PPPL-2842
UC-420

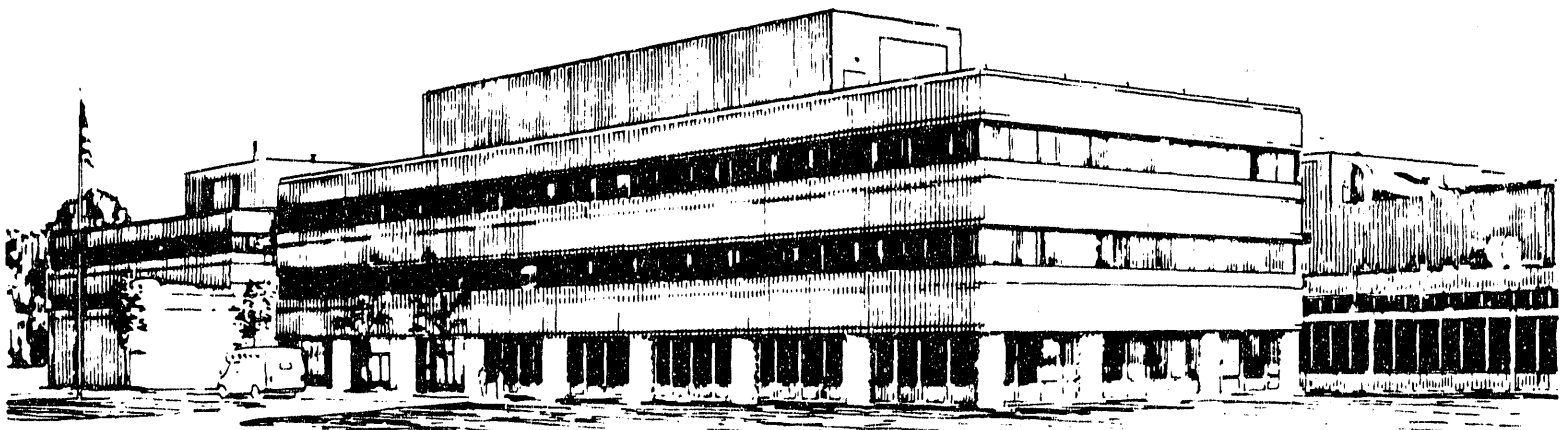# SCRAPE-OFF LAYER MODELING USING COUPLED PLASMA AND NEUTRAL TRANSPORT CODES

BY

D.P. STOTLER, D.P. COSTER, B.J. BRAAMS, ET AL.

May, 1992

PRINCETON
PLASMA PHYSICS
LABORATORY

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial produce, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Scrape-off Layer Modeling Using Coupled Plasma and Neutral Transport Codes

D. P. Stotler, D. P. Coster, B. J. Braams* A. B. Ehrhardt,
C. F. F. Karney, and M. Petravic
Plasma Physics Laboratory, Princeton University
Princeton, NJ 08543

An effort is made to refine the neutral transport model used in the B2 edge plasma code by coupling it to the DEGAS Monte Carlo code. Results are discussed for a simulation of a high recycling divertor. It appears that on the order of 100 iterations between the two codes are required to achieve a converged solution. However, the amount of computer time used in the DEGAS simulations is large, making complete runs impractical for design purposes. On the other hand, the differences in the resulting plasma parameters when compared to the B2 analytic neutrals model indicate that it would be worthwhile to explore techniques for speeding up the coupled system of codes.

*Courant Institute of Mathematical Sciences, New York University.

1

1. Introduction

The B2 code [1] is a 2-dimensional multi-fluid plasma transport code. Equations for continuity, momentum balance, ion energy balance, and electron energy balance are solved. Normally, B2 uses an analytic description of the neutral particle behavior in performing a self-consistent simulation of a scrape-off layer plasma. However, the approximations made in it are inadequate for use in detailed design work, especially for high recycling divertors. In particular, the B2 model takes into account only electron impact ionization; charge exchange and molecular reactions are ignored. For this reason, we have coupled B2 to the more complete DEGAS Monte Carlo neutral transport code [2]. DEGAS considers collision processes such as ionization, charge exchange, and dissociation. Several models for wall reflections are included. It can also handle general 3-dimensional geometries, although we assume here toroidal symmetry as in B2. Note that B2 has been coupled to the EIRENE Monte Carlo neutral code [3,] and that DEGAS has been linked with the PLANET edge plasma code [5]. In fact, the procedures discussed here should generally be applicable to codes other than B2 and DEGAS.

We have previously modeled representative TFTR supershot and ohmic discharges with the coupled codes [6]; only a simple linking scheme was utilized. We discuss here application of the coupled codes to a divertor typical of proposed burning plasma experiments [7,8]. A more involved coupling scheme is required in this case. Even after 31 iterations, some secular variation in plasma parameters persists. At this point, the peak electron temperature and density near the plate have already dropped by > 40% from their initial B2-only values, and the plasma profiles along the plate have changed qualitatively. The amount of computer time required for the DEGAS calculations prevents the iterations from being carried further; a complete run of the coupled codes is too long to be practical. However, because of the significant differences in the results relative to those obtained with the B2 analytic neutral transport model, it is worth expending some effort to speed up the coupled system.

2.   Basic coupling procedure

A minimal procedure for coupling B2 and DEGAS consists of the following steps.

1. Run B2 to convergence using its analytic neutrals model.

2. Create DEGAS namelist input using a file produced by B2.

3. Run DEGAS; at the end, have it generate a file containing particle and energy source rates.

4. Have B2 read this file and restart with the plasma obtained at the end of the previous run;

5. At each time step during the B2 run, renormalize input source rates by the total current to the plate.

6. Repeat steps (2) through (5) until plasma variations are negligible.

In step (2), B2 provides DEGAS with information about the plasma grid, density, temperature, flow velocity, and the particle flux to the target plate.

We have modeled representative TFTR supershot and ohmic discharges with this simple coupling scheme [6]. For these cases, 4 - 5 iterations were required between the two codes in order to reach a converged solution. In both runs, the final peak particle flux to the limiter was $\geq 40\%$ higher than that found with the B2 analytic neutrals model alone. The magnitude of these differences indicates the need for a detailed neutral transport model such as the one provided by DEGAS if quantitative analyses of experimental data are to be carried out. Other examples are provided in Ref. [9].

3.   Simulations of a high recycling divertor

One of the principal uses of the coupled B2-DEGAS code will be to aid in the design of divertors for future devices such as ITER [10] and BPX [8] (formerly known as CIT [7]). In this section, we describe extensions to the

basic procedure which are required to simulate the high recycling regimes expected for these devices.

In a high recycling divertor, the interaction between the divertor plasma and the neutral gas is highly nonlinear, and the simple procedure outlined in section 2 fails to work. For instance, it is possible for the source rate returned by DEGAS to be so large as to immediately radiate all of the power flowing into the SOL. A slower approach to the desired self-consistent solution is required.

First, we begin the run with a recycling coefficient $\mathcal{R}$ which is well below unity, say, $\mathcal{R} = 0.9$. As iterations between the two codes progress, $\mathcal{R}$ can be raised slowly to the desired value (e.g., $\mathcal{R} \simeq 1$). For the purposes of this investigation, however, we hold it fixed at 0.9.

Secondly, we reduce gradually the contribution of the analytic B2 neutrals model to the solution and smooth out the contributions provided by subsequent DEGAS simulations. The algorithm we use for doing this can be written as

$$S_n(t) = I_{plate,n}(t) \left\{ f \left[\frac{S_{D,n}}{I_{D,n}} \right] + (1 - f) \left[\frac{S_{n-1}}{I_{plate,n-1}} \right] \right\}. \tag{1}$$

In this equation, S_n represents the 2-dimensional ion source rate in B2 at the n-th iteration between the two codes; $I_{plate,n}$ is the total current to the target plate. The normalized source rate $S_{n-1}/I_{plate,n-1}$ from the previous run is read in along with the source information provided by DEGAS $S_{D,n}$; $I_{D,n}$ represents the total current to the target plate used in the DEGAS calculation. The two contributions are combined with an arbitrary factor f to form S_n. The array $S_n/I_{plate,n}$ is then written out by B2 for use in the next run. Here, we take $f = 0.5$. The t argument of S_n and $I_{plate,n}$ indicates that the source rate is continuously renormalized to match the total current as B2 iterates. The source term appearing in the continuity equation is $\mathcal{R}S_n(t)$ (there is no net absorption in the DEGAS calculation).

To achieve optimum convergence, the differences between successive values of $S_{D,n}$ should be due only to the changes in the plasma provided by the B2 run between them. In practice, there is some amount of Monte Carlo noise inherent in $S_{D,n}$. By increasing the number of flights and by splitting flights [2], the variance in the regions of greatest interest can be reduced to

4

an acceptable level. Unfortunately, at least for the present problem, this increases substantially the computer time relative to that required for the calculations of section 2.

When modeling an up-down symmetric double-null divertor, the B2 code is typically applied to just the outer, lower quadrant of the scrape-off layer (from midplane to the target plate); empirically, the outer half receives the greater heat flow [8]. In order to use the rectangular reference mesh of DE-GAS most efficiently [2], it is a good idea to pare down the B2 grid to include only the region near the target plate.

Since B2 is usually restricted to a curvilinear, orthogonal mesh with flux surfaces as one coordinate, it is in general not possible to utilize the exact shape of divertors and limiters. DEGAS has no such limitations, so we have developed a mechanism for augmenting the grid to allow it to meet the material boundaries (the zones corresponding to those used by B2 are unaltered). In this way, the boundary conditions used by DEGAS can be chosen in a more realistic fashion. The densities and temperatures within these additional zones are assumed to fall exponentially (with specified scale lengths) from the values at the nearest edge of the B2 grid down to a predetermined minimum.

The example we consider is a 2.1 m version of CIT [7]; the plasma mesh used in DEGAS is shown in fig. 1. The B2 grid from which it is derived is an analytic approximation to a numerical equilibrium [7] with major and minor radii of $R = 2.1$ m and $a = 0.65$ m, respectively, an elongation of 2, a toroidal field on axis $B_T = 10$ T, and a plasma current $I_p = 11$ MA. Only a few zones in the private flux region have been added; the remainder of the material boundary in the divertor region is enclosed within the B2 mesh.

The primary assumptions made in B2 for this simulation are: temperatures $T_e = T_i = 500$ eV and densities $n_e = n_i = 5 \times 10^{19}$ m^{-3} along the core plasma boundary; ion mass $= 2.5$ AMU (equal mix of D and T); thermal and particle diffusivities $\chi_e = 3$ m^2/s, $\chi_i = D = \chi_e/3$ (no anomalous pinch term); and a plate recycling coefficient of $\mathcal{R} = 0.9$. Parallel transport is classical; perpendicular transport is anomalous with the aforementioned diffusivities. The electron parallel heat flux is given by [1] $q_{\parallel} = q_f q_{SH}/(q_f + q_{SH})$, where q_{SH} is the Spitzer-Härm value and $q_f = c_q n_e T_e \sqrt{T_e/m_e}$ with $c_q = 0.1$. The ion densities and fluxes are divided equally among deuterium and tritium

when they are transferred to DEGAS.

Thirty-one iterations of the coupled codes have been made for this simulation. The evolution of the peak electron temperature at the plate sheath $T_{e,max}$ and the total current to the plate I_{plate} is shown in fig. 2. Global quantities such as I_{plate} do not vary a great deal as the iterations progress. The peak temperatures and densities at the divertor plate sheath, however, fall by nearly 50%. The peak heat flux (electron plus ion) to the target increases by 15%.

The initial and final plasma profiles near the plate are disparate, as is exemplified by fig. 3. The density profiles of the initial and final run differ to an even greater extent; the location of the peak value on the plate sheath moves from well outside the separatrix to directly adjacent to the separatrix.

The reasons for the extent of these alterations are apparent when one considers the approximations made in the B2 neutral transport model. First, B2 treats only electron impact ionization, while analysis of the data produced by DEGAS indicates that dissociation and charge exchange are also important in this problem. The poloidal and radial spreading of the ion source in B2 is performed as if the neutrals had a constant velocity [1]. In DEGAS on the other hand, a recycled neutral starts out with a velocity that is determined from a detailed wall reflection model; as the neutral propagates into the plasma, its velocity can be altered by a charge exchange event. Finally, in distributing the ion source rate along a flux surface, B2 limits the number of ions deposited in the zone directly in front of the plate sheath to be no more than 50% of the total for that flux surface. After 31 iterations between the two codes, however, we find that DEGAS predicts a source rate distribution which would clearly exceed this limit. In fact, the source rate density in many of the zones adjacent to the sheath is more than an order of magnitude greater than that found further away from the plate.

4. Improvements to the coupled system

These results indicate that a careful calculation of the SOL plasma behavior requires a detailed neutral transport model such as that provided by DEGAS. However, on the order of 100 iterations [3] may be needed to achieve convergence between the plasma and neutral transport codes; for example,

fig. 2 indicates that noticeable variations in the plasma parameter values persist even after 31 iterations. Given that each of the present DEGAS simulations requires approximately an hour of computer time (on a Cray-2), a complete calculation would be too long to be of practical use.

We are consequently investigating methods of speeding up and improving the coupled B2-DEGAS system. The simplest approach would be to use the results of a coupled calculation to enhance the quality of the analytic neutrals model in B2. Namely, there are adjustable parameters in the B2 model such as the poloidal and radial velocity of neutral atoms. By comparing the ion source rate computed by B2 against a DEGAS source based on the same plasma, it would be possible to calibrate the B2 model against the more detailed DEGAS result. Doing this would not only improve the quality of B2-only runs, but also provide a better first plasma for use in future coupled B2-DEGAS runs. Work along these lines is under way.

The success of the B2-EIRENE codes [3,4] indicates that a reasonably fast coupled system can be developed. We discuss below the steps we could take to incorporate into B2-DEGAS some of the techniques developed for B2-EIRENE. These methods could be applied to other codes as well.

The plasma-neutral transport system could be enhanced either by speeding up DEGAS or by increasing the efficiency of the coupling (note that the run time required by B2 is not significant). For example, it makes sense to have the plasma code call for a recalculation of the ion source rate whenever the plasma conditions have changed substantially (i.e., begin calling DEGAS well before B2 converges) [3,4]; this would alleviate problems with high energy loss rates for $\mathcal{R} \simeq 1$.

If the neutral density profile were passed to B2 instead of the ion source rate and if B2 had access to the atomic reaction rate data, the ion source rate could be updated continuously as the plasma temperature and density evolved [3,4]. In practice, however, a more approximate procedure would have to be used since B2 cannot treat adequately certain reactions such as charge exchange.

The number of flights used in DEGAS could be reduced if correlated sampling were employed [11,12]. This is a method for determining the differential change of source rate with respect to variations in the background plasma. The simplest implementation of this procedure would involve recording the

initial random number seed of each Monte Carlo flight in the first DEGAS run and starting each flight in subsequent runs with the same seed it had in the initial run [11]. This technique would largely eliminate run-to-run variations due to Monte Carlo noise without requiring a large number of flights.

Some savings in run time could be obtained by paring down the number of profiles kept by DEGAS to the handful that are required by the plasma code [11]. The full set could be re-enabled during the final run in order to obtained detailed results for subsequent analysis.

Since a substantial fraction of the time used in the DEGAS calculations is spent generating pseudo-random numbers, it would also be worthwhile to improve the speed of the random number generator. Efforts along these lines are under way.

5. Conclusions

Detailed analyses of experimental data and predictions of future devices require greater accuracy than is provided by the analytic neutral transport model in the B2 edge plasma code. To improve the treatment of neutral transport in B2, we have linked it to the Monte Carlo neutral transport code DEGAS and presented here initial results of the coupled system for limiter and divertor geometries. Unfortunately, it appears that, in the case of high recycling divertors at least, the amount of computer time required to complete a run is too large to make this a practical technique. On the other hand, the differences in the results relative to those obtained with the B2 neutrals model are sufficiently large to make it worthwhile to search for ways to speed up the coupled plasma-neutral transport system. The most promising possibility is the use of correlated sampling. With it, the number of flights used in DEGAS could be decreased without impeding the ability of the plasma code to react to changes in the neutral density and vice-versa.

Acknowledgments

References

[1] B. J. Braams, Computational Studies in Tokamak Equilibrium and Transport, Thesis, University of Utrecht, 1986.

[2] D. Heifetz, D. Post, M. Petravic, J. Weisheit, and G. Bateman, J. Comp. Phys. 46 (1982) 309.

[3] M. F. A. Harrison, E. S. Hotston, and G. P. Maddison, Commission of the European Communities, NET Report Nr. 100, EUR-FU/80/91-100 (1991).

[4] G. P. Maddison et al., in: Proc. 18th European Conf. on Controlled Fusion and Plasma Physics, 1991, Berlin, Part III, p. 197.

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

[6] D. P. Stotler et al., in: 1990 IEEE Int. Conf. on Plasma Science, Oakland, p. 88.

[7] R. Parker et al., in: Proc. 12th Int. Conf. on Plasma Physics and Controlled Nuclear Fusion Research, 1988, Nice, Vol. 3, p. 341.

[8] R. J. Goldston et al., Princeton Plasma Physics Lab, Burning Plasma Experiment Report X-910311-PPL-22 (1992); to appear in Fusion Technol. (1992).

[9] R. Budny, M. G. Bell, D. Coster, D. K. Owens, and D. Stotler, in: these Proceedings (PSI-10).

[10] ITER Conceptual Design Activity Final Report, ITER Documentation Series No. 16 (International Atomic Energy Agency, Vienna, 1991).

[11] D. Reiter, IPP KFA Jülich, Private Communication (1991).

[12] J. Spanier and E. M. Gelbard, Monte Carlo Principles and Neutral Transport Problems (Addison-Wesley Publishing Company, Reading, Massachusetts, 1969).

Figures

Fig. 1. Geometry of 2.1 m CIT [7] used in DEGAS calculations. The divertor plate is represented by the bottom edge of the mesh; the X-point is on the left edge near the middle of the grid.

Fig. 2. Values of (a) the maximum T_e on the plate sheath and (b) the total ion current to the plate I_{plate} at the end of each B2 run for 31 iterations of the coupled B2 and DEGAS codes.

Fig. 3. Initial (solid line; B2 analytic neutrals model) and final (dashed; after 31 iterations of the coupled codes) T_e as a function of distance along the plate sheath relative to the separatrix.
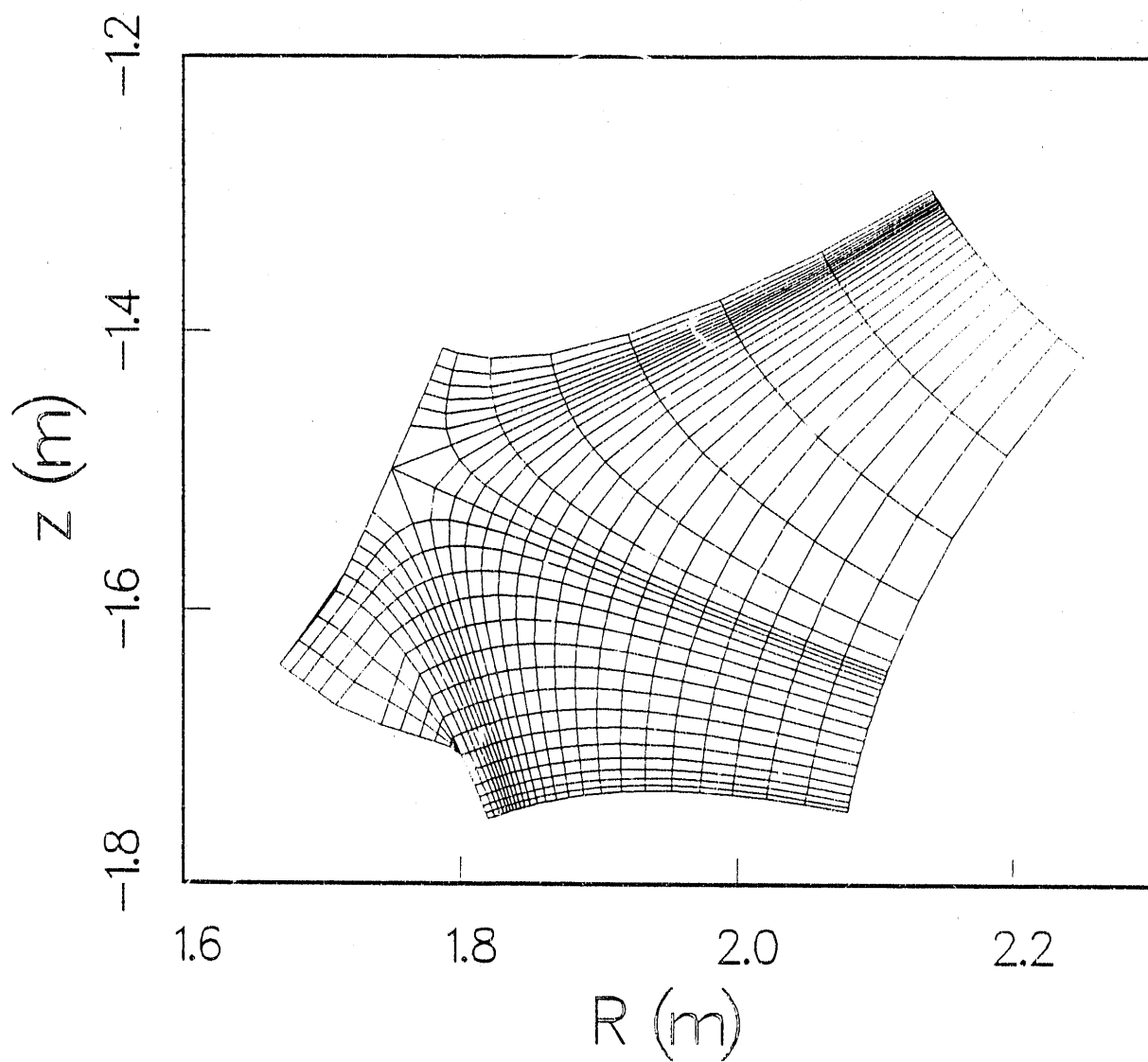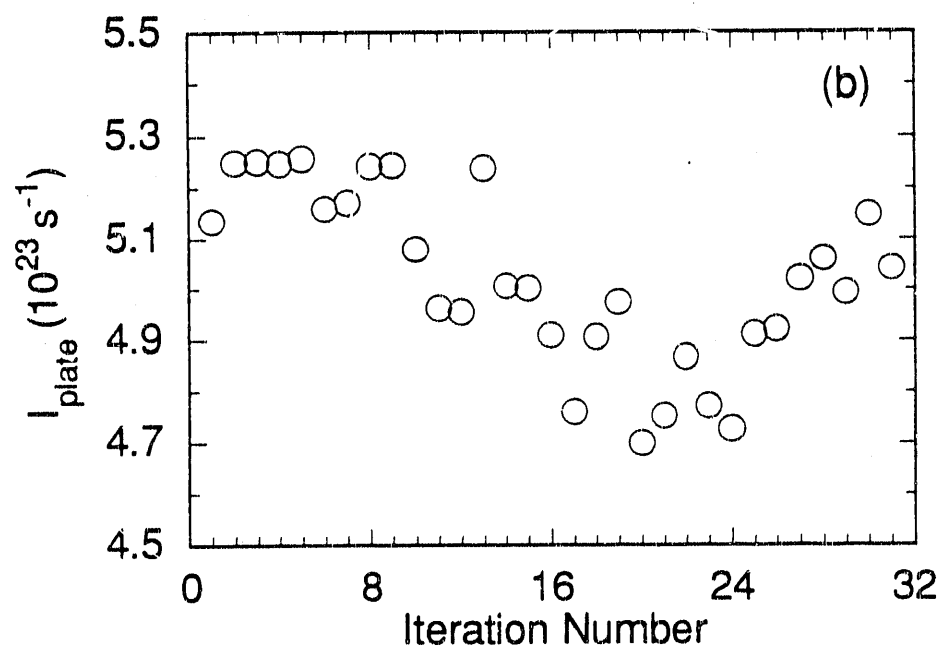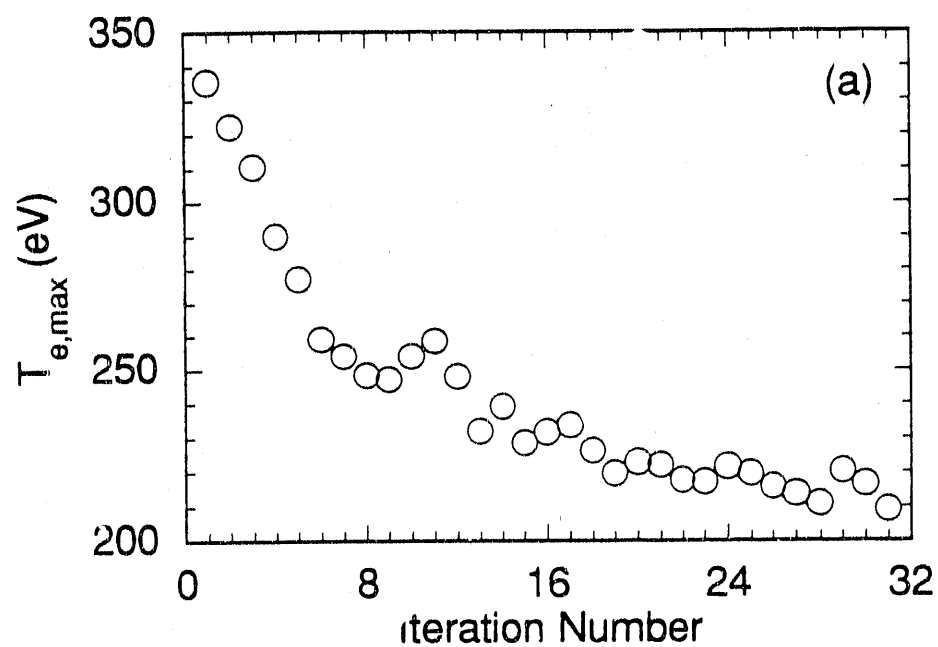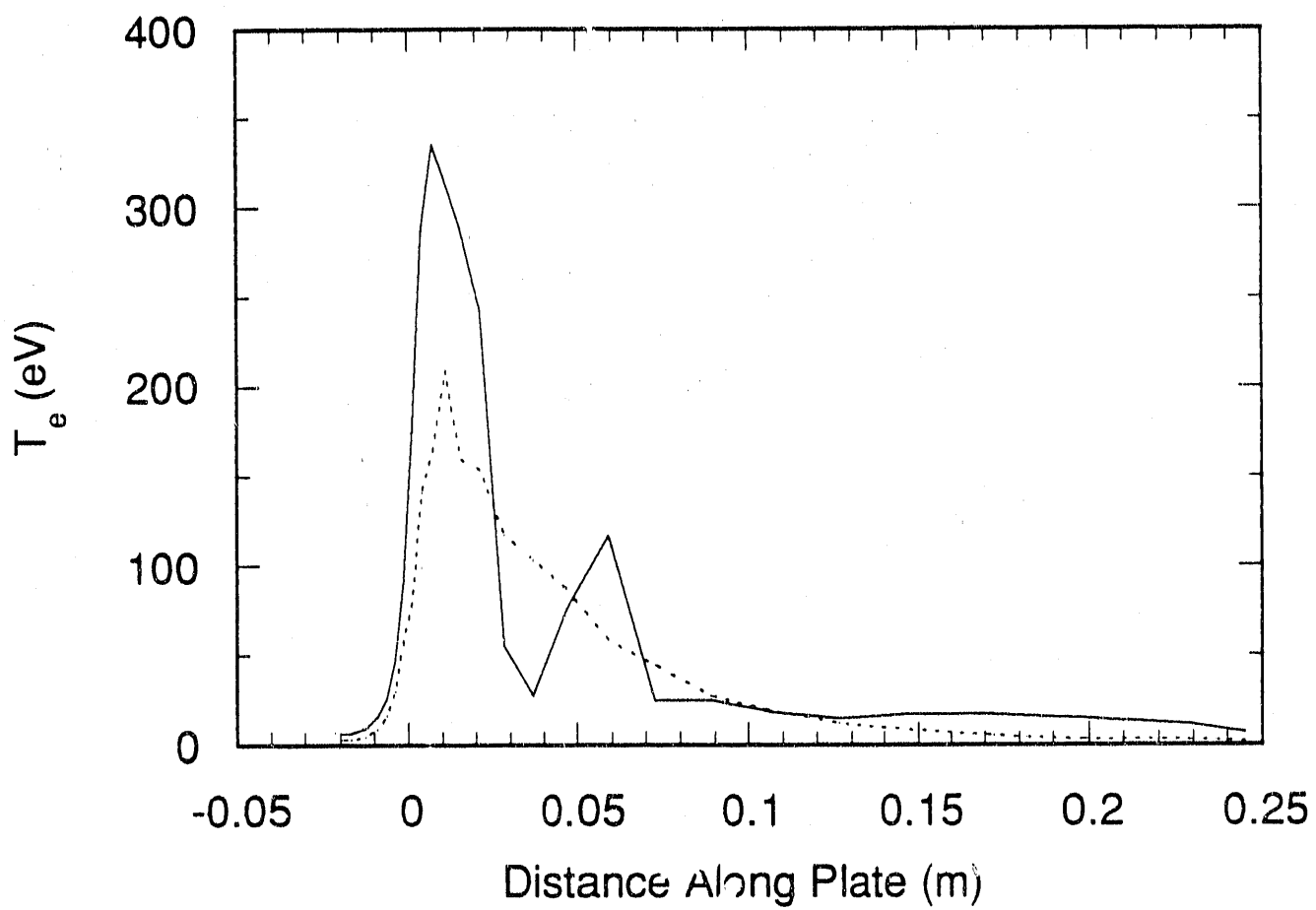
Fig. 1

Fig. 2

Fig. 3

14

Dr. F. Paoloni, Univ. of Wollongong, AUSTRALIA

Prof. M.H. Brennan, Univ. of Sydney, AUSTRALIA

Plasma Research Lab., Australian Nat. Univ., AUSTRALIA

Prof. I.R. Jones, Flinders Univ, AUSTRALIA

Prof. F. Cap, Inst. for Theoretical Physics, AUSTRIA

Prof. M. Heindler, Institut für Theoretische Physik, AUSTRIA

Prof. M. Goossens, Astronomisch Instituut, BELGIUM

Ecole Royale Militaire, Lab. de Phy. Plasmas, BELGIUM

Commission-European, DG. XII-Fusion Prog., BELGIUM

Prof. R. Bouciqué, Rijksuniversiteit Gent, BELGIUM

Dr. P.H. Sakanaka, Instituto Fisica, BRAZIL

Instituto Nacional De Pesquisas Espaciais-INPE, BRAZIL

Documents Office, Atomic Energy of Canada Ltd., CANADA

Dr. M.P. Bachynski, MPB Technologies, Inc., CANADA

Dr. H.M. Skarsgard, Univ. of Saskatchewan, CANADA

Prof. J. Teichmann, Univ. of Montreal, CANADA

Prof. S.R. Sreenivasan, Univ. of Calgary, CANADA

Prof. T.W. Johnston, INRS-Energie, CANADA

Dr. R. Bolton, Centre canadien de fusion magnétique, CANADA

Dr. C.R. James,, Univ. of Alberta. CANADA

Dr. P. Lukác, Komenského Universzita, CZECHO-SLOVAKIA

The Librarian, Culham Laboratory, ENGLAND

Library, R61, Rutherford Appleton Laboratory, ENGLAND

Mrs. S.A. Hutchinson, JET Library, ENGLAND

Dr. S.C. Sharma, Univ. of South Pacific, FIJI ISLANDS

P. Mähönen, Univ. of Helsinki, FINLAND

Prof. M.N. Bussac, Ecole Polytechnique,, FRANCE

C. Mouttet, Lab. de Physique des Milieux Ionisés, FRANCE

J. Radet, CEN/CADARACHE - Bat 506, FRANCE

Prof. E. Economou, Univ. of Crete, GREECE

Ms. C. Rinni, Univ. of Ioannina, GREECE

Dr. T. Mual, Academy Bibliographic Ser., HONG KONG

Preprint Library, Hungarian Academy of Sci., HUNGARY

Dr. B. DasGupta, Saha Inst. of Nuclear Physics, INDIA

Dr. P. Kaw, Inst. for Plasma Research, INDIA

Dr. P. Rosenau, Israel Inst. of Technology, ISRAEL

Librarian, International Center for Theo Physics, ITALY

Miss C. De Palo, Associazione EURATOM-ENEA , ITALY

Dr. G. Grosso, Istituto di Fisica del Plasma, ITALY

Prof. G. Rostangni, Istituto Gas Ionizzati Del Cnr, ITALY

Dr. H. Yamato, Toshiba Res & Devel Center, JAPAN

Prof. I. Kawakami, Hiroshima Univ., JAPAN

Prof. K. Nishikawa, Hiroshima Univ., JAPAN

Director, Japan Atomic Energy Research Inst., JAPAN

Prof. S. Itoh, Kyushu Univ., JAPAN

Research Info. Ctr., National Instit. for Fusion Science, JAPAN

Prof. S. Tanaka, Kyoto Univ., JAPAN

Library, Kyoto Univ., JAPAN

Prof. N. Inoue, Univ. of Tokyo, JAPAN

Secretary, Plasma Section, Electrotechnical Lab., JAPAN

S. Mori, Technical Advisor, JAERI, JAPAN

Dr. O. Mitarai, Kumamoto Inst. of Technology, JAPAN

J. Hyeon-Sook, Korea Atomic Energy Research Inst., KOREA

D.I. Choi, The Korea Adv. Inst. of Sci. & Tech., KOREA

Prof. B.S. Liley, Univ. of Waikato, NEW ZEALAND

Inst of Physics, Chinese Acad Sci PEOPLE'S REP. OF CHINA

Library, Inst. of Plasma Physics, PEOPLE'S REP. OF CHINA

Tsinghua Univ. Library, PEOPLE'S REPUBLIC OF CHINA

Z. Li, S.W. Inst Physics, PEOPLE'S REPUBLIC OF CHINA

Prof. J.A.C. Cabral, Instituto Superior Tecnico, PORTUGAL

Dr. O. Petrus, AL I CUZA Univ., ROMANIA

Dr. J. de Villiers, Fusion Studies, AEC, S. AFRICA

Prof. M.A. Hellberg, Univ. of Natal, S. AFRICA

Prof. D.E. Kim, Pohang Inst. of Sci. & Tech., SO. KOREA

Prof. C.I.E.M.A.T, Fusion Division Library, SPAIN

Dr. L. Stenflo, Univ. of UMEA, SWEDEN

Library, Royal Inst. of Technology, SWEDEN

Prof. H. Wilhelmson, Chalmers Univ. of Tech., SWEDEN

Centre Phys. Des Plasmas, Ecole Polytech, SWITZERLAND

Bibliotheek, Inst. Voor Plasma-Fysica, THE NETHERLANDS

Asst. Prof. Dr. S. Cakir, Middle East Tech. Univ., TURKEY

Dr. V.A. Glukhikh,Sci. Res. Inst. Electrophys.I Apparatus, USSR

Dr. D.D. Ryutov, Siberian Branch of Academy of Sci., USSR

Dr. G.A. Eliseev, I.V. Kurchatov Inst., USSR

Librarian, The Ukr.SSR Academy of Sciences, USSR

Dr. L.M. Kovrizhnykh, Inst. of General Physics, USSR

Kernforschungsanlage GmbH, Zentralbibliothek, W. GERMANY

Bibliothek, Inst. Für Plasmaforschung, W. GERMANY

Prof. K. Schindler, Ruhr-Universität Bochum, W. GERMANY

Dr. F. Wagner, (ASDEX), Max-Planck-Institut, W. GERMANY

Librarian, Max-Planck-Institut, W. GERMANY

Prof. R.K. Janev, Inst. of Physics, YUGOSLAVIA

END

DATE
FILMED

6 /12/ 92