segment of the target extends from midway to the last target point until midway to the next target point. Again, note that this does not correspond exactly to the fluid code or grid definitions of the target segment which utilize the cell vertices to define the target. DIVIMP still contains this definition as a result of compatibility with earlier versions and because the grid resolutions are sufficiently fine, this has not caused any obvious problems. One now has the length and the orientation for each target segment (in the poloidal plane).

2.3.2 Specifying the Wall Location

The other aspect of particle/grid interaction is the location and nature of the particle boundaries in DIVIMP. Two kinds of walls, which may coincide, need to be specified. One of these is specified for ions which follow magnetic field lines and for which transport is only defined within the grid region. The second wall specification applies to neutral transport. Neutrals travel in straight lines. Furthermore, they interact directly with the true vessel wall surfaces via reflection and perhaps other processes. In addition, the vessel wall surfaces may in fact be sources for impurity neutrals and thus it is important to be able to define a physically accurate representation of the vessel wall which defines the boundary for neutral transport. The impurity ions followed by DIVIMP may reach the outer boundary region at the edge of the grid. The location of this boundary is controlled by the Wall Option and Trap (Private Plasma) Wall Option. The nature and behaviour of the particles when they strike this surface is controlled by the *Ion Periphery Option*. These options will be described in detail in this section.

Wall locations:

Wall Option 0: The boundary surface for neutrals and ions is defined to be midway between the center points of the outermost real plasma cells and the ring of boundary cells that lies outside that. Just as at the targets, the outermost ring has an additional ring encircling the entire SOL that is used for fluid code boundary conditions. The ion transport surface in this Option is defined to be halfway between the cell centers. This approximates the polygon edge boundary. The neutrals are also restricted by this boundary.

Wall Option 1: The boundary surface is at the cell centers of the boundary ring of cells around the SOL. The reason for including this Option initially was to increase the spatial extent of the plasma region for specific JET grids that did not extend sufficiently far out into the SOL and at a time when it was not possible to generate a grid with certain desired characteristics.

Wall Option 2: The wall for ions is specified as in Option Zero, midway between the outermost cell centers. The neutral wall is specified by a set of R,Z coordinates entered in the input data file. The list of coordinates specifies the end points of wall segments starting with the first point that will connect to the edge of the outer target and loop around the plasma to the last point that will be joined to the end point of the inner target for a JET geometry with the X-point at the top of the grid. For an ASDEX-Upgrade geometry with the targets at the bottom of the grid and everything else organized the same, the designations of outer and inner targets are reversed. The neutrals are constrained to travel anywhere within the space defined by the piece-wise wall specification which is joined to the targets and the Trap Wall specification (see below) so that it completely encloses a region with no gaps.

Wall Option 3: Identical to Option Two except that the ion wall is at the outermost ring as in Option One. The neutral wall is specified as in Option Two.

Wall Option 4: This is identical to Option Two except that the neutral wall specification has been hard-coded into DIVIMP for specific JET shots.

Wall Option 5: This is identical to Option Three except that the neutral wall specification has been hard-coded into DIVIMP for specific JET shots.

In a similar fashion, the walls for neutrals can be independently specified in the Trap region. The Trap region is the segment of wall lying between the two targets and enclosing the trapped or Private Plasma region. The interpretation of the ion wall in this region uses the general Wall Option specified above.

Trap Wall Option 0 and 1: As in the main SOL, there is a boundary ring at the outer edge of the Trap (Private Plasma) region. Option Zero places the neutral wall midway between the center points of the cells on the last plasma ring and the cells of the boundary ring. Option One places the neutral walls at the center points of the boundary cell ring. These two Options treat neutrals in the same way as they are treated in Wall Options 0 and 1 respectively (listed above).

Trap Wall Option 2: The neutral wall is formed by joining the adjacent end points of the inner and outer targets that are next to the Private Plasma region. This gives a region of empty space between the targets and allows for the possibility of a neutral being created at one target and then being ionized near the other target.

Trap Wall Option 3: The neutral wall is specified by a set of line segments, defined by their end-points, which are entered in the input data file. These line segments are linked to the end points of the targets and allow physical structures for neutrals to be defined between the two targets.

2.3.3 Specifying the Wall Characteristics:

The other aspect of defining the walls is the way they are interpreted when the particle strikes the wall. This is presently easy for neutrals and somewhat more complex for ions. There is currently only one option for neutrals. A neutral is either lost from the system when it strikes the wall or it is specularly reflected, where the angle of incidence equals the angle of

reflection. Other reflection and/or re-emission options are possible and can easily be added but are not currently supported. This option is called the *Neutral Reflection Option*.

The interpretation of the wall for ions has many more possibilities. These are specified in the input by the value of the Ion Periphery Option and the effects of these Options are described below. These Options are necessary because the simplest approach of just stopping the ion transport at this boundary, does not, in general, provide a reasonable model of the behaviour of the ions in the peripheral region. There is both magnetic field and plasma in these regions although the grids do not typically penetrate deeply into the periphery. Understanding of the peripheral regions of the edge is slight, unfortunately. For these reasons a variety of Options have been developed to describe different types of ion behaviour when reaching the periphery.

Ion Periphery Option 0: Hard Wall. In this situation, any ions striking the wall boundary defined by the location options are assumed to stick to the wall and are removed from the system as a result. This gives a very strong sink action for ions at the edge of the plasma boundary, perhaps, in some cases, an unrealistically strong sink action.

Ion Periphery Option 1: Reflecting Wall. This is the opposite of Option 0 just described. All ions striking the boundary are bounced back into the plasma. For example, if a particle would have found itself carried a distance X past the boundary on a cross field diffusive step - then it is repositioned a distance $-X$ inside the boundary. Ions can not be lost to the walls. This Option significantly increases the run time required for a case and can result in unrealistically large impurity densities in some cases, since ions can only be lost from the plasma by reaching the targets.

Ion Periphery Option 2: No wall. Ions are tracked and are always associated with the outermost ring, but when they travel past the wall boundary nothing happens except that they are allowed to build up an unlimited cross-field diffusive displacement. There are no wall sinks present and the only particle loss mechanism will be along the field line to the targets (excluding recombination and other similar non-transport processes). Since the particle is always associated with the outermost cell which has a finite

volume - this option can result in inaccurate densities for the periphery cells, but may give a physically reasonable “sink action” at the periphery.

Ion Periphery Option 3: A simple model of the far periphery is used which includes diffusion and characteristic loss times along the field line to the target. There are three parameters used to specify this simple empirical model of the periphery region beyond the ion grid. First, there is a characteristic parallel loss time specified for the region. While an ion is in the periphery it may have a chance to be transported along the field line to the target. There is one characteristic loss time, τ_{loss} - typically 1 msec, which is arbitrarily specified. If in any timestep Δt , a random number is chosen such that it is less than $\Delta t/\tau_{\text{loss}}$, then the particle is removed and assumed to have struck the target in the peripheral region. The other two parameters are the diffusion coefficient (D_{\perp}) in the peripheral region and the width of the peripheral region (S_{wall}). If a particle is not removed to the target it is allowed to cross field diffuse at each time step a distance of $\pm \sqrt{2 D_{\perp} \Delta t}$. If it travels a distance of S_{wall} from it's injection point then it is assumed to have struck a vessel wall surface and is recorded as being deposited in the wall section associated with the cell from which it entered the boundary region. In addition it is removed from the system. If, on the other hand, the particle diffuses back past it's starting point then it is reintroduced into the main plasma grid at the point where it originally exited.

There is one other Option that affects the behaviour of ions in the peripheral region when Ion Periphery Option Three is selected. Ions which have hit the far periphery target may be reintroduced into the plasma via a neutral impurity launch at the corner of the target nearest to the point where the particle was lost into the peripheral region. This option is turned on or off by the *Periphery Recycle Option*.

2.3.4 Grid cell volumes

The volumes of the grid cells are very important since accurate values are required to properly calculate all the quantities which are being modeled. DIVIMP itself is in effect a cylindrical code, with quantities calculated per

meter of toroidal length. One thus speaks of cell areas rather than cell volumes. These are referred to in the code as “KAREAS” (Usually NIMBUS, see sec. 8, also assumes a cylindrical geometry, however, corrections based on the local value of R_i of cell I can be made for a proper toroidal treatment.) For illustration we take an example from a non-orthogonal grid JET G50501 for cell (9,5) indicated in Figure 2.3 and Table 2.1. The cell center at (9,5) has immediate neighbours of (9,4) and (9,6) and (8,5) and (10,5). If one finds the point midway between (9,5) and each of these cell centers it yields four of the points marked with a “+” and included in the area called the cell area estimate in Figure 2.3. The other 4 points on this boundary are calculated by taking the midpoints between these midpoints and the ones calculated from the cells (9,4) and (9,6). One thus ends up with 8 points that approximately define the area of the cell. This space is marked with “+”s. One joins these together to form an 8 sided figure (note that it is actually 8-sided although the example in figure 2.3 may appear to be only 4-sided, the 8 “+” signs on the figure define the end-points of the 8 sides.) that defines the cell area, KAREAS, which is the quantity generally used in DIVIMP.

Also defined in DIVIMP and calculated, though not currently used, are the quantities KAREA2 and KVOLS. KAREA2 is calculated by using the vector dot products of the polygon vertices (if these are defined) for each cell. The quantity KVOLS represents a toroidally corrected cell volume where KAREAS is multiplied by $2 * \pi * R_i$ where R_i is the R-coordinate of the cell center. KAREA2 is used for cell areas in the pindiv.d3a module (NIMBUS Sec.8). The cell area can also be calculated for JET grids by calculating the quantity $V = H_p \times H_\theta \times \Delta\theta \times \Delta\rho$ (sec 2.2).

2.4 Non-Orthogonal Grids - General

To be completed - as part of the on-going development of this Guide.

3.0 Background Plasma Specification

Since DIVIMP only follows the impurity particles, the plasma background has to be separately specified, as input to DIVIMP. That is, one has to specify the 2-D distributions of: T_e , T_{iB} , n_e , v_B (background drift velocity along \bar{B}), E (electric field along \bar{B}).

A basic distinction can be made between predictive and interpretive work using DIVIMP.

For predictive work one has no choice but to “calculate everything”, i.e., there is no experimental information. The most obvious approach is then to use a 2-D edge fluid code such as EDGE2D, B2, or LEDGE, where, generally, the input assumptions are rather global ones. (e.g. the total power outflow from the core plasma into the edge plasma outside the separatrix; the “upstream” density — ideally on the separatrix, and halfway between the targets, or at the outside mid-plane; the cross-field transport coefficients, $\chi_{\perp}^{e,i}$, D_{\perp} ; boundary conditions at the targets, and at the last poloidal rings in the SOL and Private Plasma.) Ideally such 2-D edge fluid codes are directly coupled to 2-D or 3-D Monte Carlo hydrogen neutral codes, such as NIMBUS, EIRENE, DEGAS, or some other neutral hydrogen code. The neutral code provides the ionization rate, momentum loss/gain terms (from neutral-ion interactions), and electron/ion cooling/heating terms (from e/n, i/n interactions) for the fluid code’s conservation equations. In turn, the fluid code must provide the neutral hydrogen code with 2-D distributions of n_e , T_e , T_{iB} . Thus, the two codes have to be coupled and operated iteratively.

DIVIMP can then employ such hydrogenic (neutral plus plasma) code output as the input needed to specify the plasma background. Information on such couplings are given in Sec. 8.

For such predictive work, the question arises as to whether or not it is valid to treat the “plasma background” as something fixed, and unchanged by the impurity behaviour. Clearly, this will generally not be correct —

although it is not generally clear how large an error is involved. Thus, one might decide to use a multi-fluid 2-D edge code, in which the impurity ions are also treated as fluids — rather than use DIVIMP. Most of the edge fluid codes can be operated this way, although convergence is more difficult. An alternative approach, under development at Jülich, will couple B2, EIRENE and DIVIMP iteratively, with B2 not run in the multi-fluid mode. This approach may enjoy the following benefits:

- (a) the edge plasma is often only marginally collisional, raising concern about the validity of fluid modeling; although the hydrogenic particles would still be modeled as fluids, the impurity treatment via DIVIMP would be quasi-kinetic, in as much as no assumption is made about mean-free-paths being short.
- (b) fluid models, in order to converge in reasonable times, use only a single energy equation for all the ions, i.e., at each point in space all ions have the same temperature. In reality the impurities may be poorly thermalized relative to the hydrogenic ions — possibly influencing their parallel transport. This aspect is readily dealt with in DIVIMP.

Turning to interpretive work: in the best of all possible worlds one would have complete 2-D experimental mappings of the plasma background n_e , T_e , T_{iB} , v_B , and E . No modeling of the plasma background would be needed. Any influence of impurities on the plasma background, e.g., radiative cooling of the electrons, would be automatically accounted for. Unfortunately, such an ideal situation is far from realization. Nevertheless, it seems clear that, in order to minimize the uncertainties involved in this already very uncertain exercise in data interpretation, *one should take as much input as possible from experiment, endeavoring to have to calculate as little as possible.*

It is fairly common now, on divertor tokamaks, to have Langmuir probes distributed across the target plates. Thus one can have experimental values for at least n_e , and T_e at this most critical of locations. The reasons for this being the most critical location at which to have experimental information are:

- (a) this is the location of the most intense production of impurities; the production rate is controlled by the plasma conditions at the targets.
- (b) although it is not initially obvious, it can be shown by a relatively simple argument, see Sec. 3.1.1, that when modeling the SOL plasma, the solutions are much less sensitive to all parameters (i.e., uncertainties) when one works upstream from boundary conditions at the target rather than “from the top down” (the necessary approach in 2-D edge fluid modeling); at least for the “high recycling” regime there is much less sensitivity; for the “low recycling” regime, there is even less problem since n and T are approximately constant along each field line. This matter is further explored in Sec. 3.1.1.
- (c) it is advantageous to be able to start out one’s interpretation of impurity behaviour at the source of the impurities (although it must be acknowledged that not all impurities do originate at the targets). It is also helpful to have reliable experimental data for that key location, at least, since then one can then model the plasma upstream from that location, which starts to encounter additional uncertainty. Fortunately, however, one can use the very impurity measurements themselves to help one make this “walk upstream” more reliable. The spatial distributions of the very lowest charge states, e.g., CI, CII — and their (Doppler) temperatures, if also available — are only sensitive to the plasma conditions rather near the targets. Thus, by using these, e.g., CI, CII, data one can reduce the uncertainties in the modeling of the plasma background in the region just upstream of the target. Then one is ready to model a little further upstream, modifying and correcting the model by data from, e.g., the CIII emission. One can then proceed further and further upstream, using data from successively higher charge states to improve the reliability of the background model. Thus one ends up not only interpreting the impurity data, but unraveling the plasma background as well. One uses the impurities as a diagnostic of the plasma background. This procedure depends on being able to work upstream from boundary conditions at the target.

3.1 The SOL Options Within DIVIMP for Onion-Skin Modeling of the Plasma Background in the SOL

3.1.1 Introduction

In Onion-Skin Modeling, OSM, one proceeds on the assumption that each flux tube in the SOL can be modeled independently, based on the specific, individual plasma boundary conditions for each flux tube. It should be noted that one is not assuming that each flux tube is actually independent of its neighbours: after all, the reason that the values of n and T at the target, for a specific flux tube, have the values they do, and not some other values, is precisely because of the effect of the neighboring flux tubes. The essential assumption in OSM is that the dependence of the individual flux tube on its neighbours is effectively included within the boundary values of n and T — and need not be explicitly included otherwise.

It is clear that this assumption is valid in the case of “low recycling,” where n and T are essentially constant along any individual flux tube. The cause of the cross-field variation from flux tube to flux tube is a separate issue — and one can totally bypass it when one has measurements of n and T across the target (or indeed, for “low recycling”, if one has measurements across the SOL at any point along its length).

For divertors the interesting regime, however, is the “high recycling” one where significant variations of n and T exist along \bar{B} . In that case, while it is not strictly true that one can model each flux tube without directly involving its neighbours, it will now be shown that this is still usually a good approximation. The reason for this is that, in the “high recycling” regime, upstream plasma conditions are very insensitive to almost any modeling assumptions. Thus, when modeling upstream from target boundary conditions the solution is very robust. (Precisely the opposite is the case when modeling from “top down”).

This claim can be illustrated using a simple Two-Point Model (2PM). In OSM one is looking for expressions such as $T(s)$, $n(s)$, where s is measured along \bar{B} , on the particular flux tube, from $s = 0$ at, for example, the outside target of a single-null divertor, to $s = S_{\max}$ at the inside target, with $L = 1/2 S_{\max}$ being the distance midway between the two targets. In the case of a 2PM, on the other hand, one is simply seeking the relation between $n(L)$, $T(L)$ and $n(0)$, $T(0)$. Consider here a 2PM for the “high recycling” situation where the hydrogen neutrals recycling from the target are all ionized in a vanishingly thin layer just in front of the targets; thus parallel heat convection is unimportant, except at the target sheath, and parallel heat conduction is dominant along the SOL. Assume further that $T_e = T_i$; thus parallel electron heat conduction is involved. It is readily shown that if all of the heat input to the flux tube occurs at $s = L$, then:

$$\frac{T(L)}{T(0)} = \left[1 + \frac{7}{2} \frac{q_{\text{para}} L}{\kappa_{0e} [T(0)]^{7/2}} \right]^{2/7} \quad (3.1)$$

where q_{para} = parallel heat flux density in the tube [W/m²]
 $\kappa_{0e} = 2000$ if T in [eV] , and $Z_{\text{eff}} = 1$
 $(\kappa_{0i} = 59)$

One also has:

$$(1 - f_{\text{rad}}) q_{\text{para}} = \gamma n(0) c_s(0) kT(0) \quad (3.2)$$

where f_{rad} = fraction of q_{para} which is radiated away in the divertor before reaching the target

γ = sheath heat transmission coefficient ≈ 7
 $c_{s0} = [2kT(0)/m_i]^{1/2}$

One also has pressure balance along the SOL:

$$(1 + [M(0)]^2) n(0) kT(0) = f_p n(L) kT(L) \quad (3.3)$$

where we will take the Mach Number, $M = v/c_s$, $M(0) = 1$ here; f_p gives the pressure loss due to neutral friction, viscosity or any other effects, between the two points.

When people use the expression “high recycling” they usually mean this to imply that a substantial temperature drop exists along the SOL. While it is true that spatially-extended recycling results in parallel convection playing a larger role along the SOL, thus reducing T-gradients somewhat, it is not true that when ionization occurs only very close to the plate, and thus convection is unimportant, that a large T-drop is guaranteed. Combining Eqs. (3.1) to (3.3) and setting $f_p = 1$, $f_{rad} = 0$, a substantial temperature drop exists along the SOL, i.e., $T(L) \gg T(0)$ when:

$$q_{para} \gtrsim 600 [T(0)]^2/L \quad (3.4)$$

for T in [eV]; or, expressed in terms of upstream conditions, when:

$$q_{para} \lesssim 1.5 \times 10^{-28} [n(L)]^{7/4} L^{3/4} \quad (3.5)$$

(One may note that the inequalities are in opposite senses depending on whether upstream or downstream conditions are referenced; so far as the operation of a tokamak is concerned, upstream conditions are the ones that are externally set or controlled, e.g., $n(L) \approx \bar{n}_e$, with \bar{n}_e controlled by fueling; thus one must not have too high a value of q_{para} if one wants to achieve a large T-drop.)

Nevertheless, it is true that the desirable regime of divertor operation is the “Large Temperature Gradient Regime” (a more specific term than “High Recycling Regime”), so let us assume $T(L) \gg T(0)$. Thus, Eq. (3.1) becomes:

$$T(L) \approx \left(\frac{7}{2} \frac{q_{para} L}{\kappa_{0e}} \right)^{\frac{2}{7}} \approx \left(\frac{7}{2} \frac{L}{\kappa_{0e}} \frac{\gamma n(0) c_s(0) k T(0)}{(1 - f_{rad})} \right)^{\frac{2}{7}} \quad (3.6)$$

One can thus see the robustness of upstream conditions to changes in downstream ones. This is due to the $2/7$ power in Eq. (3.6), and to the fact that one is in the Large Temperature Gradient Regime.

One may also note from Eq. (3.1) the effect of changing the arbitrary assumption that all of the heat influx to the tube occurred at $s = L$. In reality, the heat influx occurs along the length of the tube, and varies according to the local value of the cross-field density and temperature gradients and to the local values of χ_\perp and D_\perp . This latter aspect, the possible spatial variations of χ_\perp and D_\perp , is potentially a troublesome one, since we have essentially no knowledge of how these quantities vary with local plasma conditions (for that matter, even SOL-averaged values are uncertain). The usual assumption that χ_\perp and D_\perp are constant is rather arbitrary. Thus, should it turn out that a modeling result were to depend at all sensitively on local values of χ_\perp and D_\perp , the modeling results would be unreliable. Fortunately that is not the case when modeling upstream from target conditions as can be seen from Eq. (3.1): suppose that the heat influx occurred, not all at $s = L$, but uniformly over the length; in that case the factor $7/2$ inside the bracketed expression in Eq. (3.6) would change to $7/4$, giving only a small change in $T(L)$, since $(0.5)^{2/7} \approx 0.82$. A similar argument shows that $n(L)$ is also robust for modeling uncertainties.

Clearly one cannot push this last argument to extremes: suppose all the heat came into the flux tube just near the X-point, which is located, say at $L_X/L = 0.1$; then a factor of $(0.1)^{2/7} = 0.52$ is involved — still not an overwhelming effect, but not negligible. Or suppose that 99% of the heat flow into the divertor were radiated before reaching the target - then a factor $(0.01)^{-2/7} \approx 3.7$ would be involved, i.e., $T(L)$ would be $\approx 3.7X$ higher, based on the same target conditions but neglecting divertor radiation. Nevertheless, it is clear that upstream conditions are very robust to modeling uncertainties. Even crude estimates of corrections to account for actual spatial distribution of heat influx or for f_{rad} — as could be achieved with an iterative approach — should result in rapid convergence to fairly reliable final values for upstream quantities in terms of downstream ones.

The opposite is the case when proceeding from “top down”, the results at the target are very sensitive to the upstream conditions. Combining Eqs. (3.2), (3.3) and (3.6):

$$T(0) = \frac{m}{2e} \left[\frac{2 (1 - f_{rad}) q_{para}}{\gamma f_p n(L) T(L)} \right]^2 \quad (3.7)$$

where $e = 1.6 \times 10^{-19}$ if $T(0)$ is in [eV]. Here one sees that $T(0)$ varies as $(1 - f_{rad})^2$, f_p^{-2} , $[n(L)]^{-2}$, $[T(L)]^{-2}$, and so is very sensitive to variations or uncertainties in these quantities. The density, $n(0)$, is even more sensitive, varying as f_p^3 , $[n(L)]^3$, $(1 - f_{rad})^{-2}$. Clearly, when modeling the SOL “top down”, as in all 2D fluid modeling, predictions of plasma conditions near the target are highly volatile, and thus of uncertain reliability.

The approach taken here, with the SOL Options, is to carry out Onion Skin Modeling — using, whenever possible, measured experimental plasma conditions at the targets, and modeling in the upstream direction. If experimental radial scans of plasma conditions are also available further upstream, say above the X-point, this provides very valuable additional information for constraining and defining the Onion Skin Model.

In the next section, the various SOL Options are described. As will be evident, the low-numbered Options are really just prescriptions rather than proper models. For the latter, one solves the conservation equations (mass, momentum, energy) to calculate $n(s)$, $T(s)$, $v(s)$, etc. It is also useful, however, to be able to simply prescribe a 2D plasma background, in order to quickly check for various effects; it is likely that we do not really know what all the important terms are to put in the conservation equations, so we do not want to be constrained to use only those 2D plasma backgrounds which result from solving the conservation equations.

With regard to the prescription-type *SOL Options*, these are also specified in part by *Temperature Gradient Options*, also described in the following.

One possible approach to interpreting a set of experimental data using DIVIMP would be to try a very simple SOL Option first — why not one that simply keeps n and T constant along each flux tube? Who knows? — Maybe such a simple assumption will match all the available data to within experimental uncertainty. If so, then what is the justification for postulating some more complex SOL plasma background? The standard scientific procedure is to first examine the simplest postulate that fits the measurements. It is difficult to argue that solving the conservation equations is, somehow, more “physical,” than just arbitrarily prescribing some $n(s)$, $T(s)$, $v(s)$. That argument would be valid if we knew all the important terms to include in the conservation equations — but generally we do not.

If the simplest prescriptions do not give DIVIMP output for impurity behaviour that matches the experimental data, then one might try “playing with” the SOL Options which allow one to arbitrarily prescribe more complex $n(s)$, $T(s)$, $v(s)$ variations (always with target boundary conditions maintained, however), to see roughly what it will take to get agreement. Such an exercise may provide clues as to what is going on, and perhaps indicate what are important terms in the conservation equations. One could then try SOL Options which are based on solving the conservation equations to see what results are obtained. Thus one would proceed in a manner which attempts to incorporate as much experimental input as possible at each step, in building up a picture of the impurity and plasma background in the edge, simultaneously, while only incorporating more physical processes when and if the experimental data forces one to do so.

For sufficiently extreme conditions, it is clear that an Onion Skin Model approach, based on boundary conditions at the target, must fail. Consider, for example, the case of complete divertor detachment, where n_e at the target goes to zero. In such cases one could still use an OSM approach, but based on a radial scan of n_e and $T_{e,i}$ at some location upstream as boundary conditions. This solution may not enjoy the benefits of robustness seen when the OSM is used from the targets: upstream from the point of measurement, the solution would have the same characteristic robustness as is seen when the measurements are made at the targets; however, downstream from the point of measurement the calculated values may be

very sensitive to the precise values of the measured quantities and thus would lack the robustness of the upstream solutions. Furthermore, as already noted, the assumption that the cross-field sources of heat (and particles) are distributed uniformly along the SOL cannot be correct generally. Even if this usually introduces only small errors in calculating the upstream values from the downstream ones, there may be certain regimes where the error would be unacceptably large. One can tackle this problem using iterative methods and assigning cross-field fluxes proportional to local cross-field gradients (assuming the cross-field particle and heat diffusivities are spatially constant). Such a study is presently (April 1995) underway, directed at establishing the limits of applicability of the Onion Skin Model approach. For situations where an OSM approach is not viable, then the standard 2-D edge fluid code approach will be required.

3.1.2 The SOL Options

The description of SOL Options is divided into two sections. The first describes the SOL Options numbered less than 10 and the Temperature Gradient Options. The SOL Options numbered up to 10 specify solely the behaviour of the background flow velocity and the electric field. They do not make any statements about the temperature. Temperature prescriptions are handled by the Temperature Gradient Options and prescriptions for density at the targets are handled by the Plasma Decay Option. The Plasma Decay Options are in fact used to input the target conditions for all Options. These Options are described first.

One other aspect of specifying the background plasma must also be kept in mind. There are portions of the grid that do not lie in the SOL - the first number of rings lie within the core plasma. Since there is little diagnostic information about the edge of the core region and furthermore, since prescribed conditions here have only a minimal effect on impurity transport in the SOL, the prescription for this region is minimal. The density and temperature are assumed to be constant along each ring in the core. In addition, the density and temperature are assumed to rise by a specified amount for each ring going deeper into the core. This quantity is specified in the input. Finally, the initial or base values from which the core plasma values are calculated are taken from the values of density and temperature

at the midplane ($L = S_{\max} / 2$) position on the separatrix ring. Thus, if the separatrix ring is ring 8 and the Δn value was set to 1.0×10^{18} , and the density at the midplane on ring 8 was 10^{19} , then the density on ring 7 would be 1.1×10^{19} and on ring 6 1.2×10^{19} and so on for the core plasma rings. A similar prescription is used for temperature with a rise of 100 eV / ring being a typical value. More sophisticated prescriptions for the core could be readily implemented.

Symmetry Assumptions

In all of the present (May, 1995) SOL Options each flux tube is divided into halves, $0 < s < L$, $L < s < 2L$ where $L = \frac{1}{2} S_{\max}$ and S_{\max} = plate-to-plate distance for that flux tube. The SOL Options are then assigned, essentially symmetrically, to the halves, thus taking into account sign changes for v_B and E . One generally can specify different target n and T at each end, for each flux tube, so the resulting $n(s)$, $T(s)$, etc., profiles are not necessarily symmetric. Furthermore, discontinuities in these background quantities generally occur at $S=L$.

Specifying the Target Conditions: Plasma Decay Options

These are straight forward and are only briefly summarized. They control the values specified for the background conditions and, in the absence of any other specified gradients, the values that will be applied to the whole plasma.

Plasma Decay Option 0: The temperatures and densities at the target are specified for the separatrix ring and then a constant step (also specified) is applied for each ring displacement from the separatrix. (e.g. T_e at the separatrix is specified as 50 eV and a ΔT_e of 5 eV is specified - then the next outboard ring from the separatrix would have a target temperature of 45 eV and so on).

Plasma Decay Option 1: This is similar to Option 0 except that instead of a linear decay as one steps out by rings, the ring target temperature becomes:

$$T_{\text{ring}} = T_{\text{sep}} \exp (-d/\lambda_t)$$

Where T_{sep} is the temperature on the separatrix, λ_t is the e-folding distance for T across the target and d is the distance on the target from the separatrix ring to the ring being calculated. All of n , T_e and T_{iB} are specified in the same format.

Plasma Decay Options 2,3,4: All of these Options read the data for each ring individually from the input file. Option 2 - reads one set of data and applies it to both targets. Option 3 - reads data individually for both targets but only for the main SOL - the Private Plasma region is specified separately (usually as a low constant temperature and density.) Option 4 reads data for both targets and for both the main SOL and Private Plasma. Finally, if no data has been specified for a ring the code assigns data from the closest preceding ring number that has been specified. For example, if data were specified for rings 12, 13 and 14 but not for 15 and 16, then the code responds by assigning the target conditions for 14 to both 15 and 16 as well.

Simple Prescriptive Specifications

3.1.2.1 SOL Option -1

Note: This is a relatively complicated prescription, and is thus out of logical order.

One is free to prescribe any $T_e(s)$, $n(s)$ using T-Gradient Options, sec 3.1.3. This particular SOL Option itself actually specifies a model for $v(s)$ (one which is really only valid for $T_{e,i} = \text{const}$ along \vec{B}). It is based on the assumption that the hydrogenic ionization is spatially uniform over $0 < s < f_L L$ at one rate, S_{near} [particle/m³/s], then uniform at S_{far} over $f_L L < s < L$. One has to specify f_L , also:

$$f_s = \frac{f_L S_{\text{near}}}{(1 - f_L) S_{\text{far}}} \quad (3.8)$$

(One does not have to specify either S_{near} or S_{far} as these are fully constrained by specifying f_L , f_s together with the assumption that the plasma flow to the target equals the integrated source over $0 < s < L$.) Then the Mach Number of the background plasma:

$$M = v_B/c_s = q^{-1} + (q^{-2} - 1)^{1/2} \quad (3.9)$$

where v_B = plasma background velocity,

$$c_s = (k(T_e + T_{iB})/m_B)^{1/2}$$

$$q = \begin{cases} (1 + f_s)^{-1} [(f_s/f_L)(s/L - f_L) - 1] & \text{for } 0 \leq s \leq f_L L \\ (1 - f_L)^{-1} (1 + f_s)^{-1} (s/L - 1) & \text{for } f_L L \leq s \leq L \end{cases} \quad (3.10)$$

The value of E is also calculated from:

$$E = \frac{T_e}{eL} \frac{M(1 + M^2)}{(1 - M^2)} \quad (3.11)$$

Note that v_B , M , $E \rightarrow 0$ as $s \rightarrow L$. As $s \rightarrow 0$ one has $M \rightarrow -1$, $v_B \rightarrow -c_s$; also $E \rightarrow -\infty$. In principle the latter result should not unduly influence impurity ion transport, which should only be sensitive to potential drops, not the value of E , and it can be shown that the potential drop between any point $s > 0$ and $s = 0$ remains finite. However, the mesh in DIVIMP has finite resolution — indeed it can be rather coarse, even near the targets. Thus one can end up assigning to E , in the first cell, some extremely large (negative) value, keeping that constant over the entire width of the first cell. This is unphysical and potentially very distorting. One may therefore wish to assign $E = 0$ in the first cell.

3.1.2.2 SOL Option O

The simplest prescription of all: $v_B = E = 0$. One is free to specify $n(s)$, $T_{e,iB}(s)$ using T-Gradient Options, sec 3.1.3.

3.1.2.3 SOL Option 1 [N15]

This is the simpler version of SOL Opt -1, where the source is now assumed to be constant $0 < s < L$. Strictly, the model is again for isothermal conditions but one is, in fact, free to specify any $n(s)$, $T_{e,iB}(s)$ using the T-Gradient Options, sec 3.1.3.

$$M = v_B/c_s = [(s/L) - 1]^{-1} + [((s/L) - 1)^{-2} - 1]^{1/2} \quad (3.12)$$

$$E = \frac{T_e}{eL} \frac{M(1 + M^2)}{(1 - M^2)} \quad (3.13)$$

Note: $M, v_B, E < 0$ for $0 \leq s \leq L$. As with SOL Opt-1, $M \rightarrow -1$, $v_B \rightarrow -c_s$ at $s = 0$ and $M, v_B, E \rightarrow 0$ as $s \rightarrow L$. As with SOL Opt -1 one has to be careful with $E(s \rightarrow 0) \rightarrow -\infty$ and it may be best to assign $E = 0$ in the first cell.

3.1.2.4 SOL Option 2 [N7]

A simple, arbitrary prescription, approximation to SOL Opt -1:

$$v_B = -c_s(1 - s/L) \quad (3.14)$$

$$E = -kT_e/(2eL) \quad (3.15)$$

One is free to prescribe $n(s)$, $T_{e,iB}(s)$ using the T-Gradient Options, sec 3.1.3.

3.1.2.5 SOL Option 3 [N7, N19]

Another arbitrary prescription, approximating SOL Opt-1:

$$v_B = -1.33 c_s(1 - s/L) \quad (3.16)$$

$$E = (kT_e/(e\pi L))(1 - s/L) \quad (3.17)$$

One is free to prescribe $n(s)$, $T_{e,iB}(s)$ using the T-Gradient Options, sec 3.1.3.

3.1.2.6 SOL Option 4 [N55]

Another arbitrary prescription, approximation to SOL-Opt. 1:

$$v_B = -c_s(1 - s/L) \quad (3.18)$$

$$E = -(kT_e/(2eL))(1 - s/L) \quad (3.19)$$

One is free to prescribe $n(s)$, $T_{e,iB}(s)$ using the T-Gradient Options, sec 3.1.3.

3.1.2.7 SOL Option 5 [N123]

v_B = specified constant, E = specified constant (positive or negative). One can prescribe $n(s)$, $T_{e,iB}(s)$ using T-Gradient Options, sec 3.1.3.

3.1.2.8 SOL Option 6

This option allows one to specify the background plasma velocity in a very simple fashion with limited variation.

E = specified constant

$$V_B = \left\{ \begin{array}{lll} V_0 & \text{for} & 0 \leq s < C_1 \times S_{max} \\ M_1 \times V_0 & \text{for} & C_1 \times S_{max} \leq s < C_2 \times S_{max} \\ M_2 \times V_0 & \text{for} & C_2 \times S_{max} \leq s \leq L \end{array} \right\} \quad (3.20)$$

The values of V_0 , C_1 and C_2 are specified in the DIVIMP input file. The temperatures are specified using the Temperature Gradient Options, sec 3.1.3.

3.1.2.9 SOL Option 7

This option allows one to specify the background plasma velocity in a very simple fashion with linear variation along the field lines.

E = specified constant

$$V_B = \left\{ \begin{array}{ll} \text{from } V_0 \text{ at } s = 0 & \text{to } M_1 \times V_0 \text{ at } s = C_1 \times S_{max} \\ \text{from } M_1 \times V_0 \text{ at } s = C_1 \times S_{max} & \text{to } M_2 \times V_0 \text{ at } s = C_2 \times S_{max} \\ \text{from } M_2 \times V_0 \text{ at } s = C_2 \times S_{max} & \text{to } V = 0 \text{ at } s = L \end{array} \right\} \quad (3.21)$$

The values of V_0 , C_1 and C_2 are specified in the DIVIMP input file. The temperatures are specified using the Temperature Gradient Options, sec 3.1.3.

3.1.2.11 SOL Option 8

This was a LIM option that is not implemented in DIVIMP.

3.1.2.12 SOL Option 9 [N327]

Simple prescription:

$$v_B = -c_s \quad (3.22)$$

$$E = -kT_e/(2eL) \quad (3.23)$$

One can specify $n(s)$, $T_{e,iB}(s)$ using T-Gradient Options, sec 3.1.3.

3.1.2.13 SOL Option 10: Flow Reversal Prescription [N353]

Flow is reversed for specified SOL Rings and for specified portions of those Rings. The Rings are identified, in this Option, by a numbering system which is now little used elsewhere: each SOL Ring is assigned a “K-number”, $K = 1$ for the separatrix (i.e., first SOL) Ring, $K = 1.05$ for the next, 1.10 for the next, etc. (These K-numbers had direct significance in the DIVIMP1 code based on the magnetic field produced by two parallel, equal currents.) Flow reversal occurs for $fR_{min}S_{max} \leq s \leq fR_{max}S_{max}$ where $E = 0$ and $v_B = fR_M \times c_s$ at $s = fR_{min}S_{max}$, decreasing (in magnitude) linearly to 0 at $s =$

$fR_{\max}S_{\max}$. One must assign values to fR_M , fR_{\min} , fR_{\max} , K_{in} , K_{out} , where the flow reversal zone includes SOL Rings K_{in} to K_{out} .

For the non-reversed SOL Rings, also for the portions of the reversed SOL Rings which are not reversed, one uses SOL Opt -1, and therefore also has to specify f_S , f_L .

Clearly, this Reversed Flow Prescription is rather a “roughed-in” one, and its purpose is to make a quick check to see if Flow Reversal is a probable explanation for an observation. Rather than simply guess what values to assign to fR_{\min} , etc., one could be guided by running the NIMBUS code, see Sec.8, to see which flux tubes experience an “Ionization Excess”, and over what length. One can also use the somewhat more sophisticated approach of 3.1.9 “Flow Reversal”, based on the “Flux Recirculation Options.”

One can use T-Gradient Option to specify $n(s)$, $T_{e,iB}(s)$, sec 3.1.3.

3.1.3 Temperature Gradient Options

At this point, before continuing with the more model based SOL Options, it is appropriate to describe the rest of the prescriptive background plasma Options. The SOL Options described so far are incomplete without a prescription for the background temperature evolution. This function is accomplished with the Temperature Gradient Options which vary from simple linear specifications to applications of the simple Two Point Model, mentioned above, assuming only parallel heat conduction and treating electrons and ions separately. The electron and ion Temperature Gradient Options are identical in form except that the electron Options use the electron characteristics (T_e and κ_{0e}) and the ion Options use ion characteristics (T_{iB} and κ_{0i}). For this reason the following summarizes the Options together with any differences in the Options noted as one goes along.

Temperature Gradient Option 0: This is an example of the simplest prescription. The temperature ramps linearly from $f_{e,i} B_t \times T_{e,i} B_0$ at the target to $T_{e,i} B_0$ at $f_{e,i} B_L \times S_{\max}$ and then remains constant out to $s = L$. This Option

provides a simple prescription with which one can test the significance of background temperature variations on the observed quantities.

Temperature Gradient Option 1: This is a slightly more complex Option than 0. It involves two linear regions with different slopes. Again the background would be prescribed based on measured target conditions and perhaps some measurement that would supply approximate information on the variation of the velocity in the near target region. The temperature starts at $f_{e,i} B_t \times T_{e,i} B_0$ at the target and goes to $f_{e,i} B_{t2} \times T_{e,i} B_0$ at $f_{e,i} B_{L1} \times S_{\max}$ and then to $T_{e,i} B_0$ at $f_{e,i} B_{L2} \times S_{\max}$. It then remains constant at $T_{e,i} B_0$ out to $s = L$.

Temperature Gradient Option 2, 3, 4, 5, 6, 7: All of these options utilize the same basic Two Point Model for solving for $T_{e,iB}$. The only differences between the various Options are the value used for q_{para} - the power flux input that is used in the following equation and the 7/2 or 7/4 factor that relies on the power source assumption as outlined in the Two Point Model summary.

$$T_{e,iB} = \left(T_{e,iB0}^{7/2} + C_M \times \frac{q_{\text{para}} \times S}{\kappa_{0e,i}} \right)^{\left(\frac{2}{7}\right)}$$

Where for the various options the values of C_M and q_{para} are defined as follows:

Option 2: $C_M = 7/4$, q_{para} is input directly and is the same for all rings. Inner and outer plate temperatures are the same. The 7/4 factor is relevant for heat input to the flux tube occurring uniformly over its length.

Option 3: $C_M = 7/4$, $q_{\text{para}} = (2kT_{iB0} + 5kT_{e0}) \times n_0 \times V_0$ different for each ring. Inner and outer plate temperatures are the same.

Option 4: $C_M = 7/4$, $q_{\text{para}} = (2kT_{iB0} + 5kT_{e0}) \times n_0 \times V_0$ different for each ring. Inner and outer plate temperatures are allowed to differ.

Option 5: $C_M = 7/4$, $q_{para} = (5kT_{e0} \times n_0 \times V_0)$ for electrons, $q_{para} = (2kT_{iB0} \times n_0 \times V_0)$ for ions, different for each ring. Inner and outer plate temperatures are allowed to differ.

Option 6: $C_M = 7/2$, $q_{para} = (2kT_{iB0} + 5kT_{e0}) \times n_0 \times V_0$ different for each ring. Inner and outer plate temperatures are allowed to differ. The factor $7/2$ corresponds to the case where the heat influx to the flux tube all occurred at the upstream end.

Option 7: $C_M = 7/2$, $q_{para} = (5kT_{e0} \times n_0 \times V_0)$ for electrons, $q_{para} = (2kT_{iB0} \times n_0 \times V_0)$ for ions, different for each ring. Inner and outer plate temperatures are allowed to differ.

This finishes the simple background plasma prescriptions. The density is typically set to be constant for each ring in these simple prescriptions but is allowed to vary from ring to ring.

3.1.4 Conservation Equation SOL Options

The following Options are more theoretically based than the preceding descriptions. Furthermore, the Options here tie together the specifications for the background n, T_e, T_{iB}, v_B and E in an interdependent fashion based on the conservation equations for the individual species, unlike the previous prescriptions which allowed all of the individual parameters to be specified completely independently of each other. In this aspect they are more comprehensive descriptions. These Options should provide a methodology of constructing a reasonable background plasma where various effects may be considered and when operated with other codes in a feedback mode (NIMBUS or EIRENE for hydrogenic neutral calculations) may provide a good approximation for the background plasma.

3.1.4.1 SOL Option 12 [TN401, TN404, TN408, TN413, TN433, TN461, TN462]

This is the first SOL Option to solve the 3 conservation equations for $n(s)$, $T(s)$, $v(s)$. Thus one does not use the T-Gradient Options here. SOL Option 12 assumes $T_e = T_{iB}$ and that all of the parallel heat transport is via electron conduction. It is assumed that all of the heat input occurs at $s = L$. Radiative cooling is allowed for though one must prescribe the spatial variation of $P_{rad}(s)$ [W/m³] using one of the Radiative Source Options, see 3.1.7. Then $T(s)$ can be calculated directly without having to solve for $n(s)$ and $T(s)$ simultaneously (as one does have to do when convection is included, SOL Option 14, etc.):

$$T(s) = \left[T_0^{7/2} + \frac{7}{2\kappa_{0e}} \left(q_{para0} \times s + \int_0^s ds' \int_0^{s'} ds'' P_{rad}(s'') \right) \right]^{2/7} \quad (3.25)$$

where T_0 = plasma temperature at target (assigned individually for each flux tube and each end).

$\kappa_{0e} = 2000$ if T is in [eV], and $Z_{eff} = 1$

$q_{para0} = (2kT_{iBo} + 5kT_{eo}) n_0 c_{so}$

(strictly, one should not be free to assign $T_{iBo} \neq T_{eo}$ in this Option, but, in fact, one can). (Note that q_{para0} is in [W/m²].)

n_0 = plasma density at target (assigned separately for each flux tube, each end).

$c_{so} = ((kT_{eo} + kT_{iBo})/m_i)^{1/2}$

One then has the particle conservation equation:

$$\Gamma(s) \equiv n(s) v(s) = n_0 c_{so} + \int_0^s S_p(s') ds' \quad (3.26)$$

where $S_p(s)$ = ionization source strength [particles/m³/s] which has to be specified using one of the Ionization Source Options, see Sec.3.1.6. These latter Options are arranged to ensure that $\Gamma(L) = 0$ (and assuming there is no flow reversal either).

One also has the momentum equation:

$$n(s) [2kT(s) + m(v(s))^2] = 4n_0kT_0 \equiv p_0 \quad (3.27)$$

where it has been assumed that:

- (a) there is no momentum loss due to friction, etc.,
- (b) $|M| = 1$ at the target.

Note that since one has separately calculated $T(s)$, one now has just 2 coupled equations to solve for $n(s)$, $v(s)$. Noting that $\Gamma(s)$ is also completely specified one can write all of the following:

$$v^2 - \frac{p_0 v}{m\Gamma} + \left(\frac{2kT}{m}\right) = 0 \quad (3.28)$$

$$M^2 - \frac{p_0}{mc_s\Gamma} M + 1 = 0 \quad (3.29)$$

$$n^2 - \frac{p_0}{mc_s^2} n + \frac{\Gamma^2}{c_s^2} = 0 \quad (3.30)$$

There is advantage in using the last equation to obtain $n(s)$ first since one can then find $v(s) = \Gamma(s)/n(s)$ without running into the problem of dividing by zero (when solving for $v(s)$ first, one has the problem of dealing with $\Gamma(s)/v(s)$ where $v(s)$ and $\Gamma(s)$ both go to zero at some point).

One can illustrate a separate problem, however, by considering $M(s)$:

$$M = \left(\frac{p_0}{2mc_s\Gamma} \right) + \left[\left(\frac{p_0}{2mc_s\Gamma} \right)^2 - 1 \right]^{1/2} \quad (3.31)$$

namely, the phenomena of a Supersonic Transition in the midst of the flow. Of course, one usually assigns $|M| = 1$ at $s = 0$, and so it may be surprising

that the flow should reach $|M| = 1$ for some $s > 0$. Nevertheless, this can certainly happen. The term $(p_0/2mc_s\Gamma) < 0$ since $\Gamma(s) < 0$. At $s \rightarrow 0$ this term $\rightarrow -1$ so one has $M = -1$, as one has assigned. For $s > 0$ it is clearly necessary that there be no imaginary square root in the equation for $M(s)$. This, however, will happen if $T(s)$ (i.e., $c_s(T)$) rises very rapidly while $\Gamma(s)$ falls slowly: that can make the term $(p_0/2mc_s\Gamma)^2 < 1$. This is a classical cause of Supersonic Transitions in edge plasmas. What to do about it? Presently incorporated in most of the SOL Options is the simple, arbitrary prescription that whenever an imaginary root is encountered, $v(s)$ is simply assigned the local value of c_s . In this way, the energy (temperature) and particle conservation equations continue to be satisfied at every point, but the pressure/momentum equation is violated. A separate print-out is available showing how the total pressure, i.e., $p_{\text{total}} = n(kT_e + kT_i + mv^2)$, varies from point-to-point, so that one can see how $p_{\text{total}}(s)$ varies. Presumably if it does not vary greatly from p_0 , then the reliability of the solution cannot be greatly compromised — bearing in mind that the real situation is not inviscid and frictionless anyway, i.e., p_{total} is probably not really constant.

The proper approach is to abandon the assumption that $|M| = 1$ at the target. This is discussed in Sec. 3.1.4.6 (SOL Option 22).

The value of the electric field is given by Ohm's Law (the parallel momentum equation for the electrons):

$$-\frac{dp_e}{ds} - enE + \frac{enj}{\sigma_{\parallel}} - 0.71 n \frac{dkT_e}{ds} = 0 \quad (3.32)$$

We take $j = 0$ and so:

$$E = -\frac{1}{en} \frac{d(nkT_e)}{ds} - \frac{0.71}{e} \frac{d(kT_e)}{ds} \quad (3.33)$$

This is used in all the following SOL Options.

3.1.4.2 SOL Option 13 [See Note list for SOL Option 12]

As SOL Option 12 but now one follows $T_e(s)$, $T_{iB}(s)$ separately, assuming parallel heat conduction for both. Thus, again, one does not use the T-Gradient Options:

$$T_e(s) = \left[T_{e0}^{7/2} + \frac{7}{2\kappa_{0e}} \left(q_{\text{para}0} \times s + \int_0^s ds' \int_0^{s'} ds'' P_{\text{rad}}(s'') \right) \right]^{\frac{2}{7}} \quad (3.34)$$

$$T_{iB}(s) = \left[T_{iB0}^{7/2} + \frac{7}{2\kappa_{0i}} q_{\text{para}0i} \times s \right]^{\frac{2}{7}} \quad (3.35)$$

$$\Gamma(s) \equiv n(s) v(s) = n_0 c_{s0} + \int_0^s S_p(s') ds' \quad (3.36)$$

$$n(kT_e + kT_{iB} + mv^2) = 2n_0(kT_{iB0} + kT_{e0}) \equiv p_0 \quad (3.37)$$

$$q_{\text{para}0e} = 5kT_{e0}n_0c_{s0} \quad (3.38)$$

$$q_{\text{para}0i} = 2kT_{iB0}n_0c_{s0} \quad (3.39)$$

where one has to specify n_0 , T_{e0} , T_{iB0} , $P_{\text{rad}}(s)$, $S_p(s)$. The values $\kappa_{0e} = 2000$, $\kappa_{0i} = 58.9$ are fixed.

3.1.4.3 SOL Option 14 [See Note list for SOL Option 12, also TN458, TN623.]

Here convection is included — at least the dominant term is:

$$q_{\text{para}\{\text{cond}\}} \equiv \left(\frac{5}{2} kT + \frac{1}{2} mv^2 \right) \Gamma \quad (3.40)$$

Thus, it is always acceptable to take:

$$q_{\text{para}\{\text{cond}\},e} \approx \frac{5}{2} kT_e \Gamma \quad (3.41)$$

while for the ions, the similar approximation is less good, but is used here since it is much simpler to handle:

$$q_{\text{para}\{\text{cond}\},i} \approx \frac{5}{2} kT_i B \Gamma \quad (3.42)$$

In SOL Option 14 it is assumed that $T_e = T_{iB}$. Thus:

$$\frac{d}{ds} \left(5\Gamma kT - \kappa_{oe} T^{5/2} \frac{dT}{ds} \right) = -P_{\text{rad}}(s) \quad (3.43)$$

$$\Gamma = nv = n_0 c_{so} + \int_0^s S_p(s') ds' \quad (3.44)$$

$$n(2kT + mv^2) = 4n_0 kT_0 \equiv p_0 \quad (3.45)$$

$$q_{\text{para}0} = (2kT_{iB0} + 5kT_{e0})n_0 c_{so} \quad (3.46)$$

Note: one needs $q_{\text{para}0}$ as a boundary condition for solving the energy equation. Note: one can solve the energy equation directly to obtain $T(s)$, without need of solving for $n(s)$, $v(s)$ — since $\Gamma(s)$, $P_{\text{rad}}(s)$, $q_{\text{para}0}$, T_{e0} , T_{iB0} are all fully specified in advance. This is not possible to do when the kinetic energy part of the convected energy is included, $\frac{1}{2} mv^2 \Gamma$, since then one has to solve for $n(s)$, $v(s)$, $T(s)$ simultaneously. This is done in SOL Option 22 using Runge Kutta methods.

3.1.4.4 SOL Option 15 [See Note list for SOL Option 12, also TN461, TN742.]

This was an attempt to replicate SOL Option 13, but with the assumption that the heat influx occurred uniformly along $0 \leq s \leq L$, rather than all at L . This changes the $\frac{7}{2\kappa_0}$ factor to $\frac{7}{4\kappa_0}$ — which is all that has been changed to date (Feb. 1995). This is not sufficient, however, and so this SOL Option should not be used. It will be corrected as follows:

$$\frac{d}{ds} \left(-\kappa_0 T^{5/2} \frac{dT}{ds} \right) = P_{in}(s) - P_{rad}(s) \quad (3.47)$$

where we will, in fact, allow for a general assumption about the spatial distribution for the heat input, $P_{in}(s)$ [W/m³]. This gives:

Equation (3.48)

$$T^{7/2}(s) = T_0^{7/2} + \frac{7}{2\kappa_0} \left(q_{para0} \times s - \int_0^s ds' \int_0^{s'} ds'' P_{in}(s'') + \int_0^s ds' \int_0^{s'} ds'' P_{rad}(s'') \right)$$

where $P_{in}(s)$ is subject to the constraint:

$$\int_0^L P_{in}(s) ds = q_{para0} + \int_0^L P_{rad}(s) ds \quad (3.49)$$

Example: $P_{rad} = 0$, $P_{in}(s) = P_{in0}$, uniform; then:

$$P_{in0} = q_{para0} / L \quad (3.50)$$

and

$$T^{7/2}(s) = T_0^{7/2} + \frac{7}{2\kappa_0} \left[s \times q_{para0} - \frac{1}{2} \frac{s^2 \times q_{para0}}{L} \right] \quad (3.51)$$

giving:

$$T^{7/2}(L) = T_0^{7/2} + \frac{7}{4\kappa_0} L \times q_{para0} \quad (3.52)$$

To implement this Option it is necessary to set:

$$P_{in}(s) = P_0 f(s) \quad (3.53)$$

where P_0 is a constant and $f(s)$ gives the spatial form of $P_{in}(s)$. One will then be free to specify arbitrary $f(s)$, while P_0 will then be given by the above

constraint. A form $f(s) = a + bs + cs^2$, with $a, b, c, \geq 0$ specifiable may be adequate.

3.1.4.5 SOL Option 21 Detached Plasma Prescription [TN988]

It is assumed that there are three regions:

- A. the “cushion”, $0 \leq s < L_1$. No radiation.
- B. a radiation + conduction zone, $L_1 \leq s < L_2$.
- C. conduction-only zone, $L_2 \leq s < L$.

Electron Temperature: T_{e0} is taken to be specifiable, L_1/L_3 and L_2/L_3 are specified. T_{e1} , the value at the start of Region B is also specified by specifying $TR1 = T_{e1}/T_{e0}$. In Region A, $T_e(s)$ is linear.

In Region B:

$$T_e^{7/2}(s - L_1) = T_{e1}^{7/2} + \frac{7}{2\kappa_{oe}} \left[q_0(s - L_1) + \frac{1}{2} (s - L_1)^2 q_{rad}^{total} / L_{rad} \right] \quad (3.54)$$

where

$$q_0 = \left(5 + \frac{\varepsilon}{kT_{e0}} \right) n_0 c_{s0} k T_0 \quad (3.55)$$

with $\varepsilon = 15$ eV, $c_{s0} = (kT_{e0}/m_i)^{1/2}$, i.e., we are neglecting the T_{i0} contribution to c_{s0} since often we will assume $T_{i0} \ll T_{e0}$. The default value for m_i is for DT, so $c_{s0} = 6190 T_{e0}^{1/2}$ [m/s] for T_{e0} in [eV]. The value of q_{rad}^{total} [W/m²] is specified by specifying $QR = q_{rad}^{total}/q_0$. One also defines $L_{rad} = L_2 - L_1$.

In Region C:

$$T_e^{7/2}(s - L_2) = T_{e2}^{7/2} + \frac{7}{2\kappa_{oe}} [q^{tot}(s - L_2)] \quad (3.56)$$

where

$$q^{tot} \equiv q_0 + q_{rad}^{total} \quad (3.57)$$

Ion Temperature: In Region A, T_{iB0} is specified, constant. In Regions B and C: $T_e = T_{iB}$. Thus there can be a jump in T_{iB} at L_1 .

Density: n_0 is specified, also n_1 by specifying $NR1 \equiv n_1/n_0$. $n(s)$ increases linearly in Region A. In Regions B and C: assume pressure constant. Thus $n(s) = n_1 (T(s)/T_1)^{-1}$.

Plasma Velocity v_{DT}^+ : At target $v_0 = c_{s0}$. For Region A: $v(s) = n_0 v_0 / n(s)$, since it is assumed that there is no ionization in the “cushion.” In Regions B and C: $v(s)$ decreases linearly to zero at specified distance L_V , specified by specifying $VR1 = L_V/S_{max}$.

3.1.4.6 SOL Option 22.

In order to bring in both parts of convected heat, which requires the simultaneous solution of the three conservation equations, a Runge Kutta method is used [TN892]. At the same time, a number of additional terms were added to the two temperature equations. Thus:

For electrons:

$$\frac{d}{ds} \left(\frac{5}{2} k T_e \Gamma - \kappa_{oe} T_e^{5/2} \frac{dT_e}{ds} \right) = -P_{re}(s) \quad (3.58)$$

where

$$P_{re}(s) = P_{rad} + P_{Helpi} + P_{ei} \quad (3.59)$$

These various terms are described below. Thus:

$$\frac{dT_e}{ds} = \frac{1}{\kappa_{0e} T_e^{5/2}} \left[\frac{5}{2} k T_e \Gamma + q_{para0,e} + \int_0^s P_{re}(s') ds' \right] \quad (3.60)$$

For ions:

$$\frac{d}{ds} \left(\frac{5}{2} kT_{iB} \Gamma + \frac{1}{2} m v^2 \Gamma - \kappa_{oi} T_{iB} \frac{dT_{iB}}{ds} \right) = -P_{ri}(s) \quad (3.61)$$

where

$$P_{ri}(s) = P_{cx} - P_{ei} \quad (3.62)$$

Thus:

$$\frac{dT_i}{ds} = \frac{1}{\kappa_{oi} T_i^{5/2}} \left[\frac{5}{2} kT_i \Gamma + \frac{1}{2} m v^2 \Gamma + q_{para0,i} + \int_0^s P_{ri}(s') ds' \right] \quad (3.63)$$

When convection is present, one has to change the prescriptions for the ion sheath heat transmission coefficient [TN982]. Now equation (3.64):

$$q_{para\{conv\},i} \rightarrow \left(\frac{5}{2} kT_{iB0} + \frac{1}{2} m v_0^2 \right) \Gamma_0 = \left(\frac{5}{2} kT_{iB0} + \frac{1}{2} M_0^2 (kT_{e0} + kT_{iB0}) \right) \Gamma_0$$

and so, unless one makes:

$$\gamma_i = \frac{5}{2} kT_{iB0} + \frac{1}{2} M_0^2 \times (kT_{e0} + kT_{iB0}) \quad (3.65)$$

and thus calculates:

$$P_{i0} = \gamma_i kT_{iB0} \Gamma_0 \quad (3.66)$$

(noting that this uses T_{iB} , not T_e , in the expression for P_{i0}), then the $q_{para\{cond\},i}$ may give a negative contribution just upstream of the target. Assuming this to be unphysical, one changes to the above prescription for γ_i when convection is present.

Particle conservation is given as before, see SOL Option 12. Thus $\Gamma(s)$ is specified. The momentum equation now allows for neutral friction [TN1215]:

$$\begin{aligned} n \left(kT_e + kT_{iB} + m v^2 \right) &= n_0 \left(1 + M_0^2 \right) (kT_{e0} + kT_{iB0}) + \int_0^s S_{mom}(s') ds' \\ &= p_0 + \int_0^s S_{mom}(s') ds' \end{aligned} \quad (3.67)$$

$$= p(s)$$

where $S_{\text{mom}}(s)$ is the momentum loss rate, see below. One thus proceeds as before but with $p(s)$ in place of p_0 .

The terms in the temperature equations:

(a) Pei: thermal equilibration between electrons and ions [TN463]

$$P_{ei} = \frac{1.14 \times 10^{-32} n_B^2 (T_e - T_{iB})^{3/2}}{m_B (T_e)^{3/2}} \quad (3.68)$$

P_{ei} in [W/m³], n_B [m⁻³], T [eV], m_B [AMU]).

It is to be noted that the inclusion of P_{ei} in the present modeling which calculates upstream, from boundary conditions at the target, can cause T_e and T_{iB} to grow further apart, when P_{ei} is turned on, compared with it is off [TN1191, TN1194]. This can even result in one of T_e or T_{iB} actually decreasing with increasing s , even hitting zero, and going negative. Such unphysical behaviour is due to assuming that just any combination of n_0 , T_{e0} , T_{iB0} is physically possible, and can fit with monotonically increasing $T_{e,iB}(s)$. This is not true when P_{ei} is included. Thus, one must be alert when turning P_{ei} on to watch for “crashes” in T_e or T_{iB} . If that happens, one has evidently assumed impossible combinations of n_0 , T_{e0} , T_{iB0} or has not included sufficient physics in the model itself. If one assumes that n_0 and T_{e0} measured experimentally, are correct and are without error, then it must be T_{iB0} which is wrong (one might have assumed $T_{iB0} = T_{e0}$ initially, in the absence of direct measurements of T_{iB0}). One would therefore change T_{iB0} in the direction to stop the crash. It may also be the case that moving n_0 and T_{e0} around, within their error bars, would avoid the crash.

(b) Helpi, “Hydrogen Energy Loss per Ionization” [TN652, TN864] allows for the cooling to the electrons caused by the inelastic collisions associated with recycle of the hydrogenic neutrals. One defines first the number $Helpi$:

$$\text{Helpi} = 17.5 + \left(5 + \frac{37.5}{T_e}\right) \left(1 + \frac{0.25}{T_e}\right) \log_{10} \left(\frac{10^{21}}{n_e}\right) \quad (3.69)$$

the Harrison expression (*Nucl. Technol./Fusion* 3 (1983) 432) where Helpi and T are in [eV], n_e is in [m^{-3}]. Then:

$$P_{\text{Helpi}}(s) = \text{Helpi} \times S_p(s) \times 1.6 \times 10^{-19} [\text{W}/\text{m}^3] \quad (3.70)$$

Later an option will allow for the direct transfer of P_{Helpi} from PIN-NIMBUS, sec.8.

(c) P_{cx} : Charge Exchange Cooling/Heating of the Ions. As a first option:

$$P_{\text{cx}}(s) = \left(\frac{3}{2}\right) kT_{\text{IB}} \times 1.6 \times 10^{-19} \times \text{CEICF} \times S_p(s) \quad (3.71)$$

where CEICF = Charge Exchange Ion Cooling Factor, is to be specified. Here only cooling is possible. When $P_{\text{cx}}(s)$ is directly transferred from PIN-NIMBUS, cooling or heating of the ions will result.

Specifying $S_{\text{mom}}(s)$ [TN1215]: this is done by specifying the total strength of the momentum loss by specifying f_{fric} :

$$\int_0^L S_{\text{mom}}(s') ds' = p_0 \left(\frac{1}{f_{\text{fric}}} - 1 \right) \quad (3.72)$$

and using a Momentum Source Option (see sec 3.1.8) the characteristics of $S_{\text{mom}}(s)$ can be specified.

3.1.5 Supersonic Transition Mid-Stream

As already discussed in Sec. 3.1.4.1 (SOL Option 12), imaginary roots can be encountered in the solutions for $v(s)$ or $n(s)$, at some particular value of s , when the boundary condition $M_0 = -1$ is used. The preferred resolution of this problem is to change M_0 until this is just avoided. For illustration

consider the simplest case where $T_e = T_{iB}$ and with electron parallel heat conduction only (thus $T(s)$ is established, independent of the solutions for $n(s)$, $v(s)$). For simplicity assume $\Gamma(s) = n_t v_t (1 - s/L_i)$ as an illustration of one source possibility; L_i would approximately be the hydrogen ionization distance. One also has the conservation of momentum:

$$n(2kT + mv^2) = n_0(2kT_0 + mv_0^2) \quad (3.73)$$

where $v_0 = M_0 c_{s0}$. Define $M = v/c_{s0}$ (this does not require that we assume isothermal flow; M is merely a convenient variable). Then one obtains:

$$M(s) = \frac{(1 + M_0^2)}{2M_0(1 - s/L_i)} \pm \left[\left(\frac{1 + M_0^2}{2M_0(1 - s/L_i)} \right)^2 + \frac{T(s)}{T_0} \right]^{1/2} \quad (3.74)$$

where we now have to consider the possible meaning of both “+” and “-” solutions.

Define

$$A(s) = \left[\frac{1 + M_0^2}{2M_0(1 - s/L_i)} \right]^2 \quad (3.75)$$

Consider first the simple case where $T(s) \approx T_0$, i.e., isothermal flow. For $M_0 = -1$, (see fig 3.1) one can readily show that $A(s) \geq 1$ for all s , so there is no risk of imaginary roots. The boundary condition $M_0 = -1$ is thus the natural one for isothermal flow.

Now consider the case where $T(s)/T_0$ is an increasing function of s (see fig 3.2). For A_1 , $M_0 = -1$; for A_2 , $|M_0| = |M_0^*| > 1$ and the A -curve just touches the $T(s)/T_0$ curve at one point; for A_3 , $|M_0| > |M_0^*|$.

It is evident that the correct boundary condition is $M_0 = M_0^*$. For $|M_0| < |M_0^*|$ imaginary roots are encountered. For $|M_0| > |M_0^*|$ one

cannot switch over from the “-” solution to the “+” solution at any point without involving a discontinuity. For $M_0 = M_0^*$ one can switch branches at the point where $A = T(s)/T_0$ since at that point the quantity in the square root is zero. The two branches are of the following form. For $|M_0| < |M_0^*|$, see figure 3.3a, for $M_0 = M_0^*$, see figure 3.3b and for $|M_0| > |M_0^*|$ see figure 3.3c.

For $s < s^*$, one needs to use the - sign, in order to have supersonic flow. At some point one needs to switch to the other branch if one is to have $v \rightarrow 0$ at some $s > s^*$. One can only do this smoothly for one choice of M_0^* .

Thus, the algorithm in DIVIMP searches for the value of $|M_0| > 1$ which causes the two branches to just touch at one point. Unfortunately, the solutions are very sensitive near s^* at the transition and can be rather choppy (without the addition of viscosity). This choppiness is usually confined to a small Δs region and is just ignored, or smoothed over. Smoother algorithms will be sought for a later SOL Option.

3.1.6 Ionization Source Options

Please refer to the DIVIMP User Guide for more detailed information on the Option specifications. More detailed descriptions dealing with the justifications for these Options will be forthcoming in later releases of the DIVIMP Guide. Please note that there are two sets of Ionization Source Options specified in different places. One set applies to SOL Options 12 through 15, the second set applies to SOL Option 22.

3.1.7 Radiative Source Options

Please refer to the DIVIMP User Guide for more detailed information on the Option specifications. More detailed descriptions dealing with the justifications for these Options will be forthcoming in later releases of the DIVIMP Guide. Please note that there are two sets of Radiation Source

Options specified in different places. One set applies to SOL Options 12 through 15, the second set applies to SOL Option 22.

3.1.8 Momentum Source Options

The following momentum source options are currently only used by SOL option 22. (sec 3.1.4.6).

(a) Momentum Source Option 0:

$$S_{\text{mom}}(s) = \begin{cases} S_{\text{mom0}}, \text{ constant} & 0 \leq s \leq L_m S_{\text{max}} \\ 0, & L_m S_{\text{max}} \leq s \leq \frac{1}{2} S_{\text{max}} \end{cases}$$

so
$$S_{\text{mom0}} = \frac{p_0}{L_m S_{\text{max}}} \left(\frac{1}{f_{\text{fric}}} - 1 \right)$$

(b) Momentum Source Option 1:

$$S_{\text{mom}}(s) \equiv S_{\text{mom0}} \times \exp(-s/L_m S_{\text{max}})$$

$$S_{\text{mom0}} = \frac{p_0 (1/f_{\text{fric}} - 1)}{L_m S_{\text{max}} (1 - \exp(-L/L_m S_{\text{max}}))}$$

(c) Momentum Source Option 2: proportional to the ionization source, but still based on f_{fric} :

$$S_{\text{mom}}(s) = \frac{S_p(s)}{\int_0^L S_p(s') ds'} \times p_0 \left(\frac{1}{f_{\text{fric}}} - 1 \right)$$

(d) Momentum Source Option 3: proportional to the ionization source directly:

$$S_{\text{mom}}(s) = R_{\text{cx/iz}} S_p(s)$$

where $R_{\text{cx/iz}}$ (the ratio of charge exchange rate to ionization rate) is a specified number.

- (e) Momentum Source Option 4: S_{mom} is taken directly from PIN-NIMBUS output, see Sec. 8.

3.1.9 Flow Reversal Options

The neutrals which recycle from the targets will be re-ionized in some complicated 2-D pattern which is virtually guaranteed to result in more/less ionization occurring on any given flux tube than the ion outflow from that flux tube to the target. Those tubes which experience an “ionization excess” will have a “watershed”: plasma which is created between the target and the “watershed” will flow toward the target (thus the location of the “watershed” will be just such that the integrated particle source in this near-target region will equal the ion flow to the target for that tube), while the plasma created beyond the “watershed” will flow in the reverse direction, gradually decaying away as this “excess plasma” cross-field diffuses into adjacent flux tubes which experienced an “ionization deficit.” Thus, overall particle balanced is achieved via reversed flow and cross-field diffusion.

In SOL Opt. 10 this situation could be specified in a very ad hoc way. This can be achieved slightly less artificially through the “Flux Recirculation Options” defined below.

The most physical approach would use NIMBUS or EIRENE, Sec.8, to calculate the 2-D hydrogenic ionization distribution. This still requires certain ad hoc prescriptions:

- (a) One first calculates the fraction of ionization occurring in the core, $f_{\text{iz}}^{\text{core}}$

If this is large enough, then it is likely that all the SOL flux tubes will have an “ionization deficit” and there will be no flow reversal anywhere.

In any case one must have a method of dealing with f_{iz}^{core} . The simplest prescription is to just ignore it and to renormalize the total ionization source strength outside the separatrix to equal the total target flux. This is not generally very satisfactory since f_{iz}^{core} gives rise to a very important “impurity flushing action,” extending over the entire length of the SOL: f_{iz}^{core} gives rise to a cross-field “source” for parallel flow in the SOL flux tubes, particularly the ones near the separatrix, and over their entire length. Thus, a better prescription would be to assign f_{iz}^{core} uniformly to all the SOL flux tubes over their lengths.

- (b) One has to assign the “excess ionization” existing above the “watersheds” of the tubes with reversed flow, to the tubes which are not reversed. The simplest method is to take the total excess of all the tubes and to assign it uniformly over the other tubes.

In a more sophisticated approach one would iterate the SOL Option with NIMBUS, assigning both f_{iz}^{core} and the “ionization excess” proportionally to the local cross-field density gradient — based on the (possibly wrong) assumption that cross-field transport is proportional to cross-field density gradients and $D_{\perp} = \text{constant}$.

Flux Recirculation Option

This flag turns flux recirculation in Options 12 to 15 on and off. Flux recirculation is allowed for through the assumption of over and under ionization on each flux tube. The source characteristics when the Flux Recirculation Option is on are specified by the next entry. Note that if a multiplication factor of 1.0 is used, this is equivalent to no flux recirculation since the ionization on the ring is equal to the net influx. However, it does allow the following entry to be used to specify different source characteristics for each ring.

0— Flux Recirculation Off
1 — Flux Recirculation On

Flux Recirculation — Source Specifications

The first line contains the description of the entry. The second line has headings and then the number of lines to follow in the table of flux recirculation data. The contents of the table are:

Ring number	Flux mult factor	Source Length	Source	Decay Length
-------------	------------------	---------------	--------	--------------

These specify the characteristics of the ion source for each ring. The Flux Multiplication Factor represents the quantity of over/under ionization to be found on that ring/flux-tube. A value of 1.0 for this results in no flux recirculation (i.e., outflux = ionization). A value of 0.5 means that there will be 1/2 as much ionization on the flux-tube as there is flux to the plates, and a factor 2.0 will result in twice as much ionization. This results in flow reversal or increased flow to the plates occurring in the calculation of the background velocities in SOL 12 to 15. The Source Length and Source Decay Length are the same as are generally specified except that they can be customized for each flux tube.

3.2 Plasma Backgrounds from 2-D Edge Fluid Codes

This will include some comments on using both B2 and EDGE2D generated background plasmas. To be completed.

4.0 Impurity Particle Sources

4.1 Types of Sources

The simplest type of source is to inject ions, of specified charge, at specified location — point source or spatially distributed. See Sec. 4.2.

The second type of source is neutrals launched from a surface (e.g. due to sputtering as calculated by DIVIMP) or from within the plasma (e.g. simulating situations like a gas puff or pellet injection). Target or wall sources. Sec. 4.3.

The third type is using alternative codes such as NIMBUS to calculate the distribution of the initially sputtered impurity neutrals with DIVIMP starting from the point where the neutrals are ionized. Target and wall sputtering. Sec. 4.4.

Finally, when impurity ions hit the target, self-sputtering can be permitted. Sec. 4.5.

Whether particles are started as neutrals or ions is set by the Control Switch: Set to 0 turns on the NEUT subroutine within DIVIMP which calculates the impurity neutral behaviour, set to 1 the NEUT subroutine is not invoked and ions are directly injected according to several different prescriptions.

4.2 Injection of Impurities as Ions

Injection Option 0: This is disregarded when NEUT control switch is not 0.

Injection Option 1: Injects ions at a specified (R, Z) location with a specified value of velocity along \vec{B} , v_0 .

Injection Option 2: Ions are injected uniformly on a given Ring between specified points $INJ1 \cdot S_{\max}$ and $INJ2 \cdot S_{\max}$ (relative to both target plates, equidistant from both targets). Specified v_0 .

Injection Option 3: As 2 but injection just near one target.

Injection Option 4: Primary sputtered impurity neutrals are calculated by NIMBUS as a result of following the hydrogenic background behaviour, Sec. 4.4. The ionization profile is used to generate a probability map for ion injection in DIVIMP. The initial ion energy, to give v_0 , is taken from the average energy of the impurities in the cell in which they are ionized as calculated by NIMBUS.

Injection Option 5: Injects ions uniformly on a specified Ring between specified locations $INJ1 \cdot S_{\max}$ and $INJ2 \cdot S_{\max}$ (relative to both plates). The initial velocity along \bar{B} is calculated from:

$$v_{init} = rg \cdot v_0 \quad (4.1)$$

where v_0 is specified and $rg = \sqrt{-2 \cdot \ln(X1)} \cdot \cos(2\pi X2)$ with $X1, X2$ random numbers drawn uniformly on $[0, 1]$.

Injection Option 6: As 5 but injected just near one target.

4.3 Launch as Neutrals

4.3.1 Basic Aspects

The principal type of source here is sputtering (although evaporative and free space sources can also be simulated). For target sputtering, the impurity production rate is therefore taken to be proportional to the incident flux density of background ions, as received per m^2 of target surface:

$$\Gamma_{B0} = n_0 \times M_0 \cdot c_{s0} \times (B_0/B) \times \cos(\theta_0) \quad (4.2)$$

where “0” refers to “target” and will generally be different for each Ring and at each target; $c_{s0} = [k(T_{e0} + T_{iB0})/m_i]^{1/2}$; the factor $\cos \theta_0 = 1$ when the target is orthogonal to the magnetic flux surfaces; see Sec.2.4. The values of n_0 , M_0 , T_{e0} , T_{iB0} are externally specified as part of *SOL Options*, Sec.3.1, or generated as a result of the specified SOL option or if an external source for the plasma background (e.g. a 2-D plasma background previously generated) has been specified then these quantities must all be provided by the external source. The values of $(B_\theta/B)_0$ and $\cos \theta_0$ are extracted from the Grid data. (see Sec.2.)

In DIVIMP the impact energy of the background ions is taken to be:

$$E_{\text{impact}} = 2kT_{iB0} + 3ZBkT_{e0} \quad (4.3)$$

One may note that this differs from that assumed in NIMBUS, Sec.8. A correction should be made to deal with cases when $|M_0| > 1$, but has not yet been done in DIVIMP (May,1995).

One thus has all the information needed in order to perform the physical sputtering calculation based on the Bohdansky formulae and the stored sputtering data to calculate yields, Y ; this is done via the *Sputtering Options*, Sec. 4.3.2. DIVIMP then calculates the total “Primary” sputtered flux (“primary” in that it is due to impact by the background ions):

$$f_{\text{impurity}}^{\text{total}} = \sum Y \times \Gamma_{B0} \times w_0$$

where the sum is over all target segments, and $w_0 \equiv$ width of segment, Sec.2. This quantity is listed in the print-out as “Total Primary Integrated Flux*Yield”, for each target separately.

DIVIMP then picks a segment from which to launch an impurity neutral, in a Monte Carlo way, weighted according to $Y\Gamma_{B0}w_0/f_{\text{impurity}}^{\text{total}}$.

For each segment, one knows the direction of the normal, \bar{N}_t , to the surface of the segment, from the magnetic data. In order to know at what angle the sputtered neutral should be launched, the angular distribution is specified by the *Vel/Angle Flag* Sec. 4.3.3; \bar{N}_t provides the reference direction.

It is also necessary to specify the velocity distribution of the sputtered neutrals. This is also done via the *Vel/angle flag*, Sec.4.3.3.

The neutral is now launched at $t = 0$ from the mid-point of the selected segment, with direction and velocity from the *Vel/angle flag*. It travels in a straight line until it is ionized. The probability P that in a given time interval Δt it will be ionized is given by:

$$P = \Delta t / \tau_{\text{izn}} \quad \text{where} \quad \tau_{\text{izn}} = [n_e \langle \sigma V \rangle_{\text{izn}} (T_e, n_e)]^{-1} \quad (4.5)$$

where $\langle \sigma V \rangle_{\text{izn}}$ is calculated from the chosen atomic data base, Sec.6.1. Thus the neutral is stepped along the straight line until it is ionized in a Monte Carlo way.

The 2-D spatial distributions of the neutral density and of the neutral ionization rate is thus calculated.

The spatial location of the ionization of each individual neutral particle is stored until all the neutrals have been launched. The ion-following part of DIVIMP then takes each of these starting locations to inject a single-charged ion. The neutral routine saves a value for the velocity of the ion based on the velocity of each individual neutral at the point where it was ionized, and then starts each individual ion with these particular velocities. (*Initial Ion Velocity* Option; see DIVIMP User Manual.)

4.3.2 The Sputter Options

Sputtering Option 0: Sputtering by background plasma ions only (no self-sputtering), $E_{\text{impact}} = 2kT_{\text{IB0}} + 3ZBkT_{\text{e0}}$, is used to calculate the yield.

In this Option it is taken that the maximum energy which can be transferred to the sputtered neutral is given by:

$$E_{\max} = E_{\text{impact}} \gamma(1 - \gamma) - E_{\text{bd}} \quad (4.6)$$

where $\gamma = 4[m_B m_t / (m_B + m_t)]^2$ where m_t = mass of target atom (usually $m_t = m_I$, of course, but this is left free to be specified) and E_{bd} = surface binding energy. The values of E_{bd} are simply stored as an atomic data base and since the values are sometimes in question, the value used is listed in the print-out.

The sputtered neutral velocities are chosen using the Velocity/Angle Flags Option (Sec. 4.3.3) with the maximum Velocity of the injected neutral limited by the maximum transferable energy, E_{\max} . The characteristic value of E_{\max} varies from target segment to target segment as the plasma temperature varies. The calculation of neutral velocity is done for every neutral launched and the limiting values depend on the local target conditions. DIVIMP converts this limiting energy to a number in the range [0,1] resulting in the following maximum limit on x (see N41).

$$x_{\max} = (1 + E_{\text{bd}}/E_{\max})^{-2} \quad (4.7)$$

The value of x_{\max} is then compared to a number drawn randomly for each neutral to be launched. If the randomly drawn number is less than the limit, the random number is used to calculate the sputtered neutral velocity, v_n . If the random number is greater than the calculated limit, it is recorded as a discarded velocity, i.e. the velocity selected did not satisfy the energy limitation condition for the local conditions. Since the value of x_{\max} may be very small under certain conditions, DIVIMP will allow only 1000 discarded velocities for a particular neutral. After accumulating 1000 discarded velocities for a particular neutral, DIVIMP then records that one neutral as a “failed launch” since it was unable to find a valid set of launch conditions for the neutral given the local conditions on the specific target segment. Usually failed launches are very rare. DIVIMP then proceeds to launching the next neutral and repeats the procedure. The case print outs refer to the “Number

of Impurity Particles to Follow” (which actually refers to the number of neutrals initially launched for a neutral case or the number of ions injected for an ion case.) The information on the number of “failed launches”, discarded velocities, E_{\max} and other information is given in the print-out.

It is usually assumed that the energy distribution of physically sputtered neutrals is given by the Thompson Distribution:

$$\frac{dY}{dE_n} = \frac{2E_{bd}E_n}{(E_n + E_{bd})^3} \quad (4.8)$$

where dY is the yield of neutrals having energies in $[E_n, E_n + dE_n]$. Such a distribution can be generated by choosing a random number x , uniform in $[0, 1]$ and setting the neutral launch velocity to:

$$v_n = \left[\frac{2E_{bd}}{mI(x^{1/2} - 1)} \right]^{1/2} \quad (4.9)$$

see N41.

The Thompson Distribution has a high energy tail which can make important, even dominant, contributions to the contamination efficiency of the source since the high energy neutrals penetrate the plasma more deeply. It is therefore important to introduce the cut-off energy, as above, which is given by $x_{\max} = (1 + E_{bd}/E_{\max})^{-2}$, see N41.

With regard to the expression to be used for E_{\max} , Lorne Horton has pointed out, A14, July 20, 1993, that since the sputtering data itself specifies the “threshold” energy for sputtering, E_{th} , then for $E_{\text{impact}} = E_{th}$ we would want to have that $E_{\max} = 0$, i.e.,

$$0 = E_{th}\gamma(1 - \gamma) - E_{bd} \quad (4.10)$$

Putting in values of E_{bd} can then sometimes give values of E_{th} which are not in agreement with the sputtering data value for E_{th} . One can force consistency in various ways. The way used in NIMBUS, and also available as

an option in DIVIMP, is to adjust (i.e., eliminate) the factor $\gamma(1 - \gamma)$ to make for constancy. Thus one would use for E_{\max} :

$$E_{\max} = E_{bd}(E_{\text{impact}}/E_{th} - 1) \quad (4.11)$$

Consultations with Eckstein, N712, TN910, indicated that none of these simple formulae are ideal, particularly for cases where the masses of the impacting and target particles are close. Thus, the choice is somewhat arbitrary and up to the user.

For self-sputtering, Eckstein (TN746) recommends the use of $E_{\max} = 0.5 E_{\text{imp}}$, (but this not used in DIVIMP as yet, May, 1995).

Sputtering Option 1: Sputtering by a specified ion type, impurity sputtering, with:

$$E_{\text{impact}} = 2kT_i B_0 + 3Z_{\text{imp}} kT_e \quad (4.12)$$

with Z_{imp} specified. Assumes $E_{\max} = E_{\text{imp}}$ for cut-off. (i.e. not currently Eckstein's recommendation).

Sputtering Option 2: This Option represents a carbon chemical sputtering source with the yields calculated according to the formulae in "Revised Formula for Chemical Sputtering of Carbon" by Garcia-Rosales and Roth. In the following E_0 is the energy of an incident deuterium atom, T is the temperature of the Target in K and Γ_{D^+} is the incident deuterium flux in $\text{cm}^{-2}\text{s}^{-1}$.

$$Y_{\text{tot}}(E_0, T, \Gamma_{D^+}) = Y_{\text{phys}}(E_0) + Y_{\text{chem}}(E_0, T, \Gamma_{D^+}) \quad (4.13)$$

Where the physical yield is described by the following:

$$Y_{\text{phys}}(E_0) = Q \cdot S_n(E_0) \left(1 - \left(\frac{E_{th}}{E_0} \right)^{2/3} \right) \left(1 - \frac{E_{th}}{E_0} \right)^2 \quad (4.14)$$

Q and the threshold energy E_{th} are fitting parameters. $S_n(E_0)$ is the stopping power and can be approximated by the following.

$$S_n(E_0) = \frac{0.5 \ln \left(1 + 1.2288 \times \left(\frac{E_0}{E_{TF}} \right) \right)}{\frac{E_0}{E_{TF}} + 0.1728 \times \sqrt{\frac{E_0}{E_{TF}}} + 0.008 \times \left(\frac{E_0}{E_{TF}} \right)^{0.1504}} \quad (4.15)$$

E_{TF} is the Thomas-Fermi energy.

The chemical yield is described by the following:

$$Y_{chem}(E_0, T, \Gamma_{D^+}) = Y_{ch,th}(E_0, T, \Gamma_{D^+}) + Y_{th,ath}(E_0, T) \quad (4.16)$$

with equation (4.17):

$$Y_{ch,th}(E_0, T, \Gamma_{D^+}) = \frac{6 \times 10^{19} \exp\left(\frac{-1}{kT} [\text{eV}]\right)}{1 \times 10^{15} + 3 \times 10^{27} \exp\left(\frac{-2}{kT} [\text{eV}]\right)} \times \left(2 + 200 \times Y_{phys}(E_0)\right) \times \left(\frac{\Gamma_{D^+}}{10^{16}}\right)^{-0.1}$$

$$Y_{ch,ath}(E_0, T) = \frac{0.05 \exp\left(E_0 \times 10^{-3} \times \left(20 - \frac{1}{kT}\right)\right)}{\left[1 + \exp\left(\frac{E_0 - 150}{25}\right)\right] \times \left[1 + \exp\left(\frac{T - 740}{25}\right)\right]} \quad (4.18)$$

These equations are used to obtain a distribution of impurity neutral production across the target due to chemical sputtering effects. The value of E_0 is the same as E_{impact} used in the previous options for the background plasma ions. The velocity and angular distribution of the injected particles is controlled by the “Velocity/Angle Flag” options. $\Gamma_{D^+} = \Gamma_{B0}$ of sec 4.3.1.

Sputtering Option 3: This allows for both primary and self-sputtering. The initial or primary sputtering is by the background ions only. For this

sputtering, the same assumptions are made as in Sputtering Option 0. When a primary impurity ion returns to the target, its individual and specific location, charge Z_I , temperature T_I , exit velocity and thus impact energy are known:

$$E_{\text{impact}} = 3Z_I k T_e + 2k T_I + 5.22 \times 10^{-9} m_I v_{\text{exit}}^2 \quad (4.19)$$

(m_I in [AMU]; E, T in [eV]; v in [m/s])

Thus, one can calculate the yield of self-sputtered secondary neutrals; call this Y_{SS2} . One uses the Bohdanský and Thompson expressions. Also $E_{\text{max}} = E_{\text{impact}}$, here. This secondary neutral, then ion, is followed through the plasma just as a primary neutral/ion but it is given weight Y_{SS2} rather than unity when it is counted in a bin, Sec. 8.1. When this secondary ion finally strikes the limiter it creates a tertiary-sputtered neutral, with a new calculated yield Y_{SS3} appropriate for the impacting conditions of the secondary ion. This particle is followed as before, but now has weight $Y_{SS2} \times Y_{SS3}$. This process is followed until the weight falls below some specified value, say 0.1, when the sequence is abandoned (as if $Y_{SSX} = 0$), and a new primary neutral is launched, arising from a primary sputtering event. In Sputtering Option 3, the self-sputtering may use a different Velocity/Angle flag from the primary sputtering.

Sputtering Option 4: This is the same as Sput.Opt.3 except that the velocity of the self-sputtered neutral is also limited by the value of E_{max} as described above.

Sputtering Option 5: This Option is identical to Sputter Option 2. The initial impurity production is from a chemically sputtered source. However, this Option will follow the self-sputtering cascade of the impurity ions as they return to the target.

4.3.3 Velocity/Angle Flag Options

The specification of the angular and velocity distribution of the released neutrals is given by the “Velocity/Angle Flag”:

Velocity/Angle Flag 0: This gives a cosine angular and a Thompson velocity distribution in a simple sense [N38]. $q = \pm \sin^{-1}[\xi]$ (actually this should be $\pm \sin^{-1}[\xi^{1/2}]$ in order to give cosine [N41]) and

$$v_n = \left(\frac{2E_{bd}}{m_{imp}} (\xi_2^{-1/2} - 1)^{-1} \right)^{1/2} \quad (4.20)$$

Velocity/Angle Flag 1: This gives a cosine and Thompson distribution projected onto 2-D space [N65]. Here one picks $\beta = \sin^{-1}((\xi_1)^{1/2})$ then $\phi = 2\pi\xi_2$ and finally $\theta = \tan^{-1}[\tan \beta \cos \phi]$,

$$v_n = \left[\frac{2E_{bd}}{m_{imp}(\xi_3^{-1/2} - 1)} \right] [\text{abs}(\cos^2\beta + \sin^2\beta \cos^2\phi)]^{1/2} \quad (4.21)$$

A maximum value of ξ_3 is imposed based on the maximum amount of momentum which can be transferred from the impacting ion to the target atom.

Velocity/Angle Flag 2: This gives a Maxwellian velocity distribution [N83]. θ is given as in Velocity/Angle Flag 1 and

$$v_n = (2kT_g/m_i)^{1/2} (|\ln(1-\xi)|)^{1/2} \quad (4.22)$$

where the gas temperature T_g is specified.

Velocity/Angle Flag 3: This is a simpler approximation to a Maxwellian [N94]. $\theta = \pm \sin^{-1}[\xi^{1/2}]$. $v_n = \sqrt{2E_{in}/m_{imp}}$ with E_{in} specified. To simulate chemical sputtering.

Velocity/Angle Flag 4: This is the same as Velocity/Angle Flag 2, but it allows for the possibility of cutting the velocity distribution off at a level that is different than the “natural” E_{\max} (just in case that prescription over- or under-estimates the number of high energy neutrals). The new $E_{\max} = \text{old } E_{\max} \times (E_{\max} - \text{Factor})$, where one specifies $(E_{\max} - \text{Factor})$.

Velocity Angle Flag 5: This similarly alters Velocity/Angle Flag 0 for an $(E_{\max} - \text{Factor})$. Also $\pm \sin^{-1}(\xi) \rightarrow \pm \sin^{-1}(\xi^{1/2})$ [N105].

Velocity/Angle Flag 6: This gives a simple gas jet with $\theta = 0$ and $v_n = (2E_{\text{in}}/m_{\text{imp}})^{1/2}$ with E_{in} specified.

Velocity/Angle Flag 7: This gives the actual distribution known to be characteristic of a Free Jet (gas flow into a vacuum) [N120]. $\theta = \pm \cos^{-1}[(1 - \xi)^{1/3}]$, $v_n = (2E_{\text{in}}/m_{\text{imp}})^{1/2}$.

Velocity/Angle Flag 8: This gives an isotropic neutral source as, e.g., from molecular breakup; thus perhaps useful for chemical sputtering [N122]. $\theta = 2\pi\xi$, $v_n = (2E_{\text{in}}/m_{\text{imp}})^{1/2}$.

Velocity/Angle Flag 9: It may be that molecular breakup is better modeled by two neutral velocities [N156]. Here $\theta = \pm \sin^{-1}[\xi^{1/2}]$, $v_n = (2E_{\text{in}}/m_{\text{imp}})^{1/2}$ but two different, specified energies E_{in} are used alternatively.

Velocity/Angle Flag 10: This gives a 3D Free Jet for 3D LIM work [N218]. The (x_n, y_n, p_n) coordinates of the neutral advances in time (launch from $(0,0,0)$ assumed as

$$y_n = v_n t \sin \beta \cos \phi, \quad x_n = v_n t \cos \beta, \quad p_n = v_n t \sin \beta \sin \phi$$

where

$$\beta = \cos^{-1}[(1 - \xi_1)^{1/3}], \quad f = 2\pi\xi_2, \quad v_n = (2E_{\text{in}}/m_{\text{imp}})^{1/2}$$

(Note: this Velocity/Angle Flag is a carry-over from LIM and needs re-interpretation for DIVIMP).

Velocity/Angle Flag 11: This gives a “2.5-D Free Jet” [N222]. This is the same as Velocity/Angle Flag 7 (the 2-D Free Jet) but the p-coordinate is assigned randomly between two specified limits $\pm p_{\max}$.

4.3.4 Neutral Launch Options

It is also necessary to specify the “Launch Option”:

Launch Option 0: Distributed launch across the divertor target surface.

Launch Option 1: At given point (R, Z).

Launch Option 2: Homogeneously along walls.

4.4 Sputtering and Neutral Transport Calculated by Other Codes

To be completed. This will describe the interfaces in place for using NIMBUS sputter sources and impurity neutral transport and ionization directly in DIVIMP.

4.5 Self-Sputtering

This is handled by Sputtering Options 3,4 and 5 above, when they are invoked. The sputtering “cascade” can be terminated at a specified number of generations, if the weight of the particles is not dropping fast enough (this can occur when a recycling impurity, such as neon, is involved and one simulates the effect of recycling at the target by setting the Yield to 1. (The “self-sputter” yield for a recycling impurity like neon is assumed to be 1. (i.e. all neon striking the target is released from the target.) The effect of pumping

is simulated by setting the Yield Multiplication Factor (YMF) to something less than 1. The difference from 1 corresponds to the pumping of gas by the target/target region.)

5.0 Impurity Transport

This chapter describes the different types of particle transport dealt with in DIVIMP and addresses the physics that guided the impurity transport aspects of the DIVIMP implementation.

5.1 Impurity Neutral Transport

Briefly, impurity neutrals travel in straight lines in the poloidal plane. The initial direction and velocity for these particles are determined by the sputter options and velocity angle flags described in section 4.3.3 and 4.3.4. They continue to travel in straight lines until they are ionized or strike another solid surface where, depending on the options specified, they will either reflect or be absorbed.

5.1.1 Change of Charge State

If the impurity particle is launched as a neutral, then the particle motion is in a straight line in (R, Z) space until ionization occurs in a Monte Carlo way. The neutral mean free path for ionization of the neutral may be very short and it may be necessary to use shorter time steps for the neutral-tracking than for the ion-tracking. The option is available to set the neutral time step, Δt_n , separately from the ion time step, Δt_i .

At each time step Δt_n , the ionization rate is calculated based on the local value of n_e , T_e , i.e., $\overline{\sigma v}_{iz}(n_e, T_e)$. A random number ξ , uniform on $[0, 1]$, is drawn. If the random number falls within $0 \leq \xi \leq \Delta t_n / \tau_{iz}$, then ionization is considered to have occurred where:

$$\tau_{iz} \equiv [n_e \overline{\sigma v}_{iz}(n_e, T_e)]^{-1}$$

The location of ionization is stored, as well as the velocity of the neutral at that point (its projection along $\bar{\mathbf{B}}$). This information is used later to start the impurity ion off in the ion-tracking part of the code.

Subsequent ionization to higher states is included, also recombination, and optionally, charge-exchange recombination. One defines:

$$\tau_{\text{ch}} \equiv [n_e(\bar{\sigma}v_{\text{iz}}(n_e, T_e) + \bar{\sigma}v_{\text{rec}}(n_e, T_e))]^{-1}$$

as the time for a change of charge state (either ionization or recombination). At each time step Δt_i a random number ξ_1 , uniform on $[0, 1]$ is drawn. If $0 < \xi_1 < \Delta t_i / \tau_{\text{ch}}$ then a change of state occurs. In that case a second random number ξ_2 is drawn. The change is recombination if $0 < \xi_2 < \bar{\sigma}v_{\text{rec}} / (\bar{\sigma}v_{\text{iz}} + \bar{\sigma}v_{\text{rec}})$, otherwise it is ionization.

The values of $\bar{\sigma}v_{\text{iz}}(n_e, T_e)$ and $\bar{\sigma}v_{\text{rec}}(n_e, T_e)$ are drawn from the atomic data base, Sec. 6, preferably from ADAS. If charge exchange recombination is included, then the 2-D spatial distribution of the atomic hydrogen density, n_{H} , has to also be specified. This can be done via an analytic prescription in which case one must also specify the relative velocity of approach of the neutral and ion, v_{rel} . To be implemented: an option where n_{H} is transferred from a NIMBUS output, also the information needed to calculate v_{rel} .

5.2 Impurity Ion Parallel Transport and Heating

5.2.1 The Parallel Force Balance on the Impurity Ions

Parallel transport and heating of the impurity ion (via thermal coupling to the background ion temperature T_{iB}) is assumed to be classical.

Thus the force on the impurity ion is given by:

$$m \frac{dv}{dt} = F_{\text{total}} = -\frac{1}{n} \frac{dp}{ds} + m \frac{(v_B - v)}{\tau_s} + ZeE + \alpha_e \frac{dT_e}{ds} + \beta_i \frac{dT_{iB}}{ds} + \dots \quad (5.1)$$

where the lack of a subscript indicates the impurity; the first term on the right is the impurity pressure gradient force per particle; the second term is due to friction with the background plasma flow at specified velocity $v_B(s)$ and Spitzer stopping time τ_s ; the third term is the electric force, specified, $E(s)$; the fourth and fifth terms are the electron and ion temperature-gradient forces, with $T_e(s)$ and $T_{iB}(s)$ specified; other forces, such as viscosity, are not considered here; s is measured along \vec{B} ; $s = 0$ at target, $s = L$ at the half-way point to the other target.

Consider first the case when (a) the only forces are the impurity pressure gradient force and the force of friction in a stagnant background plasma, i.e., $v_D = 0 = E = dT_e/ds = dT_{iB}/ds$, and (b) collisionality is strong enough that the inertia mdv/dt can be neglected, i.e., $F_{\text{total}} = 0$, and (c) $T = T_{iB}$, constant in space. One can then rearrange Eq. (5.1) to give:

$$\Gamma = nv = -D_{||} \, dn/ds \quad (5.2)$$

where $D_{||} = \tau_s kT/m = \tau_s v_{th}^2 \quad (5.3)$

It is thus seen that inclusion of the impurity pressure gradient force has the same effect on transport of particles as inclusion of parallel diffusion. This fact is used in Monte Carlo impurity transport codes, including DIVIMP where the impurity pressure gradient force is not included explicitly, but rather parallel diffusion (in space or velocity) is used.

The diffusion can be treated either as a diffusion in $s_{||}$ -space, or $v_{||}$ -space. For spatial-diffusion the s -value can be incremented at each Δt by $\pm(2D_{||} \Delta t)^{1/2}$. The next task, in that case, is to specify $D_{||}$. Here a problem arises since the basic collisional calculations for charged particles, from Spitzer, are given in terms of velocity-diffusion. One can make approximations to develop an expression for $D_{||}$ in terms of the Spitzer collision expressions (see later in this section), and this was what was

originally done in DIVIMP (thus the low-numbered “Collision Options”). This situation is fundamentally unsatisfactory, however. In addition (as Shimizu and Takizuka (1994 ITER Workshop) have pointed out) there are cases where spatial-diffusion will produce errors, relative to a correct, velocity-diffusion treatment. It is therefore recommended that the early spatial-diffusion Collision Options no longer be used (it is also recommended that the preliminary velocity-diffusion Collision Options not be used because they also involve approximations that may not be valid in all situations.) and that Collision Option 13 be used almost exclusively since it is based directly on the Spitzer collisional expressions.

When an ion transfers from one poloidal ring to another, as a result of cross-field transport, see Sec. 5.1, then the value of $s_{||}$ should not be simply carried over, but a correction should be made as follows; see fig 5.1. When the ion transfers from point 1 to point 2, the fractional separation between points, along \vec{B} , should be preserved, not the absolute $s_{||}$ -value.

Allowing for both parallel diffusion, as well as the electric field and temperature-gradient forces, one then obtains:

$$\Delta v = \langle \Delta w_{||} \rangle \Delta t + \langle (\Delta w_{||})^2 \rangle \Delta t^{1/2} r_G + \frac{Z_I e E}{m_I} \Delta t + \frac{\alpha_e}{m_I} \left(\frac{dT_e}{ds} \right) \Delta t + \frac{\beta_i}{m_I} \left(\frac{dT_{iB}}{ds} \right) \Delta t \quad (5.4)$$

where $\langle \Delta w_{||} \rangle$ and $\langle (\Delta w_{||})^2 \rangle$ are the Spitzer collision coefficients, and r_G is a random number of Gaussian distribution with $r_G^2 = 1$. Different prescriptions for α_e and β_i are available: the Temperature Gradient Coefficient Options (sec 5.2.3). Allowing for the drift velocity of the background plasma along the SOL at velocity v_B , we can write:

$$\langle \Delta w_{||} \rangle = (v_B - v) / \tau_S \quad (5.5)$$

where the value of τ_S used here is extracted with the aid of Spitzer’s Table 5.2; for simplicity we use Spitzer’s tabulated value for $x = “l_{fw}” = v / (2kT_{iB}/m_B)^{1/2} \ll 1$, although this involves some error; this gives:

$$\tau_s = \frac{m_I T_{iB} (T_{iB} / m_B)^{1/2}}{6.8 \times 10^4 (1 + m_B / m_I) n_B Z_I^2 Z_B^2 \ln(\Lambda)} \quad (5.6)$$

where in Eq. (5.6) quantities are in the convenient units: τ in [s], T in [eV], m in [AMU], n_B in [10^{18} m^{-3}]. We take $\ln(\Lambda) = 15$, fixed.

5.2.2 Parallel Diffusion and Heating of the Impurity Ions

One can also rewrite from Spitzer:

$$(\langle \Delta w_{\parallel} \rangle^2 \Delta t)^{1/2} = \left(\frac{k T_I}{m_I} \right)^{1/2} \left(\frac{2 \Delta t}{\tau_{\parallel}} \right)^{1/2} \quad (5.7)$$

where

$$\tau_{\parallel} \equiv \frac{m_I T_I (T_{iB} / m_B)^{1/2}}{6.8 \times 10^4 n_B Z_I^2 Z_B^2 \ln(\Lambda)} \quad (5.8)$$

in the same convenient units as Eq. (5.6).

The choice of the value of the calculational time step in DIVIMP, Δt , is specifiable and is usually chosen to be much smaller than the smallest value of τ_s , τ_{\parallel} for any charge state. The values of the plasma background quantities, E , v_B , dT_e/ds , dT_{iB}/ds are specified by separate models either internal to the DIVIMP code (“SOL Options”, see 3.1), or through direct coupling to 2-D edge fluid codes, such as EDGE2D/NIMBUS or B2/EIRENE, see 3.2.

The Spitzer collision times, τ_s , τ_{\parallel} , Eqs. (5.6), (5.8), are actually for 3-D motion while here we ignore the coupling between parallel and perpendicular motion. The use of these expressions for τ_s , τ_{\parallel} then encounters a small inconsistency associated with the finite value of m_B/m_I , which causes τ_s to differ from τ_{\parallel} by a factor $(1 + m_B/m_I)$ when “ T_I ” \rightarrow T_{iB} : here the value of T_I used in Eqs. (5.7) and (5.8) is calculated from:

$$\Delta T_I^f = (T_{iB} - T_I^f) \Delta t / \tau_T \quad (5.9)$$

where τ_T is the Spitzer energy transfer collision time:

$$\tau_T = \frac{m_I T_{iB} (T_{iB} / m_B)^{1/2}}{1.4 \times 10^5 n_B Z_I^2 Z_B^2 \ln(\Lambda)} \quad (5.10)$$

where the same convenient units are used as for Eq. (5.6). The superscript “f” is for “formula”, and is needed here to distinguish this from the value of T_I which can be directly extracted from the actual ion velocity distribution itself. We denote the latter by T_I^d ; “d” for “distribution”.

Ideally, of course, $T_I^f = T_I^d$. This will not happen, however, if the $(1+m_B/m_I)$ term is present in τ_s , Eq. (5.6), but absent in $\tau_{||}$, Eq. (5.8). This is seen most simply for the situation where $T_I^f = T_{iB}$: at each time step the ion velocity is incremented by $\Delta v = (kT_{iB}/m_I)^{1/2} (2\Delta t/\tau_{||})^{1/2} r_G$, giving an average value of $\langle(\Delta v)^2\rangle = (2kT_{iB}/m_I) (\Delta t/\tau_{||}) \langle r_G^2 \rangle = (2kT_{iB}/m_I) (\Delta t/\tau_{||})$; thus the power input rate, $P_{in} = \frac{1}{2} m_I \langle(\Delta v)^2\rangle/\Delta t = kT_{iB}/\tau_{||}$. For an individual ion with velocity v the energy loss rate is mv^2/τ_s and so for the velocity distribution varying as $\exp(-mv^2/2kT_I^d)$ the average power loss rate is readily shown to be $P_{out} = kT_I^d/\tau_s$. Setting $P_{in} = P_{out}$ gives $T_I^d / T_{iB} = \tau_s/\tau_{||} = (1 + m_B/m_I)^{-1} = 0.857$ for carbon in deuterium. Code runs with these values of τ_s , $\tau_{||}$ in DIVIMP, and with all forces turned off except friction and with $v_B = 0$, did indeed give a velocity distribution of C-ions with such a depressed temperature. While this discrepancy is of no practical consequence, it is potentially confusing. Rather than removing it by employing a full 3-D treatment of the ion collisions, a simple *ad hoc* 1-D approximation has been used here of re-defining $\tau_{||}$ to also have a factor $(1 + m_B/m_I)$ in the denominator. With this approximation, one then finds that $T_I^d = T_I^f$: Fig 5.2 shows the velocity distribution for C^{4+} ions which were injected as 50 eV C^{4+} into a deuterium plasma with $T_{iB} = 50$ eV, $n_e = 10^{19}$

m^{-3} constant in space; all forces off except friction with $v_B = 0$; the ions were injected very far from the target so as to give the distribution a chance to fully develop (average dwell time of ions in the plasma = 94 ms, to be compared with the Maxwellianization time, here $\approx \tau_{||} \approx 20 \mu s$). As can be seen, the ion velocity distribution follows the expected form $\exp(-mv^2/2kT_{iB})$ over about 4 orders of magnitude. When using the value of $\tau_{||}$ without the $(1 + m_B/m_I)$ factor, the velocity profile was found to obey an exponential form just as well, but the exponent corresponded to a temperature of $0.86 T_{iB}$.

It is not merely a matter of convenience to calculate T_I from T_I^f , Eq. (5.9); this also side-steps the problem that often the velocity distribution does *not* follow an exponential form to the high precision shown in Fig.5.2. Often the ions are not in a particular charge state long enough to fill out the distribution completely. Also, the background ion temperature is generally not constant in space and the impurity ions can move through changing temperature conditions before they have had a chance to fully fill out the distribution. Figure 5.3 shows the velocity distribution for C^+ to C^{4+} for injection (as C^+) into a constant plasma background of $T_e = T_{D+} = 50$ eV, $n_e = 10^{19} m^{-3}$. Injection was far from the targets so that true loss from the plasma was not a factor; ions were killed off, however, with characteristic time 1 ms. The ions were injected with an average energy of 1 eV. Figure 5.3 thus shows both the effects of heating-up, and of incomplete Maxwellianization. For this case:

State	$\tau_{ } [\mu s]$	$\tau_{iz} [\mu s]$	$T_I^f [eV]$
C^+	17	5.5	2.8
C^{2+}	33	26	23
C^{3+}	31	150	47
C^{4+}	18	>1 ms	~50

The values of T_I^d , found by making straight line approximations to the curves in Fig. 5.3, correspond approximately to T_I^f .

Fluid models assume fully Maxwellian ions and so this is a further aspect of the real situation in a plasma which is tested for when using DIVIMP, i.e., this additional aspect of partial collisionality.

As already noted, earlier applications of DIVIMP and LIM employed *spatial*, rather than *velocity* (parallel) diffusion (say $\Delta t = \tau_{\text{coll}}$, then $\Delta v = \sqrt{2} r_G v_T$ with $v_T \equiv (kT_I/m_I)^{1/2}$, giving $\Delta s = \sqrt{2} r_G v_T \tau_{\text{coll}}$ and so the parallel (spatial) diffusion coefficient $D_{||} = \langle (\Delta s)^2 \rangle / 2\tau_{\text{coll}} = (kT_I/m_I)\tau_{\text{coll}}$; previously a similar expression $D_{||} = (4kT_I/\pi m_I) \tau_{||}$ was used in DIVIMP for spatial diffusion). For the most part, results are little influenced by which assumption is made, however, as Shimizu and Takizuka have pointed out there are cases where differences are important and therefore velocity diffusion is to be preferred, since the Spitzer derivations are for velocity diffusion. Also, with regard to the above point of testing for the effect of partially-Maxwellianized velocity distributions it is necessary to use this approach. Velocity diffusion is therefore now recommended.

Finally, we may consider the question of what is “ T_I ”, actually, in the present context where individual test particles are being followed? The value of T_I^f is not really used: this is the term which appears in Eq. (5.7) but as can be seen from Eq. (5.8), it cancels out. It’s utility is in other uses of DIVIMP, e.g. for comparison with experimental (Doppler) temperatures, where T_I^f is conveniently calculated by the code. The value of T_I^d is the more physically meaningful because it is based on a particle ensemble. However, it is somewhat less convenient to compute. The values in the DIVIMP print-out for the different charge states are T_I^f .

5.2.3 The Temperature Gradient Coefficients

The values of α_e , β_i are specified by the T_eB , T_iB Gradient Coefficient Options, as given below. The Option 0 just turns these forces off. Option 1 uses coefficients from J. Neuhauser et al, Nucl. Fusion 24 (1984) 39. Option 2 is from R. Simonini and R. Taroni, private communication, 1989, and is close

to that given by Yu. L. Igitkhanov, Contrib. Plasma Phys. 28 (1988) 477. Option 2 is a step in the direction of incorporating the effect of finite impurity densities on these coefficients; here, one has to *specify* the impurity density, however. In an approach presently (April 1995) being implemented, DIVIMP will be feedback coupled iteratively to the SOL Option, with the impurity densities of each charge state being used to calculate the α_e , β_i coefficients, based on Igitkhanov's full formulation.

T_{eB} Gradient Coefficient 0: $\alpha_e = 0$

T_{iB} Gradient Coefficient 0: $\beta_i = 0$

T_{eB} Gradient Coefficient 1: [N351]

$$\alpha_e = 0.71 Z_I^2$$

T_{iB} Gradient Coefficient 1: [N351]

$$\beta_i = -3 \frac{[1 - \mu - 5\sqrt{2} Z_I^2 (1.1\mu^{5/2} - 0.35 \mu^{3/2})]}{2.6 - 2\mu + 5.4\mu^2}$$

$$\mu = m_I/(m_I + m_B)$$

T_{eB} Gradient Coefficient 2: [N412] allows for finite impurity levels:

$$\alpha_e = 1.5[1 - 0.6934 (1.3167)^{-Z_I}]Z_I^2$$

T_{iB} Gradient Coefficient 2: [N412] allows for finite impurity levels:

$$\beta_i = H(ZO) Z_I^2 \left[ZO + \left(0.5 \left(1 + \frac{m_B}{m_I} \right) \right)^{1/2} \right]^{-1}$$

$$H(ZO) = \frac{1.56(1 + 1.41 ZO) (1 + 0.52 ZO)}{(1 + 2.65 ZO) (1 + 0.285 ZO)}$$

and ZO is a parameter to be specified. In fact, $ZO = n_Z \overline{Z_I^2} / n_i$.

5.3 Impurity Ion Perpendicular (Cross-Field) Transport

At each time step, Δt , the cross-field “distance,” s_\perp , is incremented by $\pm(2D_\perp \Delta t)^{1/2}$, with D_\perp specified. At the instant the neutral is ionized — or if it is injected as an ion — it starts off located at the nearest cell center, so far as its s_\perp location is concerned. Suppose the ion had no parallel motion. Then the Δs_\perp steps would accumulate along the straight lines joining the cell center, at which the ion started, and the next cell centers in/out. When the ion has passed the midway to the in/out cell center, it then becomes associated with the new cell, for purposes of calculating densities. The s_\perp -information is not, however, discarded.

Now, imagine that parallel motion is also occurring, so that $s_{||}$ is always changing. This is dealt with as follows, see fig 5.4. At time t_1 , the ion may be associated with cell center 1, so far as its cross-field motion is concerned, and it may be 30% of the way cross-field to cell center 2. (The ion’s location is not indicated in the most general way in this figure, as the ion will generally be located part way along \bar{B} to the set of cell centers 3 and 4, and would not (generally) be on the line joining centers 1 and 2.) At time $t_1 + \Delta t$ let us suppose the ion makes a $\Delta s_{||}$ -step which takes it beyond the halfway point, along \bar{B} , to cell center 3. It now is associated with this new cell and its cross-field location is taken to now be 30% of the distance between cell centers 3 and 4 (i.e., the absolute s_\perp -value is not conserved).

One may note that if the target is coincident with one of the orthogonal (-to- \bar{B}) lines, in an orthogonal grid (a common case), then cross-field steps Δs_\perp can never carry the ion into the target. Only $\Delta s_{||}$ -steps can.

The grid does not normally extend to the very center of the plasma (Sec 2). The innermost poloidal ring in the grid is treated as a mirror for the

impurity ions. If at some particular time step the ion attempts to move a distance Δs_{\perp} which would take it inside this innermost ring by a distance $\Delta s_{\perp}'$, then instead, the ion is moved to a location a distance $\Delta s_{\perp}'$ outside the innermost ring. In the absence of a cross-field pinch, one then expects to find, inside the separatrix, a flat distribution, cross-field, of the total impurity density (summed over all charge states), assuming that there are no sources or sinks for impurity ions inside the separatrix - which is often the case. This can be a sensitive test of whether or not the cross-field steps are being properly implemented, which may be a problem for some non-orthogonal grids. In order to monitor this, it can be useful to look at radial plots of the total impurity density that extend into the core. DIVIMP printouts also include the total number of crossfield steps in the core plasma, and the average size of the crossfield steps there.

6.0 Data Sources

6.1 Atomic Data Sources

6.1.1 NOCORONA Package (Abels-van Maanen)

References: JET-DN-T (85) 27, 28, 29, “A Package for Non-Coronal Impurity Data”. Parts I, II, III. By A.E.P.M. Abels-van Maanen (see N 73).

This package of subroutines calculates the rate coefficients for ionization, recombination and radiation of impurities as a function of n_e and T_e . The radiation is broken down by charge state and also by the mechanism of production, line radiation or bremsstrahlung, for example. One can also get outputs for the total radiated power (all charge states, all mechanisms), the energy used to ionize the impurities, provided by the electron’s “ionization energy loss”, and the total “electron energy loss”.

The radiation and electron power rates are given by the NOCORONA subroutine RDLONG. One has to specify the volume n_e , T_e , n_z for each cell as input. RDLONG then outputs:

- (a) the total radiative power loss per unit volume (cm^3) in each cell [W/cm^3], also for the cell in [W],
- (b) the electron energy loss [W/cm^3], [W],
- (c) the radiation losses by type (bremsstrahlung, etc.) [W/cm^3], [W],
- (d) the ionization energy loss [W/cm^3], [W].

One can thus sum up for all the cells to obtain what is called “Total Power” [W] in DIVIMP. Now, since DIVIMP calculations are based on an influx of one ion/sec/m toroidally, and the cells were all taken to be 1 m in toroidal extent, this quantity is also the “Radiation Potential”, $E_{\text{rad}}^{\text{ion}}$

[J/particle], i.e., the amount of energy in Joules per ion during its lifetime in the system.

This value is just for the ion stages. DIVIMP can also calculate the Total Power from neutrals (for a neutral launch case), based on one neutral created per sec per m toroidally. The power radiated by both neutral and ion stages are added and the number given as PRAD in DIVIMP is based on one neutral created/s/m toroidally (i.e., the loss of neutrals which do not get ionized in the system is allowed for in the calculation.) The total PRAD is thus the usually-defined E_{rad} [Joules] per neutral entering the plasma radiated during that particle's stay in the plasma — as neutral and/or ion.

6.1.2 ADAS (H. P. Summers)

Reference: “Atomic Data and Analysis Structure (ADAS)”, H. P. Summers, JET, Aug. 22, 1994.

ADAS is a much more ambitious atomic package than NOCORONA (the data from NOCORONA are contained as an option within ADAS). The ADAS data are continually updated by Prof. Summers so that when one specifies the version of ADAS one is using, one has to specify the year of the ADAS file (the NOCORONA data is available as “ADAS 1988”, or so).

ADAS provides the same ionization, recombination, and other rates. Further, when an ionization stage has one or more metastable levels, then ADAS can provide the atomic data which permits one to follow each of the metastables as if they were all separate stages of ionization. In addition, it includes rate data for relaxation from the metastable states to the ground state, thereby allowing each state to be independently followed and still coupled to the rest of the system. ADAS then provides the data for the various ionization, recombination, relaxation and radiative rates for each of these states. Resolving the impurity system in this way is valuable since the populations of one metastable state are not very well coupled to the population in other metastable states. Thus measured line intensities are needed for transitions in each of the metastable systems, if one is to be able

to measure the total population of the stage of ionization. This then requires that each metastable be followed as a separate population. This has not yet (May 1995) been implemented in DIVIMP.

As described under PLRP (Particular Line Radiation Power), Sec. 7.2, ADAS allows for photon production not just by electron-impact from the ground state of the stage of ionization of interest, Z_j , but also via (e-i) recombination from state Z_{j+1} ; also via ionization from state Z_{j-1} ; also via charge-exchange recombination from stage Z_{j+1} (one must then also provide neutral hydrogen input, e.g., from NIMBUS, Sec. 8).

6.1.3 Sputtering Data

6.1.3.1 Physical Sputtering

Originally, physical sputtering data was taken from the Bohdanský article in the 1984 Special Issue of Nuclear Fusion, page 61 [N33]. For each pair of impacting ion species and substrate material, three constants are required to give the normal incidence, physical sputtering yields: E_{th} [eV], ETF [eV], Q . These numbers are loaded into DIVIMP for many combinations, including self-sputtering. One then uses Bohdanský's analytic expression which then only requires specifying the impact energy, E_{impact} , see Sec. 4.3.

The actual numbers (E_{th} , ETF , Q) have been changed a number of times over the years as the Garching Lab refines their data. The latest and most extensive compilation is in "Sputtering Data", W. Eckstein et al, IPP 9/82, Feb. 1993. Actually, and somewhat confusingly, this Report contains two sets of the E_{th} , ETF , Q values. Thus, to be perfectly clear which values are actually being used in the calculation, they are included in the DIVIMP print-out. See TN828.

One should note that the analytic expressions themselves have also been changed somewhat from 1984 to 1993. (For the equations currently in use see Sec.4 where the sputtering options are discussed.)

It should be noted that the calculations of physical sputtering included in NIMBUS — and the NIMBUS source can be used by DIVIMP — differ in several respects with those in DIVIMP:

- (a) the impact energy in DIVIMP is given by:

$$E_{\text{impact}} = 2kT_{\text{e0}} + 3ZkT_{\text{iB0}}$$

while in NIMBUS it is:

$$E_{\text{impact}} = R(5/3)kT_{\text{iB0}} + (5/2)ZkT_{\text{e0}} + (1/2)mc_{\text{s0}}^2$$

where R is a random number selected from $\sqrt{x} e^{-x}$ [see Note A10 from L. Horton, April 13, 1993, and TN828, A11, TN837].

- (b) the values of the 3 coefficients (E_{th} , E_{TF} , Q) can differ [A10, TN828, A11, TN837].
- (c) the analytic expressions can differ [A10, TN828, A11, TN837].

6.1.3.2 Carbon Chemical Plus Physical Sputtering

For carbon under hydrogenic impact, one can allow for simultaneous contributions from (a) physical sputtering, (b) thermally activated chemical sputtering, and (c) athermal chemical sputtering by using the expressions provided in “Revised Formula for Chemical Sputtering of Carbon”, C. Garcia-Rosales and J. Roth, 1994. See TN1209. (See Sec.4 - sputtering options.)

6.1.4 Early, Ad Hoc, Charge-Exchange Data

Charge-exchange recombination rates (also cx as it influences radiation) should now be taken from ADAS. Earlier, cx rate coefficients were loaded in from “Low Energy Charge Capture Cross Sections”, P. T. Greenland, AERE-R-11281, April 1984. See N89.

6.1.5 Early, Ad Hoc, Photon Efficiency Data (for PLRP's)

Now such data should be taken from ADAS. Originally *ad hoc* data was loaded into DIVIMP, usually only as a function of T_e (not T_e and n_e) and usually unreferenced.

7.0 DIVIMP Output

7.1 How Impurity Densities Are Calculated

7.1.1 Steady-State

For each spatial cell, which we identify for generality here by (x, y) coordinates, we can associate a number of “bins”, one for each charge state, z_I . If at time t the impurity ion that is being currently followed, number i , is in bin (x, y, z_I) then we add a “count”, C_i , to the total count of that bin. The value of C will be unity for primary-launched impurities and of lesser weight for secondary particles (e.g. those created by self-sputtering. see Sec.4.5). In addition, DIVIMP can maintain a second set of temporally resolved “bins” where the time t of the particle will fall into one of a set of temporal ranges $[t_{j-1}, t_j]$ in which $t_0 = 0$. The temporal groupings $[t_{j-1}, t_j]$ for each set of “bins” is specified in the input to DIVIMP. Thus the “bins” can be identified by four parameters, x, y, z_I, t — which makes it possible for DIVIMP to follow time dependent situations (see below for more details). Usually, however, DIVIMP is run in a “steady-state” mode where the temporal statistics on the particles are not collected.

When one has launched all the particles, total N , for the run one would then normalize the contents of the bins :

$$f(x, y, z_I, t) = \left(\sum_{i=1}^N C_i(x, y, z_I, t) \right) / N \quad (7.1)$$

(Note that the value of N allows for varying particle weights.)

The value of f is therefore the impurity density — normalized to one particle entering the “system”, see below — at location (x, y) , in charge state z_I , in time interval t seconds after launch. One can thus calculate time-

dependent densities for such an initial, instantaneous injection of particles — as from a laser blow-off experiment. If one wants to have the highest time resolution, then one has to have a very large array for the (x, y, z_I, t) bins, since one would have a separate bin for each Δt -step. This is too demanding of memory and is usually not of interest. Rather one may wish to integrate over larger time intervals. Details are given in Sec. 7.1.2.

Normally one is interested in steady-state where it is assumed that the source has been on for a very long time — longer than any probable dwell-time of an impurity particle in the system. In this case we calculate, what we will show below to be, the steady-state (normalized) densities:

$$f_{ss}(x, y, z_I) \equiv \int_0^\infty f(x, y, z_I, t) dt \quad (7.2)$$

In reality the integral can be cut off at some time longer than the longest dwell-time of any particle since $f(x, y, z_I, t) = 0$ after such a time. For steady-state calculations it is computationally very advantageous not to keep track of $f(x, y, z_I, t)$ (and then to integrate it for f_{ss}), since this requires the memory for a 4-D bin. Rather, it is sufficient to advance the count in the 3-D bin, $f(x, y, z_I)$, by $C_i(x, y, z_I, t) \Delta t$. This is equivalent to performing the temporal integral *as one proceeds*. At the present time in DIVIMP Δt is a constant at all times and so could be moved out of the integral. However, in a situation where Δt varies, it is necessary to include the timestep since a particle that resides in a particular bin for twice as long as another particle will contribute twice as much to the integral.

In present versions of DIVIMP, the ion time step Δt is also constant in space. In LIM the option is included of allowing Δt to be small in regions of space where a lot of action occurs, e.g., near the limiter, while making Δt larger where less is going on, e.g., inboard of the LCFS. If such variable Δt 's are introduced into DIVIMP then that will have to be allowed for in advancing the $C_i \Delta t$ count, i.e. one uses the local value of Δt .

In DIVIMP, the “system” is a 1 meter (toroidal) section of the torus (equivalent cylinder, actually). Thus, the normalization for the density is

based on “one ion per second entering the torus per meter toroidally”. That this is the case can be seen from the following reasoning: suppose $\Delta t = 10^{-6}$ sec; then if $\phi_{in} = 1$ ion/sec (always understood to be per m toroidally, so this point will be not repeated hereafter), then the total count C^{total} — integrated over all (x, y) and summed over all z_I — will advance by $C_i \Delta t = \Delta t = 10^{-6}$ at each time step (assuming primary-launched ions where the particle weight is unity). Suppose the dwell or confinement time is τ_p sec (and, for simplicity, that all ions deposit out after *exactly* τ_p seconds in the plasma). One imagines, however, the f_{in} continuing indefinitely, i.e., a steady-state. One then expects a steady-state total content, N^{total} given by

$$N_{total} = \tau_p \phi_{in} \quad (7.3)$$

which is seen, in fact, to be the case. Thus, f_{ss} , as defined, does give the steady-state result for a source which has been on at a constant rate for a very long time.

Thus when one wishes to calculate an absolute impurity density, it is necessary to know the absolute production rate of impurity ions/sec/m toroidally. For the case of a sputtering source this can be calculated using DIVIMP output:

- (a) “Total Primary Integrated Flux”, ϕ_B^+ , i.e., the flux of background plasma ions integrated over each target, printed separately (one adds the two to get ϕ_B^+ (“primary” here does not mean the sputtered particle, but the background ion flux.))
- (b) “Effective Yield”, Y_{eff} , which includes all the sputtering sources.
- (c) The ratio $R = (\text{“Total Number of Ions Created”})/(\text{“Total Number of Neutrals Launched”})$. One wants to allow for neutral impurity production which does not create an ion due, for example, to direct deposition of the sputtered neutral on a wall.

Thus, the normalized densities are multiplied by $\phi_B^+ Y_{\text{eff}} R$ in order to get the absolute densities. In the DIVIMP output this latter quantity is printed as “Absolute Factor for Power, Z_{eff} ”.

7.1.2 Density for the Time Dependent Case

Ref: N128

As mentioned, it is not practical to calculate or plot impurity densities for each time step Δt . For each charge state there is an “Average Dwell Time”, $\text{ADT}(z_I)$, equal to the lesser of the average time to ionize and the average time to deposit out. Generally one can only guess/estimate these numbers. Alternately one can run a steady-state DIVIMP case first to find the $\text{ADT}(z_I)$, then run the time-dependent case.

When running the time-dependent case one has to provide as input:

- (a) the $\text{ADT}(z_I)$,
- (b) “Dwell Time Factors”, e.g., 0.05, 0.5, 2, 20, say.

Then, for this example the code only has 4 “time sub-bins” for each (x, y, z_I) “bin”, namely for:

$$0.0 < t < 0.05 \text{ ADT}(z_I) ,$$

$$0.05 \text{ ADT}(z_I) < t < 0.5 \text{ ADT}(z_I), \quad \text{etc.}$$

The memory consumption is thus more manageable and the plotting of results more useful.

7.2 Particular Line Radiation Power, PLRP

Perhaps the most important output from DIVIMP is the calculation of the number of photons emitted per sec per m^3 at a given location in the

plasma for a particular spectroscopic line of some charge state of some impurity species. This is the Particular Line Radiation Power, PLRP. (actually in photons, however, rather than joules). The 2-D PLRP can be calculated by one of several methods:

1. (N81, N84, TN60) The first method is based on the DIVIMP-calculated 2-D distribution of the ionization rate of the impurity to the next ionization stage, $I_{iz}(x, y, z_I)$. In a highly-ionizing environment, where recombination can be neglected — often, but not always the case in the tokamak edge — one can take the simple approach that the ion or neutral has a certain probability of giving off a photon, characteristic of that ionization stage, before it reaches the next ionization stage. This probability is specified by a quantity termed the “photon efficiency” η , which is actually the number of ionizations per photon, i.e., the inverse of what we are after. Values of η are calculated by atomic physics codes, such as those in ADAS, Sec. 6.1.2, and η is generally a strong function of T_e , and a weak function of n_e . Typically the latter dependence is ignored in DIVIMP. Thus:

$$\text{PLRP}(x, y, z_I) = I_{iz}(x, y, z_I) / \eta \quad (7.4)$$

In earlier years, values of η were accumulated from various sources, and tabulated in the code, generally without reference. The reliability of these data are therefore uncertain. Latterly they are calculated using ADAS. However, the statistics when the PLRP calculation is based on the DIVIMP ionization rates can be very poor since an ion, in regimes where recombination is weak, will typically only enter a particular ionization state once. Therefore accumulating ionization-based statistics can result in a poor distribution in the radiation calculation. Better statistics can be obtained by utilizing the densities calculated by DIVIMP in combination with the ionization times to estimate the ionization rates,

$$I_{iz}(x, y, z_I) \approx \frac{\eta(x, y, z_I)}{\tau_{iz}(x, y, z_I)} \quad (7.5)$$

This gives a much smoother estimate of the radiation distribution.

2. The second method directly uses the ADAS code outputs. The ADAS code allows for four separate processes that can result in release of a photon by a particular stage of ionization:
 - (a) excitation from the ground state of that stage due to electron impact. This is the basic process. In fact, this is the only process that is included in the “photon efficiency” concept described above. Note that each particular stage of ionization may consist, in effect, of one or more metastable states (the ground state is, for convenience, just referred to as another metastable state in ADAS); these different metastable states are so weakly coupled that one really should treat them each as separate populations; such an approach is to be implemented. The ADAS data itself is available in two forms. The first contains data integrated over all the possible ground states of the particular ionization state. Metastable ground states, despite their importance in spectroscopic measurements are not resolved. This is typically the database which DIVIMP uses in its calculations since it does not differentiate between ground states and metastable ground states on an ionization stage. However, the ADAS data is also available in a resolved form for each ground and metastable state. When DIVIMP is modified to follow the metastable states - the ionization and rate data to do this will be available from ADAS and the data to calculate the radiative contributions for each state will also be available.
 - (b) (ordinary) electron-ion recombination from the next ionization state. This can involve recombination into an excited state, thus giving rise to a photon.
 - (c) ionization from the stage of ionization below the one of interest (into an excited state with an attendant release of a photon).

- (d) charge-exchange recombination. This requires that 2-D neutral hydrogen spatial distributions be input (e.g., from NIMBUS calculations)

One can optionally turn off each of these processes. The calculation draws the appropriate impurity densities from the DIVIMP output, and the related coefficients from ADAS, the latter depending on the local value of T_e and n_e (and for charge-exchange recombination, the T_i , T_{H0} , n_{H0} from NIMBUS). Typically the charge-exchange recombination is not used. At present process (c), ionization is also not used, as it is generally the least important process of the four.

The ADAS calculation assumes that all of the excited states “above” each metastable ground state can equilibrate very rapidly to any changes in the density of the metastable state. ADAS includes many excited states for each metastable/ground state. Thus, the problem separates into two parts:

- (a) DIVIMP follows the evolution in space and/or time of the metastable/ground states (at present, just one state for each stage of ionization).
- (b) ADAS calculates the distribution of excited states, in equilibrium with the metastable/ground state — which is only dependent on the local value of T_e , n_e , etc. Thus, the ADAS calculations can all be done in advance for various values of T_e , n_e for which the rates are tabulated, then extended via interpolation.

7.3 Spectroscopic Line-of-Sight, LOS, Integrals

7.3.1 Some Basics of Photometry

Reference: “Photometry” by J. W. T. Walsh, 1958, p. 141.

Definitions:

1. I [Watts/steradian] \equiv “Luminous Intensity” of source.
2. I_V [W/sr/m³] \equiv “Specific Luminous Intensity” of an extended, volume source.
3. B [W/sr/m²] \equiv “Luminance” of source.
4. E [W/m²] \equiv “Illumination” of receiver.

The important relation is between E and B :

$$dE = B \cos \phi_{\text{rec}} d\omega_{\text{rec}} \text{ [W/m}^2 \text{ in cone } d\omega_{\text{rec}}] \quad (7.6)$$

where: $d\omega_{\text{rec}}$ = solid angle of emitting surface as seen by the receiver,
 ϕ_{rec} = angle between normal to receiver surface and line to source.

See Fig. 7.1. One finds the total E by integrating over the entire emitter. It may seem that there is a problem in this relation between E and B : after all, the “steradian” in B relates to the solid angle subtended by the receiver, while the “steradian” for dE is $d\omega_{\text{rec}}$, the solid angle of the element of emitter. One can show, however, that these solid angles are the same, when the area of the element of emitter, and the area of the receiver are very small, compared with the separation distance z ; see Fig. 7.2 where two extreme points on the element of emitter are considered, and the solid angles subtended by the receiver are shown (both the element of emitter and the receiver are to be thought of as having 1 m² of area, although only a 2-D picture is shown here). Clearly the two angles are virtually the same as in Fig. 7.1.

7.3.2 Line-of-Sight Integrals of PLRP’s and Total Radiation (Bolometer)

Now let us consider the case of an extended volume source with a specified Specific Luminous Intensity I_V , Fig. 7.3, where we wish to calculate the Line-of-Sight, LOS, integral of the Illumination of the receiver. Consider

an increment dz along the LOS and construct a disc of radius r , thickness dz , with axis of the disc aligned with the LOS. Thus, the total Luminous Intensity of the source [W/sr] is $I_V \pi r^2 dz$ giving $I_V \pi r^2 dz 4\pi$ [W] into all space. An isotropic source is assumed here. The photons come out of the front and back surfaces of the disc, so out of the front (facing the receiver) comes $I_V \pi r^2 dz 2\pi$ [W]. Thus, for this disc:

$$B = I_V dz \quad [W/sr/m^2] \quad (7.7)$$

on the front side, shining forward. Note that here it is assumed that the receiver is aligned with the LOS, thus $\phi_{rec} = 0$. Also $d\omega_{rec} = \pi r^2/d^2$, thus:

$$dE = I_V dz \pi r^2/d^2 \quad (7.8)$$

Now, if we are interested in the “Angular-Specific Illumination” of the receiver, E_s [W/m²/sr] then this is just:

$$dE_s = I_V dz \quad (7.9)$$

Thus, for the entire integral along the LOS:

$$E_s = \int I_V dz \quad (7.10)$$

Assuming the source is isotropic, then

$$I_V = PLRP/4\pi \quad (7.11)$$

where PLRP can be in either [W/m³] or [photons/m³/s], thus

$$E_s = \frac{1}{4\pi} \int_{LOS} PLRP(z) dz \quad [W/m^2/sr] \quad \text{or} \quad [photons/m^2/sr/s] \quad (7.12)$$

If one had a 2-D, rather than 3-D system, with both emitter and receiver extending to $\pm\infty$ axially, then the $\frac{1}{4\pi} \rightarrow 2\pi$ and $sr \rightarrow \text{radian}$.

For modeling some measurements on JET (TN488, TN483, TN418, TN368), the latter has been assumed. Also, for some measurements, the acceptance angle of the viewing instrument, $\Delta\theta_{\text{acc}}$, enters because the measurements, as actually output, are for the entire signal received over $\Delta\theta_{\text{acc}}$. In that case, in order to compare code and experiment, the DIVIMP output is of:

$$\frac{\Delta\theta_{\text{acc}}}{2\pi} \int_{\text{LOS}} \text{PLRP}(z) dz \quad [\text{photons/m}^2/\text{s}] \quad (7.13)$$

where $\Delta\theta_{\text{acc}}$ must be specified.

For other measuring devices the actual output corresponds to:

$$\frac{1}{2\pi} \int_{\text{LOS}} \text{PLRP}(z) dz \quad [\text{photons/m}^2/\text{s/radians}] \quad (7.14)$$

while for others it is:

$$\frac{1}{4\pi} \int_{\text{LOS}} \text{PLRP}(z) dz \quad [\text{photons/m}^2/\text{s/sr}] \quad (7.15)$$

For JET Bolometry, (TN446, TN448, TN451, TN488), where the total power (all wavelengths) is involved the relevant comparison is with:

$$\int_{\text{LOS}} \varepsilon(z) dz \quad [\text{W/m}^2] \quad (7.16)$$

where ε is in $[\text{W/m}^3]$.

7.3.3 Line-of-Sight, PLRP-Weighted Impurity Ion Temperatures (TN75)

When Doppler-temperatures are measured they are likely to involve a LOS integral. In DIVIMP the temperature is weighted by the PLRP, in order to compare with experiment:

$$\bar{T} = \frac{\int_{\text{LOS}} T(z) \text{PLRP}(z) dz}{\int_{\text{LOS}} \text{PLRP}(z) dz} \quad (7.17)$$

7.4 Sputtering Yield and Related Information

Detailed information is printed out on the flux of background ions to the target. Each segment of the target (specified in Sec. 2) is identified by its (R, Z) component; the Yield Multiplication Factor (YMF), Sec.4, for that segment; the background ion particle flux density, “FLUXDENS” = $n_0 |M_0| c_{s0} (B_\theta/B)_0$ [ions/m²/s]; the energy of impact, “ENERGY” = $3zBkT_0 + 2kT_i B_0$; the yield as calculated, see Sec. 4, and including the YMF; the pitch angle information, “Bt/Bth” $\equiv B/B_\theta$; the length of the segment; the non-orthogonal correction, “NONORTH” (if the target is not orthogonal to the \bar{B} field in the poloidal plane, then the background ion flux density on the target has to be reduced by the further factor “NONORTH”, see Sec. 2.4).

Then, for each target, the background ion flux is integrated to give “TOTAL PRIMARY INTEGRATED FLUX” in ions per sec per m toroidally. Also given is the integral, for each target, of the background flux and sputtering yield, thus giving the total “primary” production of impurities from that target, i.e., for impact by the background ions. Lastly, the total heat flux to that target, associated with the background plasma, is given in units of Watts per m toroidally.

Let the total (both targets) primary (background ion) flux to the targets be ϕ_B^+ . Let the total neutral impurity production due to this background ion impact be $\phi_{Z,p}^0$. Then one has the “primary yield”:

$$Y_p = \frac{\phi_{z,p}^0}{\phi_B^+} \quad (7.18)$$

If self-sputtering is allowed, then the “Self-Sputtering Enhancement Factor” is printed out, SSEF. Then the Effective Yield:

$$Y_{\text{eff}} = Y_p(1 + \text{SEEF}) \quad (7.19)$$

This allows for the complete self-sputtering “cascade”. Since information is also printed out on the number of impurity ions returning to the target and the number of new impurity neutrals they produce by sputtering, one can calculate the (average) self-sputtering yield, \bar{Y}_{ss} , and thus confirm that:

$$Y_{\text{eff}} \approx Y_p/(1 - \bar{Y}_{ss}) \quad (7.20)$$

7.5 Erosion and Deposition

The following can be plotted for erosion and deposition across the targets:

- (a) Total Removal: this is due to both “primary” sputtering by the background ions and the self-sputtering “cascade”. Since all the quantities being plotted are based on *one atom of target material removed per meter toroidally per sec*, the total area under Total Removal should be unity. When one wants the *absolute* removal rate, one multiplies by the absolute *neutral* production rate, $\phi_B^+ Y_{\text{eff}}$, see Sec. 7.1.1.
- (b) Primary Removal: is just the removal due to “primary” sputtering, and so the area under this curve is less than under Total Removal, if there is any self-sputtering.

- (c) Total Deposition: if all the sputtered neutrals are ionized (i.e., if none deposit on the walls) and if all these ions return to the targets (i.e., are not lost to the “periphery”, Sec. 2.3.3), then the total area under this curve will be -1 (minus, since deposition rather than removal). If there are losses, however, then the area under Total Deposition will be between -1 and 0.

8.0 Coupling of DIVIMP to Monte Carlo Hydrogen Codes Such As NIMBUS and EIRENE

8.1 Introduction

Monte Carlo neutral hydrogen codes like NIMBUS and EIRENE function in the same way as DIVIMP, in that they require as input a full 2-D prescription of n_e , T_e , T_iB . (Thus we sometimes refer to them as “PIN” codes — “Plasma Input Neutral”.) The background ions strike the targets and are neutralized, thus giving the source for these codes. Some of the neutrals are backscattered atoms, others are thermal molecules. The neutrals are then followed including: ionization, charge-exchange, molecular dissociation, wall (or target) reflections. The output includes:

- (a) the 2-D distributions of neutral atoms, n_H , neutral molecules, n_{H_2} , and their temperatures;
- (b) ionization rates from atoms and molecules (separately and added), S_{iz}^H [ions/m³/s];
- (c) the 2-D cooling rate for the electrons due to ionization, excitation, dissociation;
- (d) the 2-D cooling/heating rate for the ions due to charge-exchange and elastic collisions with neutrals;
- (e) 2-D momentum loss/gain rate for the ions as a result of charge-exchange and elastic collisions with neutrals;
- (f) 2-D H_α photon production rates;
- (g) spatial distribution of H and H₂ fluxes to walls and targets and information on associated heat fluxes
- (h) spatially-resolved sputtering rates from walls and targets as a result of the neutral hydrogen bombardment (These “hydrogenic” codes will also often follow the sputtered impurity neutral until it is ionized; this can be an alternative to the neutral-following part of DIVIMP, when the codes are coupled.

8.2 Use of the Hydrogen Ionization Information by DIVIMP

Probably the most important use DIVIMP has for the output from these codes is the 2-D spatial distribution of the hydrogenic ionization, which is needed in the SOL Options, Sec.3. The simplest approach is to use an analytic prescription for the distribution of hydrogen ionization, Sec.3.1, guessing what a reasonable ionization length would be; thus using a SOL Option, generate some 2-D “plasma background” (n_e , T_e , T_{iB}); then call NIMBUS in the PIN-mode and see how the hydrogen ionization would actually look for such a background. If the originally estimated ionization length is approximately OK, then one could just go on with it.

At the next level of sophistication, the SOL Option directly uses the numerical ionization rate S_{iz}^{NIMBUS} , and can do so in an iterative, feed-back mode, where the plasma background evolves to a new steady-state (from the original guess).

It is important to have as realistic as possible a calculation of the 2-D S_{iz} , since this directly controls the plasma background velocity v_B , hence the frictional force on the impurity ions — typically the most important force. The 2-D v_B distribution also controls the parallel heat convection, thus the parallel temperature gradients (thus the parallel temperature gradient forces on the impurities). In addition, the 2-D S_{iz} -distribution controls the flow reversal pattern, which can have a major effect on the impurities. It would thus seem to be particularly worthwhile to operate the SOL Options iteratively with NIMBUS/EIRENE to get the most realistic spatial distribution of S_{iz} as possible.

Since the grids and target definitions are not precisely identical between NIMBUS and DIVIMP, there can be some corrections needed to get the best consistency; see Sec. 2.

8.3 Use of the Momentum and Energy Transfer Information by DIVIMP

Work is in progress to implement momentum transfer options “Momentum Source Opt”, Sec. 3.1.8, and energy transfer features for the electrons, “P_{Helpi}”, and the ions, “P_{CX}”, Sec.3.1.4, which directly use the numerical values from NIMBUS/EIRENE.

8.4 Charge-Exchange Recombination in DIVIMP

Charge-exchange recombination for impurity ions can be included in DIVIMP, through various CX Recombination Options. At present, the only supported Options involve analytic specifications of the neutral hydrogen density, n_H , and of the relative velocity of approach, v_{CX} . It is planned to implement an Option where the 2-D n_H -distribution will be imported to DIVIMP from NIMBUS for these calculations, also the information needed to calculate v_{CX} ; this will be done via ADAS.

8.5 Hydrogen Neutral Fluxes to the Walls

NIMBUS calculates:

- (a) the flux of neutral atoms and molecules to each segment of wall and target;
- (b) the average impact energy of these fluxes;
- (c) the physical sputtering rate due to these fluxes.

The latter information can be imported into DIVIMP, which can then launch “supplementary” neutrals from these wall segments, using the “Supplementary Launch Option”, see DIVIMP User Manual.

Alternatively, the entire treatment of the neutral impurities can be left to NIMBUS which will launch neutrals from both targets (due to background

ion impact) and from walls and targets (due to neutral hydrogen impact) and follow these neutrals until they are ionized. The 2-D source of singly-charged impurity ions and their initial velocities are then passed to DIVIMP.

8.6 H_α Spatial Distributions

The neutral hydrogen codes also calculate the absolute intensity of the 2-D spatial distribution of H_α light. This information, while having nothing directly to do with DIVIMP, is extremely valuable to take into consideration, along with the calculated DIVIMP distributions, when confronting the experimental data. This constitutes an additional reason for normally running NIMBUS/EIRENE with DIVIMP.

8.7 Compatibility Problems

Since DIVIMP and NIMBUS differ somewhat regarding the precise definition of the target location, the total source strength (which equals the total background ion flux to the targets) is somewhat different in the two codes. Thus, when the NIMBUS ionization rate S_{iz}^{NIMBUS} is transferred to DIVIMP a re-normalization is required in order to ensure that the total (2-D) spatial integral of S_{iz} equals the total target ion flux as calculated by DIVIMP.

A further option, when transferring S_{iz}^{NIMBUS} to DIVIMP, is to artificially prevent any flow reversal by re-normalizing the total 1-D integral of S_{iz} for each flux tube, to make it equal the target ion outflow for that flux tube, i.e., one is only using the *shape* of the spatial distribution of S_{iz}^{NIMBUS} , but not the *absolute* level. Unless this localized re-normalization is made, one will have an “ionization excess” or “ionization deficit” on each flux tube, and this will require that the reversed flows be handled in a DIVIMP SOL Option. Such Options are under development, but are not yet implemented.

Figure Captions:

Fig 2.1 Plot of the entire grid for shot geometry G50501 showing the set of polygons that define the plasma region for the DIVIMP run in this case.

Fig 2.2 Close-up plot of the G50501 grid as shown in Fig 2.1. As can be seen the “orthogonality” of the cells can vary substantially. Especially near the targets and the X-point.

Fig 2.3 Close-up of grid G50501 at the outer target in the SOL on rings 8, 9 and 10. Ring 8 is the “separatrix” ring for this grid. The area estimated by the code for cell (9,5) is marked by the “+” signs around cell (9,5).

Table 2.1 This table contains a listing of polygon information for the polygons of JET grid G50501 plotted in figure 2.3. The content of each entry is itemized in the example at the top of the table. The information has been reformatted from the raw grid format to make interpreting the contents easier and to bring out the similarities between the JET grid data and Sonnet Grid data (ASDEX Upgrade) shown in table 2.2. Also included is the cell area as calculated using the methods outlined in sec 2.3.4.

Table 2.2 Sample listing of a selection of cells for Sonnet grid Upgrade.Elements.6. The information content is similar to JET grids but lacks the ρ and θ data that allow one to easily quantify cross-field transport. This table has been reformatted from the raw ASDEX grid format.

Fig 3.1 Isothermal case. $T(s) = T_0$, constant, while $A(s)$ increases due to decreasing particle flux density $\Gamma(s)$. Therefore no risk of an imaginary root in the $v_B(s)$ solution if $v_B(0) = c_s(0)$ is assumed.

Fig 3.2 Case of $T(s)$ increasing. For $A_1(s)$, $M_0 = -1$. For $A_2(s)$, $M_0 = M_0^*$. For $A_3(s)$, $|M_0| > |M_0^*|$. For curve $A_2(s)$, $A_2(s^*) = T(s^*)/T_0$ at just one point, permitting a smooth supersonic transition at s^* .

Fig 3.3 Only for $|M_0| = |M_0^*|$ is a smooth transition possible, permitting $|M_0| > 1$, while $M \rightarrow 0$ for large s .

Fig 5.1 At time t_1 , the ion is at location A for example. At time $t_1 + \Delta t$ a $\Delta s_{||}$ -step takes the ion more than halfway along \vec{B} to the next cell, 3. As a result the ion is now assigned the location B, so far as its cross-field location is concerned.

Fig 5.2 The DIVIMP calculated velocity distribution for C^{4+} ions in a D^+/e plasma of $T_D = T_e = 50\text{eV}$, $n_e = 10^{19}\text{m}^{-3}$ for a long dwell time, $\approx 100\text{ms}$; Maxwellianization time $\approx 20\text{ }\mu\text{s}$. The horizontal scale is in units of (kT_D/m_0) , thus if the carbon ions were fully thermalized to the D^+ , their distribution would vary as $\exp(-m_0 v^2/2kT_D)$, shown as dashed lines, which is seen to be the case over 4-5 orders of magnitude.

Fig 5.3 The same as Fig 5.3 but for $1\text{eV } C^+$ ions injected into a plasma of $T_e = T_D = 50\text{ eV}$, $n_e = 10^{19}\text{ m}^{-3}$ and allowed to thermalize and ionize. The finite thermalization of the lower charge states is evident. It is also clear that the lower charge states are less fully Maxwellianized - particularly the high energy tails.

Fig 5.4 When, as a result of cross-field motion, an ion moves from one ring to another, the fractional distance between cell centres is preserved.

Fig 7.1 $B [\text{W/sr/m}^2] \equiv \text{luminance of source}$. $E [\text{W/m}^2] \equiv \text{illumination of receiver}$.

Fig 7.2 For unit area emitters and receivers, the solid angles subtended in either direction (compare Fig 7.1), and for all points (compare cases A and B here) are the same, provided that the size of the emitter or receivers are $\ll z$.

Fig 7.3 Volume source has specific Luminous Intensity, I_v [W/sr/m³].
$$E = \int_{\text{LOS}} I_v dz$$

