

**MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK**  
**GARCHING BEI MÜNCHEN**

**INFLUENCE OF ELASTIC COLLISIONS  
ON NEUTRAL GAS TRANSPORT  
IN BOUNDARY PLASMAS**

P. Bachmann<sup>1</sup>, Detlev Reiter<sup>2</sup>

IPP 8/1

Mai 1992

<sup>1</sup> Max-Planck-Institut für Plasmaphysik, Bereich Berlin,  
Association EURATOM, Mohrenstr. 40-41, O-1086 Berlin

<sup>2</sup> Institut für Plasmaphysik, Forschungszentrum Jülich GmbH,  
Association EURATOM-KfA, Postfach 1913, W-5170 Jülich

*Die nachstehende Arbeit wurde im Rahmen des Vertrages zwischen dem  
Max-Planck-Institut für Plasmaphysik und der Europäischen Atomgemeinschaft über  
die Zusammenarbeit auf dem Gebiete der Plasmaphysik durchgeführt.*

# Influence of Elastic Collisions on Neutral Gas Transport in Boundary Plasmas

Peter Bachmann<sup>1</sup>, Detlev Reiter<sup>2</sup>

<sup>1</sup> Max-Planck-Institut für Plasmaphysik, Bereich Berlin,  
Association EURATOM, Mohrenstr. 40-41, O-1086 Berlin

<sup>2</sup> Institut für Plasmaphysik, Forschungszentrum Jülich GmbH,  
Association EURATOM-KFA, Postfach 1913, W-5170 Jülich

May 19, 1992

## Abstract

An analytical solution to an one-dimensional linear kinetic transport equation (slab model) is presented and applied to investigate the influence of elastic collisions between neutral atoms and plasma ions on neutral gas transport under typical tokamak boundary conditions. By comparing solutions obtained for neutral helium and neutral hydrogen the possibility of local helium enrichment in divertors or pump limiters is considered in detail. Here we reinvestigate the inverted pump limiter concept of Prinja and Conn, however with applications to the issue of helium removal in general, e.g. also by divertors. By using a general Monte Carlo algorithm to solve the same kinetic equations, the analytical solutions are verified. Furthermore some of the simplifying approximations, which were necessary to obtain closed form analytical solutions, are then removed in the Monte Carlo solution. This allows a critical assessment of such approximations.

# Contents

1	Introduction	4
2	Analytical model	5
2.1	Model equations and boundary conditions . . . . .	5
2.2	Solution . . . . .	8
2.3	Helium enrichment . . . . .	11
3	Monte Carlo model	14
3.1	Method of solution . . . . .	14
3.2	EIRENE results and comparison with analytical results . . . . .	15
4	Conclusions	16

# 1 Introduction

The transport of neutral particles in tokamak boundary plasmas is dominated by elastic (at small plasma temperatures, below 20 eV) and inelastic interactions between the neutral and charged particles. Viscous effects on neutral gas transport can in many (but notably not in all) cases be neglected. This and comparing characteristic length and mean free paths under typical tokamak edge plasma conditions clearly points to the need for linear kinetic models for neutral particles transport.

General 3 dimensional solutions, for almost arbitrarily complex boundary conditions and collision integrals can routinely be found by using Monte Carlo simulation methods. General trends and parametric dependencies, nevertheless, can only be investigated by analytic methods. However, analytical treatment is often only possible for strongly simplified model equations. Combining these two methods of solution can be beneficial with regard to at least two aspects. As already pointed out in ref. [9], the concept of conditional expectation estimators allows to combine analytical and stochastic information in the Monte Carlo solution without violating it's applicability to very complex problems but with the potential of tremendous savings in CPU-costs.

A second aspect, discussed in this report, is the trivial fact that a Monte Carlo computer code, if sufficiently flexible, can easily be reduced to also solve exactly the approximate kinetic equations solved by the analytical methods. Thus Monte Carlo can assist to assess the effects of the simplifying assumptions on the closed form analytical solutions. In this paper we make use of this latter concept with regard to the frequently discussed issue of decoupling of neutral hydrogen and helium transport in boundary plasmas, on the basis of different atomic physics for the two particle species involved. Starting point and motivation for this present study was the analytical investigation of neutral hydrogen versus helium transport in ref. [8], which resulted in a proposal for an "inverted limiter concept" for preferential helium removal from tokamak plasmas. Apart from the point made

in ref. [11] that this issue can not be discussed in terms of neutral gas transport alone but critically depends on the mutual effects of neutral and charged particle transport, one remaining confusing fact was the significant discrepancy of the analytical solutions given in [8] and the Monte Carlo solutions for a seemingly identical kinetic equation [10]. In this report we will firstly reinvestigate this problem and show how perfect agreement between analytical and Monte Carlo treatment of this relevant kinetic equation can be achieved. Secondly we will extend the previous analytical investigation of ref. [8] to include more physical effects such as different boundary conditions, or elastic interaction between neutral and charged particles. Finally we will critically examine the approximations in the model equation by returning to Monte Carlo solutions with less restrictive assumptions.

Our analysis tends to confirm results obtained earlier by [12] on the relevance of elastic collisions (for a different configuration discussed there).

Our analysis will, in principal terms, contribute to an optimisation of the positioning of the pump duct entrance with respect to the neutralizing target, in terms of neutral particle mean free paths, for efficient helium removal.

## 2 Analytical model

### 2.1 Model equations and boundary conditions

The starting point is the linear time-independent kinetic equation for the distribution function  $f_A$  of atomic neutral particles of species  $A$

$$\vec{v} \cdot \vec{\nabla} f_A = \sum_{i,cx,el} C_A(f_A) . \quad (1)$$

We will use the following terminology and assumptions throughout this report:  $k_A$  and  $\tilde{k}_A$  denote rate coefficients,  $\nu_A$ 's the corresponding collision frequencies. The ion density is defined by  $n_{A+} := \int d\vec{v} f_{A+}$ ,  $\hat{f}_{A+} := f_{A+}/n_{A+}$  is the normalized ion velocity distribution

function and has to be specified (e.g. as Maxwellian  $\hat{f}_{A+} = \sqrt{m_{A+}/2\pi T_{A+}} e^{-m_{A+}v^2/2T_{A+}}$ , at the ion temperature  $T_{A+}$ ).  $n_{A+} = n_e$  (electron density),  $\vec{\Gamma}_A := \int d\vec{v} \vec{v} f_A$  (neutral particle flux).

The interactions of neutral atoms with the fixed, prescribed plasma background are described by the following model collision terms:

*Electron impact ionization (ei):*

$$C_A^{ei} = -k_A^{ei}(T_e)n_e f_A \equiv -\nu_A^{ei} f_A . \quad (2)$$

For the ionization rate coefficient  $k_A^{ei}$  the polynomial fits given in the database [1] are used.

*Charge exchange (cx):*

$$C_A^{cx} = -\tilde{k}_A^{cx}(T_{A+})n_e f_A + \tilde{k}_A^{cx}(T_{A+})n_e \hat{f}_{A+} N_A \equiv \nu_A^{cx}(-f_A + \hat{f}_{A+} N_A) \quad (3)$$

The cx rate coefficient  $k_A^{cx}(v, T_{A+}) := \langle v_r Q^{cx}(v_r) \rangle$  depends, in general, on both the neutral's velocity  $v$  and the ion temperature  $T_{A+}$ .  $\langle \dots \rangle$  denotes averaging over the ion velocity distribution  $\hat{f}_{A+}(v_i)$  and  $v_r = |\vec{v} - \vec{v}_i|$  is the relative velocity of the collision partners. Here we use the good approximation  $\tilde{k}_A^{cx} \cong v_r^* Q^{cx}(v_r^*)$  with  $v_r^* := (8T_{A+}/\pi m_{A+} + v^2)^{1/2}$  (cf. [2]) and furthermore, we replace  $v$  by  $v_{A+}$ ,  $v_{A+} := \sqrt{T_{A+}/m_{A+}}$  (thermal velocity of the ions  $A^+$ ).  $Q^{cx}$  is again taken from [1]. This replacement of the explicit neutral particle velocity dependence by  $T_{A+}$  in the cx rate coefficient removes the functional dependence of the model collision term on the neutral particle distribution function. This term then only depends on the neutral particle density  $N_A := \int d\vec{v} f_A$ . That permits to derive an integral equation for the spatial neutral particle density profile  $N_A$  (cf. [3]). After having solved this equation, one can then calculate the distribution function  $f_A$  in a second step, ie. all the higher momenta of  $f_A$ .

*Elastic collisions (el):*

$$C_A^{el} = -\tilde{k}_A^{el}(T_{A+})n_e(f_A - N_A \hat{f}_{A+}) \equiv -\nu_A^{el}(f_A - N_A \hat{f}_{A+}) \quad (4)$$

The elastic interaction is considered here in a very crude approximation only as a relaxation of  $f_A$  to the ion distribution function  $\hat{f}_{A+}$ . This relaxation is described by a rate coefficient, in which the explicit velocity dependence has again been suppressed using the same scheme as for the charge exchange collision rate:  $\tilde{k}_A^{el}(T_{A+}) \approx k_A^{el}(v_{A+}, T_{A+})$ . Thus at least particle conservation is ensured (cf. [4]). In case of elastic collisions between particles of different masses, such as collisions between helium atoms and proton ions, we assume a relaxation of the neutral particles to the energy distribution (not the velocity distribution) of the background ions. In this paper we have used the cross section evaluated in [5]. (Retaining a full BGK collision term to describe elastic collisions would lead to a nonlinear problem which can not be solved analytically (cf. [6]).)

For simplicity and because, in general, surface recycling is the dominant source of neutral particles in tokamak boundary plasmas, recombination is neglected.

We consider a planar semi-infinite half-space geometry. Then the kinetic equation in the only spatial coordinate  $x$  reads

$$v \frac{\partial f_A}{\partial x} + \nu_A^- f_A = \nu_A^+ \hat{f}_{A+} N_A, \quad (5)$$

$$\nu_A^- := \nu_A^{ei} + \nu_A^{cx} + \nu_A^{el}, \quad \nu_A^+ := \nu_A^{cx} + \nu_A^{el}.$$

This is the basic equation which we solve employing the analytic solution given in [7]. In particular we are referring here to the MODEL I ("neutrals from the wall") of [7]. In that paper it was shown, that the formal solution of (5) can be written as:

$$f_A(\eta, v) = \theta(v) f_A^+(\eta, v) + \theta(-v) f_A^-(\eta, v) \quad (6)$$

with

$$f_A^+(\eta, v) = f_A^+(0, v) e^{-\eta/v} + \int_0^\eta \frac{d\eta'}{v} e^{-(\eta-\eta')/v} \hat{f}_{A+}^+(\eta', v) \hat{N}_A(\eta'), \quad (7)$$

$$f_A^-(\eta, v) = - \int_\eta^\infty \frac{d\eta'}{v} e^{-(\eta-\eta')/v} \hat{f}_{A+}^-(\eta', v) \hat{N}_A(\eta'); \quad (8)$$



$f_{A+}^{\pm} := \theta(\pm v) \hat{f}_{A+}$ ,  $\alpha_A := \nu_A^+ / \nu_A^-$ ,  $\eta(x) := \int_0^x dx \nu_A^-(x')$ . We have made use of the fact that the product  $\hat{N}_A := \alpha_A \cdot N_A$  is a function of the generalized spatial coordinate  $\eta$  only.

The boundary condition at the left recycling surface is assumed to have the following form:

$$\begin{aligned} f_A^+(0, v) &= \Gamma_{0A} f_{0A}(v) + \int_0^\infty dv' R_A(v, -v') f_A^-(0, -v'), v > 0, \\ &\equiv \Gamma_{0A} f_{0A} + \int_0^\infty d\eta' \hat{N}_A(\eta') \int_0^\infty \frac{dv'}{v'} e^{-\eta'/v'} R_A(v, -v') \hat{f}_{A+}^-(\eta', -v'). \end{aligned} \quad (9)$$

The reflection function  $R_A$  is a linear combination of specular and diffusive reflection:

$$R_A = R_{SA} \delta(v - v') + R_{DA} F_{DA} v' \quad (10)$$

with

$$\int_0^\infty dv v f_{0A}(F_{DA}) = 1. \quad (11)$$

and  $R_{SA}$  and  $R_{DA}$  are free parameters of the model.

The second boundary condition, at infinity, is

$$f_A(\infty, v) = 0 \quad \forall v. \quad (12)$$

## 2.2 Solution

Now we solve for the neutral particle density profile. After that the full kinetic solution is obtained (eqs. (6)-(8)), using for  $\hat{f}_{A+}$  an ion velocity distribution which must be consistent with the approximations in the collision integrals eqs. (2), (3) and (4). (For example, in this report,  $f_{A+}$  is taken to be a double delta function throughout. For electrons, however, we retain a maxwellian distribution function, which is intrinsic in the rate coefficients for electron impact collisions.)

The solution for the density is taken as given in ref. [7], however with three further simplifying assumptions as compared to the full results in [7]:

1. Homogeneous plasma temperature and plasma density,
2. double delta function distribution for the ions  $A^+$

$$\hat{f}_{A^+} \approx \frac{1}{2} [\delta(v - v_{A^+}) + \delta(v + v_{A^+})], \quad (13)$$

3. monoenergetic and one-dimensional reflection function

$$f_{0A} \equiv F_{DA} = \frac{\delta(v - v_A)}{v_A}. \quad (14)$$

$v_A$  is the injection velocity of the atoms  $A$ . (Note that under these pathologic conditions and for  $v_A = v_{A^+}$ , the diffusive reflection becomes identical with the specular reflection.)

With these assumptions we obtain for the normalized density the solution [7]:

$$\begin{aligned} \widetilde{N}_A(\xi_A) := \frac{N_A}{\Gamma_{0A}/v_{A^+}} &= \frac{1 + A_A R_{DA}}{u_A} \frac{1 - u_A^2}{1 - \delta_A^2 u_A^2} e^{-\frac{\xi_A}{u_A}} \\ &+ \frac{1 + u_A}{1 + \delta_A} \frac{1 - \delta_A}{u_A} \frac{1 + \frac{1 - u_A}{1 + u_A} R_{SA}}{D_A} e^{-\delta_A \xi_A} \end{aligned} \quad (15)$$

$$D_A := 1 - (1 - \delta_A) \left( \frac{R_{SA}}{1 + \delta_A} + \frac{R_{DA}}{1 + \delta_A u_A} \right) \quad (16)$$

$$A_A := \frac{1 - \delta_A}{1 + \delta_A} \frac{1}{D_A} \quad (17)$$

with the definitions

$$\xi_A(x) := \frac{\eta}{v_{A^+}} \equiv \int_0^x dx' \frac{\nu_A^-(x')}{v_{A^+}}, \quad u_A := \frac{v_A}{v_{A^+}}, \quad \delta_A := \sqrt{1 - \alpha_A} \equiv \sqrt{\frac{\nu_A^{ei}}{\nu_A^-}} \quad (18)$$

$$A_A = |\Gamma_A^-(0)| / \Gamma_{0A} \text{ (Albedo)}. \quad (19)$$

Here the dimensionless variables  $\xi_A$  and  $\delta_A$  correspond to the optical depth and to an inverse penetration depth for generated particles, respectively.

We now proceed to calculate the higher momenta, thereby retaining the distribution functions (13) and (14). The momenta are defined by

$$M^{(n)}_A(\xi) := \int_{-\infty}^{\infty} dv v^n f_A(\xi, v). \quad (20)$$

They can be calculated using eqs. (6)-(8) to

$$M_A^{(2n)} = v_{A+}^{2n} \left[ \frac{\Gamma_{0A}}{v_A} (u_A^{2n} - 1) e^{-\frac{\xi_A}{u_A}} + N_A(\xi_A) \right], \quad (21)$$

$$M_A^{(2n+1)} = \Gamma_{0A} v_A^{2n} (1 - 1/u_A^2) e^{-\frac{\xi_A}{u_A}} - v_{A+} \frac{d}{d\xi_A} M_A^{(2n)}(\xi_A), \quad (22)$$

$$M_A^{(0)} \equiv N_A, \quad M_A^{(1)} \equiv \Gamma_A. \quad (23)$$

If the first term of both equations can be neglected the diffusion approximation results. These terms vanish exactly for  $u_A = 1$  (i.e. for  $v_A = v_{A+}$ ) or for  $v_A \rightarrow 0$ . Both cases will be considered below. We note here that the perfect reduction of the full kinetic solution to the diffusion approximation for  $u_A = 1$  is a consequence of the assumption 2 of a one-dimensional monoenergetic ion velocity distribution. In general, and in particular for the three-dimensional ion distribution function in ref. [8], the diffusion solution is, at best, only approximate, even for otherwise identical conditions.

Using eqs. (15) and (22) the particle flux can be calculated to

$$\begin{aligned} \tilde{\Gamma}_A(\xi_A) := \frac{\Gamma_A}{\Gamma_{0A}} &= \frac{1}{u_A^2} \frac{1 - u_A^2}{1 - \delta_A^2 u_A^2} \left( \delta_A^2 u_A^2 + A_A R_{DA} \right) e^{-\delta_A \xi_A} \\ &+ \delta \frac{1 + u_A}{1 + \delta_A u_A} \frac{1 - \delta_A}{1 - \delta_A u_A} \frac{1 + \frac{1 - u_A}{1 + u_A} R_{SA}}{D_A} e^{-\delta_A \xi_A}. \end{aligned} \quad (24)$$

We next discuss a few special cases:

(i)  $\underline{u_A = 1}$  (thermal injection velocity)

reflecting left boundary

$$(R) \quad R_{SA} + R_{DA} = 1 : \tilde{N}_A = \frac{e^{-\delta_A \xi_A}}{\delta_A}, \quad \tilde{\Gamma}_A = e^{-\delta_A \xi_A} \quad (25)$$

absorbing left boundary

$$(0) \quad R_{SA} = R_{DA} = 0 : \quad \widetilde{N}_A = \frac{2}{1 + \delta_A} e^{-\delta_A \xi_A}, \quad \widetilde{\Gamma}_A = \frac{2\delta_A}{1 + \delta_A} e^{-\delta_A \xi_A} \quad (26)$$

These results are exact within the model assumptions, in particular with eqs. (13) and (14).

(ii)  $u_A \rightarrow 0$  (low velocity injection)

$$(R) \quad R_{DA} = 1, \quad R_{SA} = 0 : \quad \widetilde{N}_A = \frac{1 - \delta_A}{\delta_A} e^{-\delta_A \xi_A}, \quad \widetilde{\Gamma}_A = (1 - \delta_A) e^{-\delta_A \xi_A} \quad (27)$$

$$(0) \quad R_{DA} = R_{SA} = 0 : \quad \widetilde{N}_A = (1 - \delta_A) e^{-\delta_A \xi_A}, \quad \widetilde{\Gamma}_A = \delta_A (1 - \delta_A) e^{-\delta_A \xi_A} \quad (28)$$

These are approximate solutions, as well as  $u_A = 0$  is an unphysical limiting case only.

## 2.3 Helium enrichment

The first analytical treatment of the problem was given in [8] for a slab model with absorbing left wall. Elastic interaction had not been taken into account there so that for helium atoms the plasma is a purely absorbing medium. In this section we will show how the boundary conditions and in particular the elastic interaction may influence local helium enrichment. The results of the foregoing section are used to calculate the helium enrichment factor, which is defined by the ratio of helium to hydrogen normalized particle fluxes

$$\eta := \frac{\widetilde{\Gamma}_{He}}{\widetilde{\Gamma}_H}. \quad (29)$$

The interaction processes which are included are: Electron impact ionization, charge exchange (only for hydrogen) and elastic interaction ( $H/H^+$ ,  $He/H^+$ ). Describing the elastic interaction  $He/H^+$  by the model collision term (4) energy conservation is not ensured so that this description is rather crude. The rate coefficients of these processes are displayed in Figs. 1a,b.

The solution for the first special case (i), with boundary condition (R), takes a particularly simple form and we refer to it as “standard solution”  $\eta_s$ . The solution for the other special cases considered here can then be expressed in terms of this standard solution.

Special cases:

(i)  $u_H = u_{He} = 1$

$$(R) \quad \eta = \eta_s := e^{\delta_H \xi_H - \delta_{He} \xi_{He}} \quad (\text{standard solution}) \quad (30)$$

$$(0) \quad \eta = \frac{\delta_{He}}{1 + \delta_{He}} \frac{1 + \delta_H}{\delta_H} \eta_s \quad (31)$$

(ii)  $u_H \rightarrow 0, \quad u_{He} = 1$

$$(R) \quad \eta = \frac{1}{1 - \delta_H} \eta_s \quad (32)$$

$$(0) \quad \eta = \frac{2\delta_{He}}{1 + \delta_{He}} \frac{1}{\delta_H (1 - \delta_H)} \eta_s \quad (33)$$

(iii)  $u_H = 1, \quad u_{He} \rightarrow 0$

$$(R) \quad \eta = (1 - \delta_{He}) \eta_s \quad (34)$$

$$(0) \quad \eta = \delta_{He}(1 - \delta_{He}) \frac{1 + \delta_H}{2\delta_H} \eta_s \quad (35)$$

(iv)  $u_H \rightarrow 0, \quad u_{He} \rightarrow 0$

$$(R) \quad \eta = \frac{1 - \delta_{He}}{1 - \delta_H} \eta_s \quad (36)$$

$$(0) \quad \eta = \frac{\delta_{He}}{\delta_H} \frac{1 - \delta_{He}}{1 - \delta_H} \eta_s \quad (37)$$

Discussion:

The standard solution  $\eta_s$  has a very simple analytic form. In this case the enrichment factor  $\eta$  scales exponentially with the line density  $\int_0^x dx n_e$ . For temperatures for which the total collision rate for helium is larger than for hydrogen atoms, one finds an exponential increase in  $\eta$ , otherwise an exponential decrease. But this holds true only for the special case  $u_A = 1$ , condition (R) and, in particular, the ansatz (13). In this case the transport of each particle species is characterized by one single decay length. Under more general conditions this dependence is more complicated.

In order to compare our results with those of [8] we calculate helium enrichment at a distance  $a = 20\text{cm}$  into the slab, and for an electron density  $n_e = 10^{13}\text{cm}^{-3}$ . We investigate the temperature range between 3.2 eV and 100 eV. To elucidate the influence of the different interaction processes we calculate also helium "enrichment" by means of the density

$$\eta_d := 2 \frac{\widetilde{N}_{He}}{\widetilde{N}_H} \quad (38)$$

and denote  $\eta$  by  $\eta_f$  ('flux').

Now we consider the four special cases which are redefined as follows

case (i) :  $u_H = u_{He} = 1$  (R) (*standard solution*)

case (ii) :  $u_H = u_{He} = 1$  (0)

case (iii) :  $u_H = 0.1, u_{He} = 1$  (R)

case (iv) :  $u_H = 0.1, u_{He} = 1$  (0)

Quantities calculated without including the elastic interaction are denoted by a suffix 0 and displayed by a dashed line. Figs. 2a, b show that elastic interaction lowers both damping rates  $\delta_A$ . This is particularly pronounced for the helium component. In contrast  $H/H^+$  collisions only slightly affect  $\delta_H$ . As expected, for temperatures above 20 eV  $\delta_{He}$  approaches 1, i.e. the damping rate  $\delta_{He}^0$  without elastic collisions. Figs. 3a,b show how the elastic interaction lowers the total mean free paths for the both velocity combinations  $u_H = u_{He} = 1$  and  $u_H = 0.1, u_{He} = 1$ .

Figs. 4-7 show analytically calculated enrichment factors for the four special cases (i) - (iv). In general elastic interaction may affect enrichment for temperatures below 20 eV. The standard solution Fig. 3b yields a maximum enrichment factor of about 2 which is slightly increased by elastic collisions. The enrichment calculations of [8] obtained without including elastic interaction are also displayed. Our results show that such high values can only be obtained for rather unphysical model assumptions, as can be seen in the

following figures. For the case (ii) of an absorbing boundary (Fig. 5b) helium enrichment is enlarged and elastic interaction has a strong influence.

### 3 Monte Carlo model

#### 3.1 Method of solution

Linear neutral particle transport codes, based on the Monte Carlo method, are often considered as tools to empirically simulate some physical process, which is often only marginally precise defined (such as "neutral atoms penetrating a plasma boundary region"). It is, however, made clear in almost every textbook on Monte Carlo methods for neutron transport that a well defined linear transport equation is actually solved by the Monte Carlo procedure. This has also been emphasized e. g. in [9] for the plasma edge neutral gas transport code EIRENE. For the present study we have used EIRENE to solve eq. (1) in the following precise sense (loc. cit): The solution to the kinetic part of eq. (1), i. e. the left hand side, with the right hand side replaced by a delta function, yields the Greens function  $T$ , which is used as transition probability for a free flight of a test particle from one point of collision (or from the point of birth at the left boundary) to the next point of collisions. The right hand side of eq. (1) is taken as transition probability  $C$  from a pre - to a post collision state of the test particle, with exactly the same approximations retained in the collisions terms as in section 2.1.

A large set (about 100,000) of random walks starting at the left boundary with the distribution eqs. (9) and (10), is generated by alternatively applying the kernels  $T$  and  $C$  for random number generation.

Clearly, and for exact proofs of this the reader is referred to any textbook on Monte Carlo methods, the distribution of test particles is then given by  $f_A$ , the solution of eq. (1). Simply by counting, but also by employing more sophisticated "estimators", the

moments  $N_A$ ,  $\Gamma_A$  and in general  $M_A^{(n)}$  are obtained.

The major advantage of Monte Carlo methods over numerical or analytical solutions rests on the fact, that this procedure remains valid for almost arbitrarily complex boundary conditions or transport and collision kernels  $T$  and  $C$ , as long as random numbers can be generated from them.

### 3.2 EIRENE results and comparison with analytical results

A first investigation of helium enrichment due to different neutral gas transport characteristics for hydrogen and helium, and a comparison with the result in ref. [8], by using the EIRENE code, was attempted in ref. [11]. The agreement was rather unsatisfactory, whereas in view of section 3.1 it should have been perfect. In the EIRENE runs the same atomic data, collision terms and boundary conditions as in [8] had been included. This present study, and in particular the perfect agreement of Monte Carlo and analytical solutions using the formulars of ref. [7], resolve that issue. Retaining only the discrete part of the spectrum of the linear Boltzmann operator in [8] is equivalent to a diffusion like approximation. Whereas this diffusion approximation happens to be exact for the ansatz eq. (13) in the case (26) and (31), it is only approximate for the corresponding ansatz of a monoenergetic but isotropic distribution for  $\hat{f}_{A+}$  in [8]. On the other hand, this latter ansatz function is definitely closer to reality, a nearly 3 dimensional maxwellian (possibly shifted) velocity distribution. The significant disagreement between the exact (Monte Carlo) solution and the diffusion approximation for this otherwise identical model equation, clearly demonstrates the great care needed when describing neutral gas transport in the tokamak plasma edge by diffusion like approximations.

Finally, having verified perfect agreement between the general analytical solution (24) and the Monte Carlo solution we proceed from the simplified model of section 2 to a more complete one, which then, however, can be solved conveniently only by the Monte Carlo



method. In a first step, we have replaced the ansatz (13) by a 3 dimensional (in velocity space) maxwellian distribution at temperature  $T_{A+}$ .

In a second step (to be published later), we will use the full Monte Carlo model, however, for the same infinite slab configuration. In this model, neutral particles are created at the left boundary from recycling ions, employing detailed surface interaction models, and, in particular, allowing for hydrogen molecules. The charge exchange process is now correctly treated retaining the full explicite velocity dependence in the collision term. Elastic processes will be included in a more consistent way.

#### Present results:

We have verified a perfect agreement between analytical and Monte Carlo results which is within the thickness of lines in the figures. An essential result of our investigations is shown in Fig. 8 where the standard solution is displayed together with a Monte Carlo correction. The use of a full Maxwellian ion distribution function confirms our analytic estimation of a low helium enrichment factor.

## 4 Conclusions

In this report we have demonstrated the possibility of decoupling of neutral hydrogen and neutral helium transport under typical tokamak edge plasma conditions, due to significantly different atomic processes for the two particle species.

Whereas the qualitative picture of [8] remains valid, the correct results obtained in this paper lead to much smaller ratios of local neutral helium enrichment in the plasma. This overestimation in [8] was a result of the diffusion approximation used there, whereas, under the conditions investigated, a kinetic treatment (either analytically or with a Monte Carlo procedure), turned out to be necessary.

We have further shown that the elastic collision processes between neutral atoms

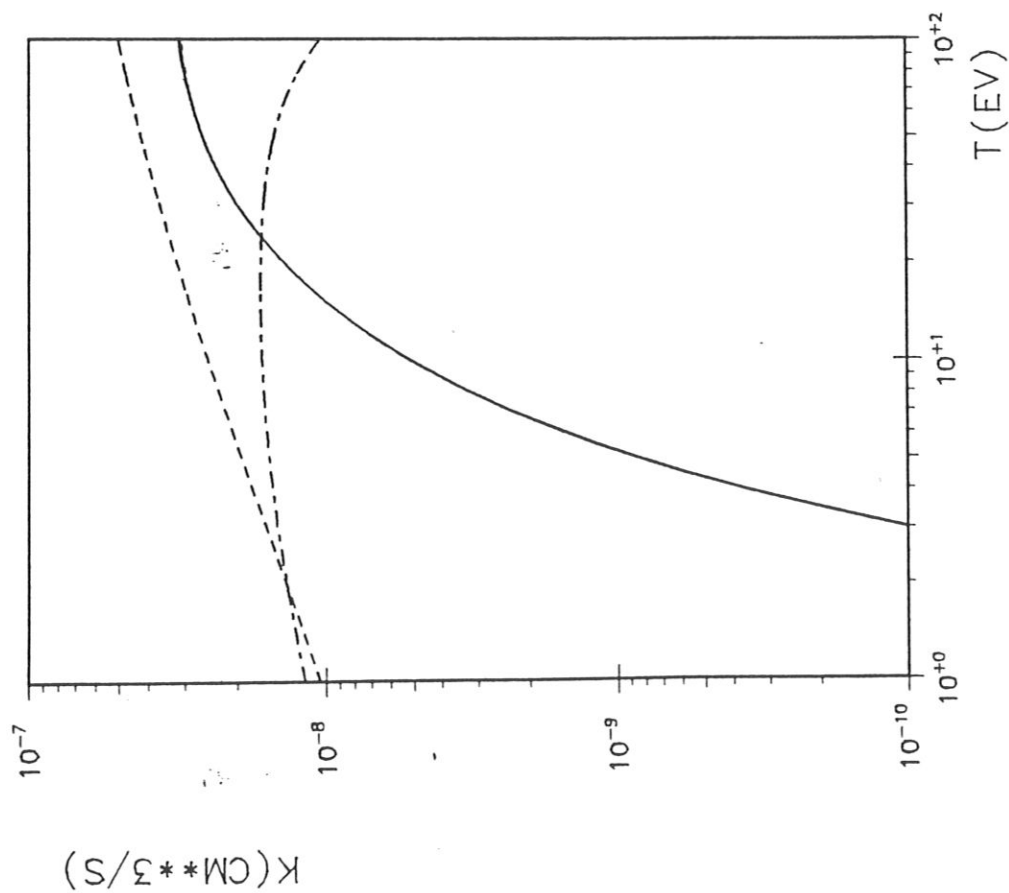
and plasma ions, usually neglected in tokamak neutral gas transport models, can play a significant part under low temperature, high density plasma conditions, which become more and more accessible near divertor target surfaces in the new large divertor tokamaks such as ASDEX UPGRADE.

We finally would like to point out, that, although not mentioned explicitly in this report, for the same reasons, which cause that decoupling of hydrogen and helium transport, the hydrogenic ions created by ionisation in the plasma tend to have much higher energies than the helium particles. This is due to more efficient thermalization, whereas helium atoms are predominantly cooled at divertor chamber surfaces without recovering their energy in the plasma. This could also be the origin of different transport characteristics of these two charged species. Mutual influence of neutral and charged particle transport then renders the problem of helium enrichment in pumping stations rather unpredictable, and results are, in general, only valid for one particular set of plasma and configurational conditions.

## References

- [1] R.K. Janev, W.D. Langer, K. Evans Jr, D.E. Post Jr, Elementary Processes in Hydrogen-Helium Plasmas, Springer Verlag 1987
- [2] E. Cupini, A. De Matteis, R. Simonini, J. Comp. Phys. 57(1985)77
- [3] A.K. Prinja, Phys. Fluids 30(1987)840
- [4] J.H.H.M. Potters, W.J. Goedheer, Nucl. Fusion 25(1985)779
- [5] P. Bachmann, D. Reiter, Elastic Processes in Hydrogen-Helium Plasmas: Cross Sections and Rate Coefficients, Max-Planck-Institut Report, in preparation
- [6] J.H. Ferziger, H.G. Kaper, Mathematical theory of transport processes (1972)
- [7] P. Bachmann, Physica Scripta 38(1988)835
- [8] A.K. Prinja, R.W. Conn, Nucl. Fusion 25(1985)1775
- [9] D. Reiter, JÜL-1947 (August 1984) and JÜL-2599 (March 1992)
- [10] D. Reiter, ITER/US/91/PH-13-01
- [11] D. Reiter et al., Plasma Physics and Controlled Fusion 33, 13 (1991) 1579
- [12] H. H. Abou-Gabal, G. A. Emmert, Nucl. Fusion 31 (1991) 407

KIH, KCXH(---), KELH(---)



KIHE, KCXHE(---), KELHE(---)

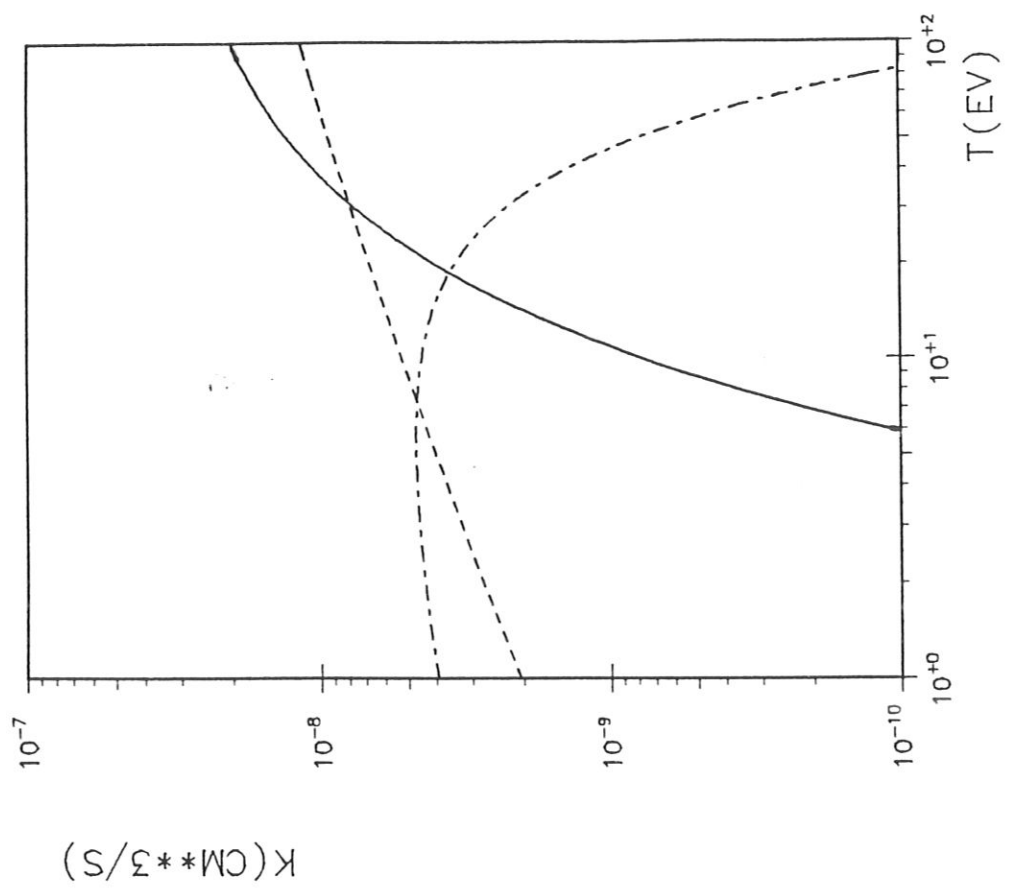
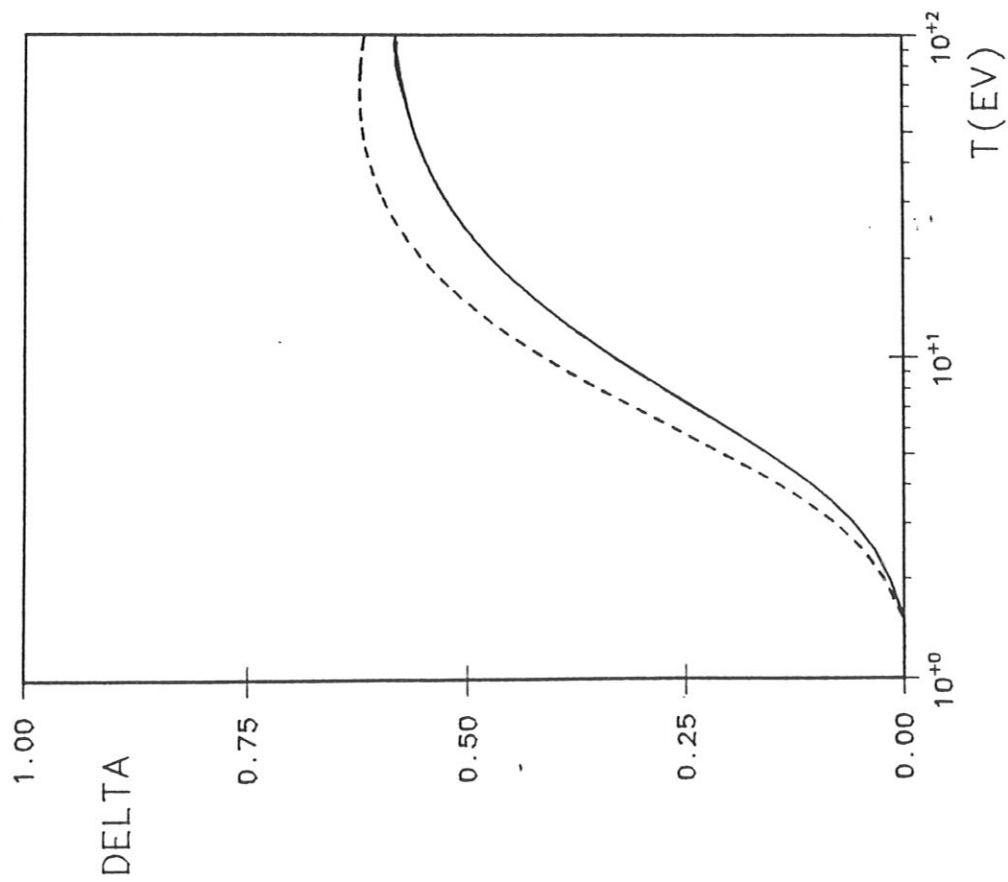


Fig. 1a,b. Rate coefficients for (a)  $H$  and (b)  $He$ : electron impact ionization (—), charge exchange (---), elastic collisions (a)  $H^+$  on  $H$  and (b)  $H^+$  on  $He$  (-.-).

DELTAH DELTAHO (- - -)



DELTAHE DELTAHEO=1

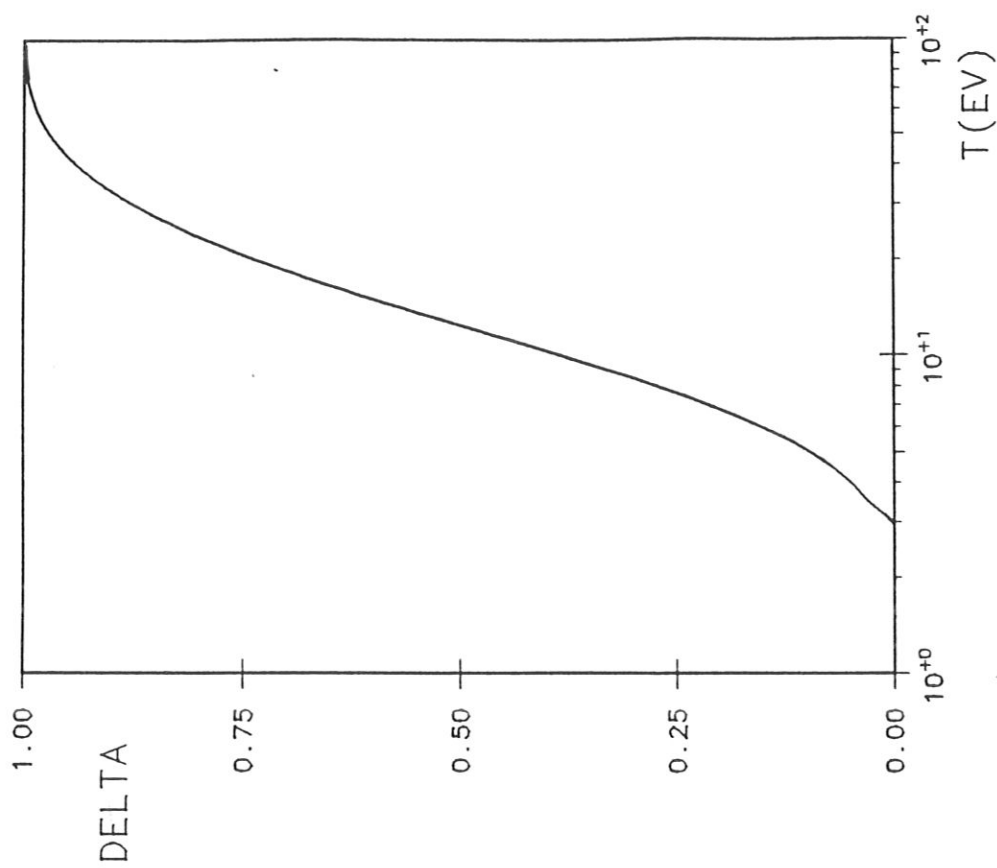


Fig. 2a,b. Damping rates (a)  $\delta_H$  and (b)  $\delta_{He}$ .

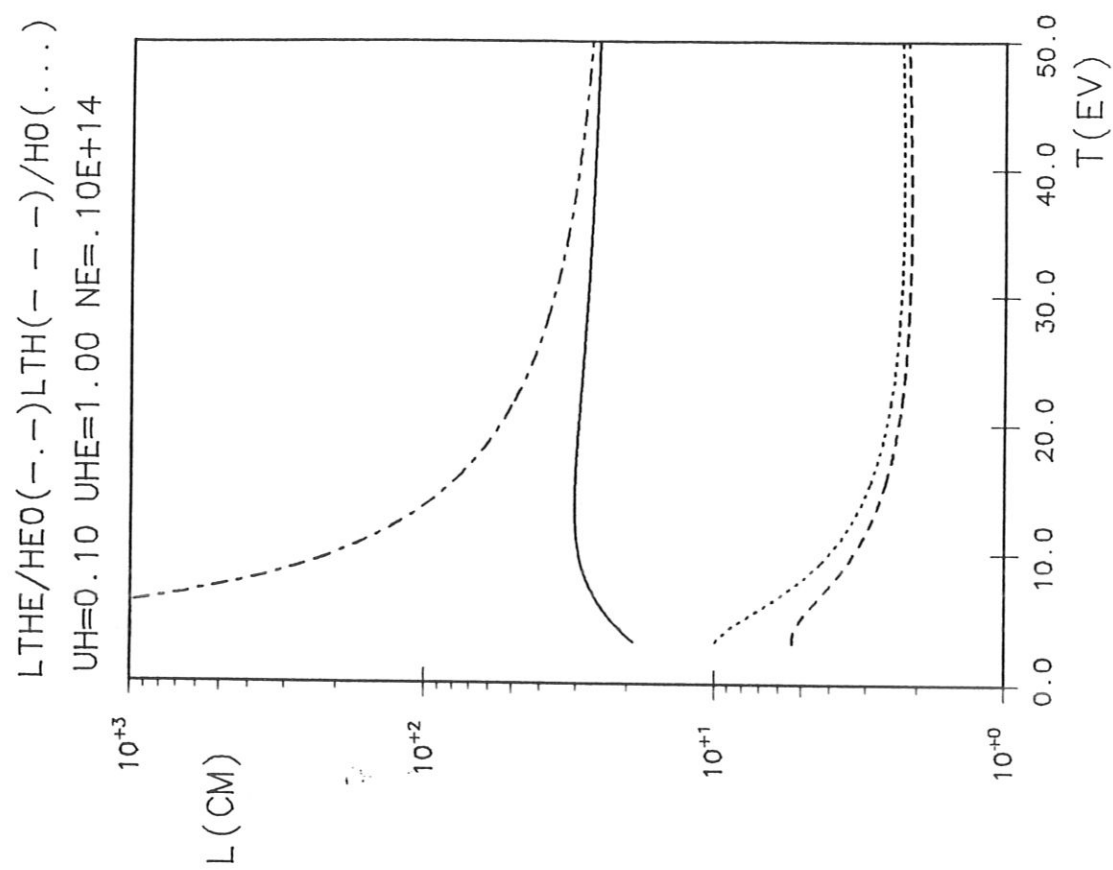
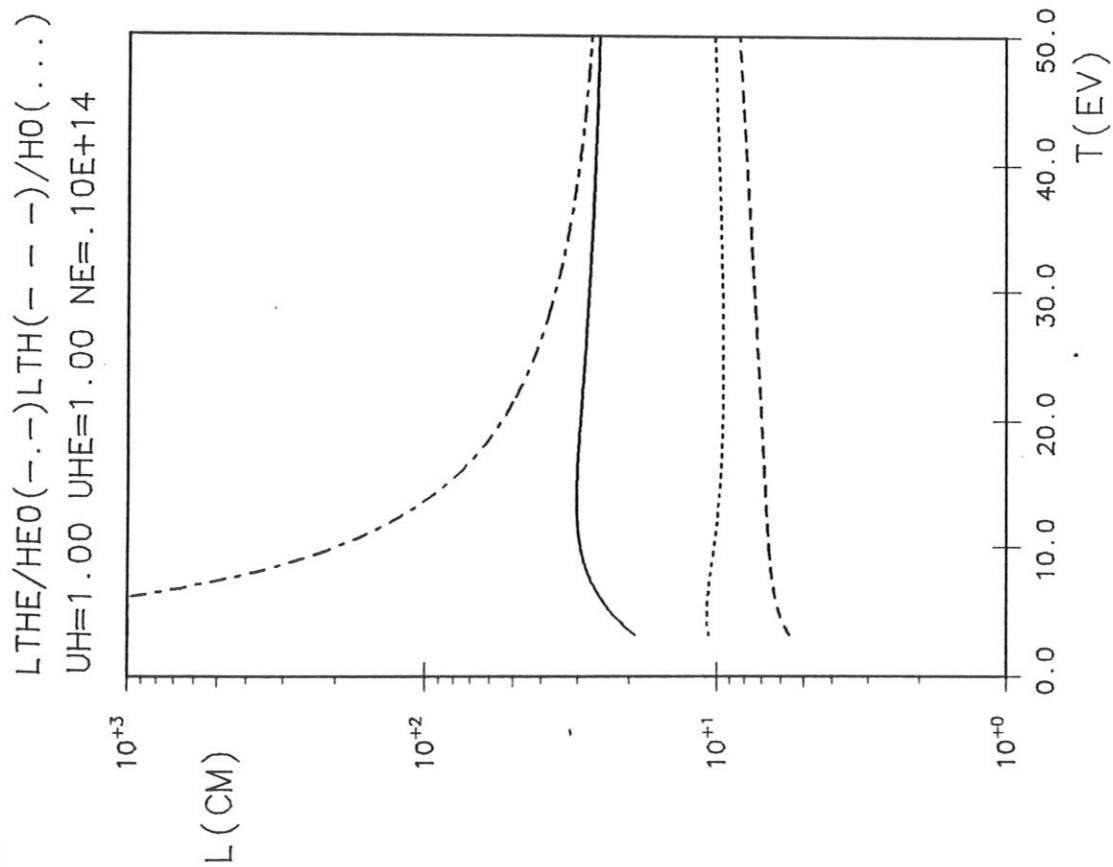


Fig. 3a,b. Total mean free paths for  $H$  (with  $(- - -)$ , without  $(\dots)$  elastic interaction) and  $He$  (with  $(-)$ , without  $(-.-)$  elastic interaction) for (a)  $u_H = u_{He} = 1$  and (b)  $u_H = 0.1, u_{He} = 1$ .

UH=1.00 UHE=1.00 NEA=.20E+15 RDH=1.0 RDHE=1.0 NO EL. (- -) REF.8 (-.-)

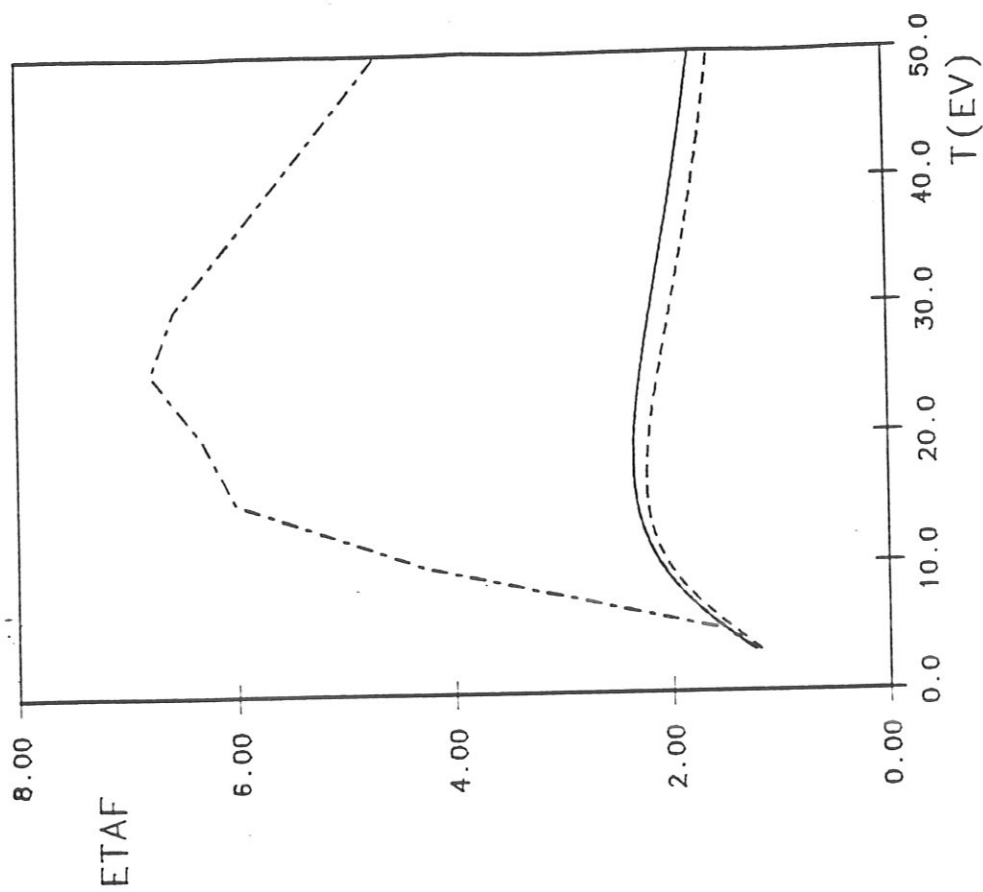
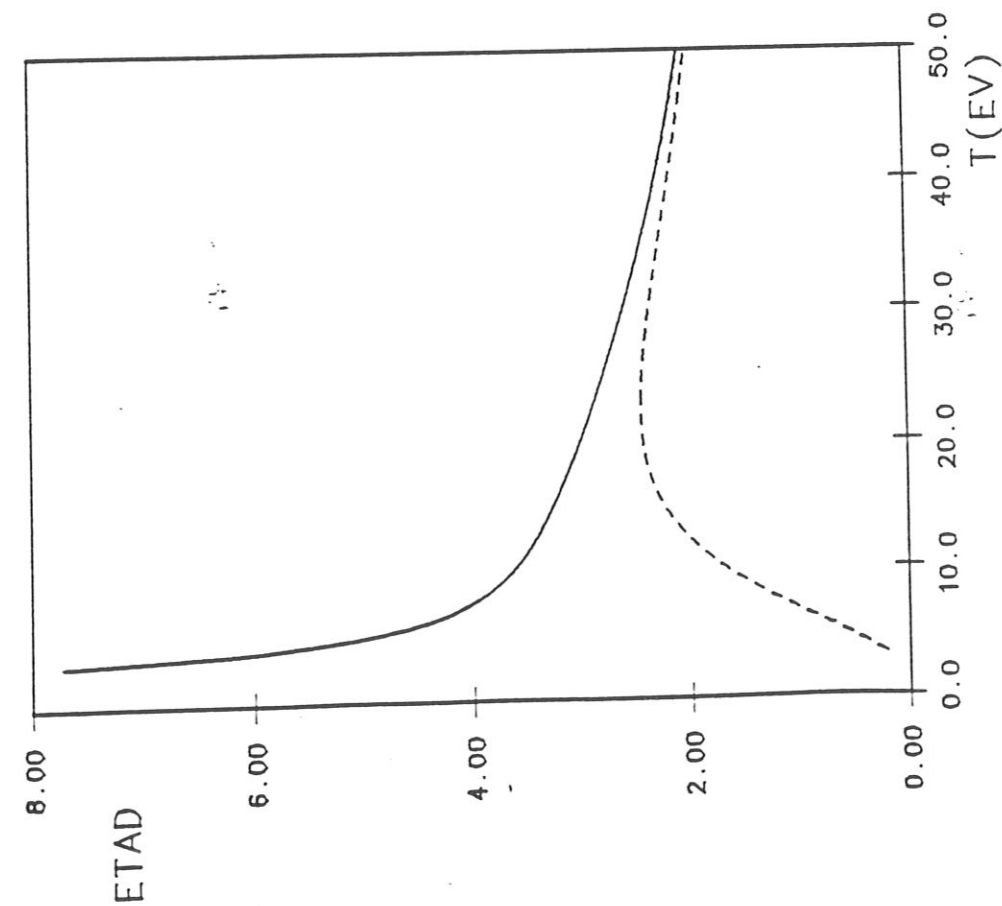


Fig. 4a,b. Analytic solutions for (a)  $\eta_d$  and (b)  $\eta_f$  for case (i) (s. text). (-.-) - result of ref. [8].

UH=1.00 UHE=1.00 NEA=.20E+15 RDH=0.0 RDHE=0.0 NO EL. (---) REF.8 (-.-)

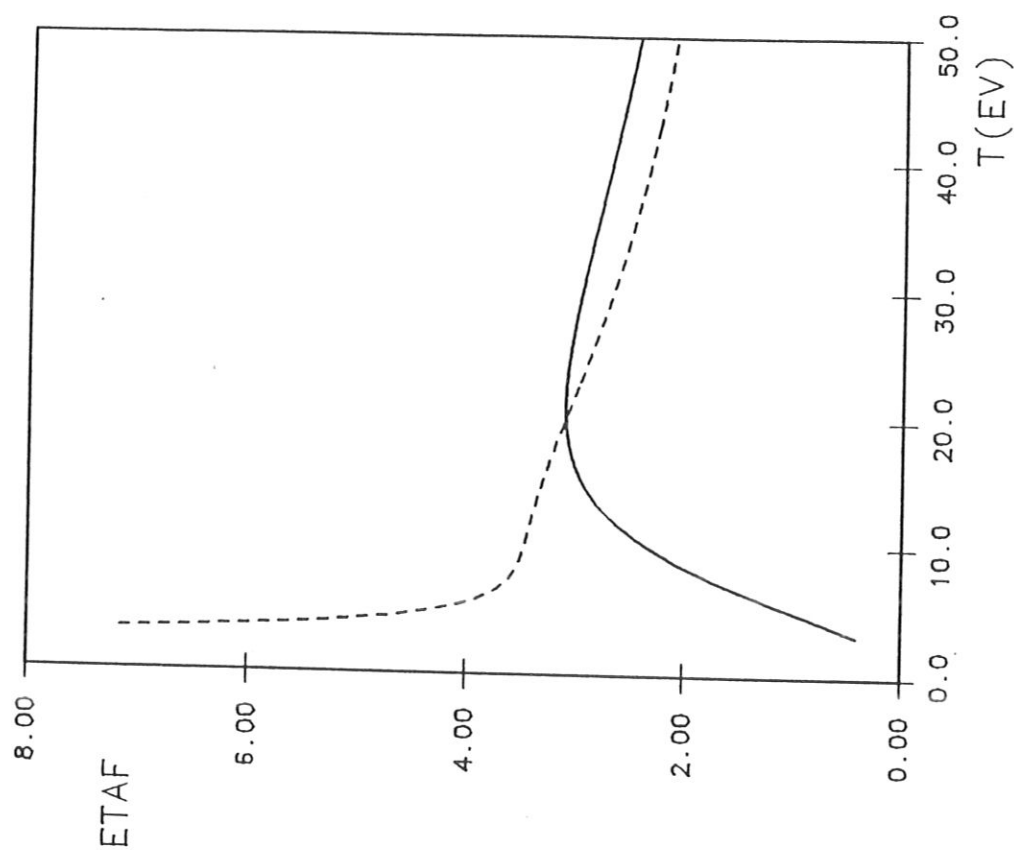
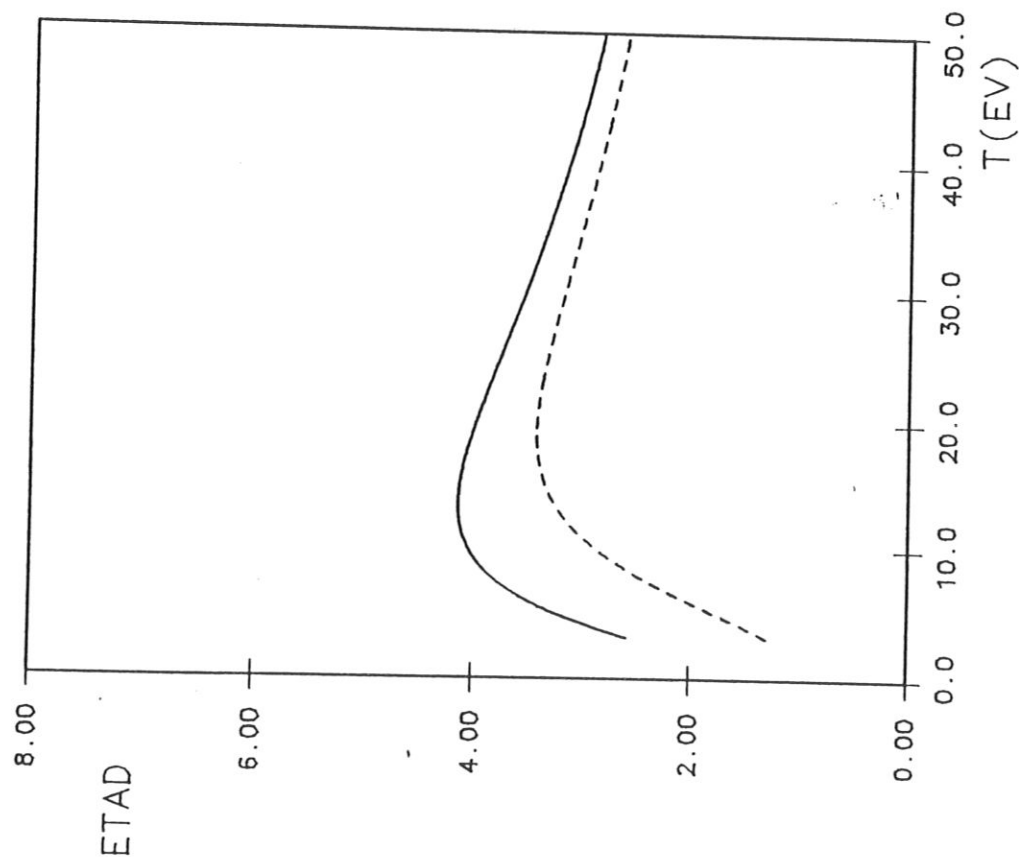


Fig. 5a,b. Analytic solutions for (a)  $\eta_d$  and (b)  $\eta_f$  for case (ii) (s. text).



UH=0.10 UHE=1.00 NEA=.20E+15 RDH=1.0 RDHE=1.0 NO EL. (- -)

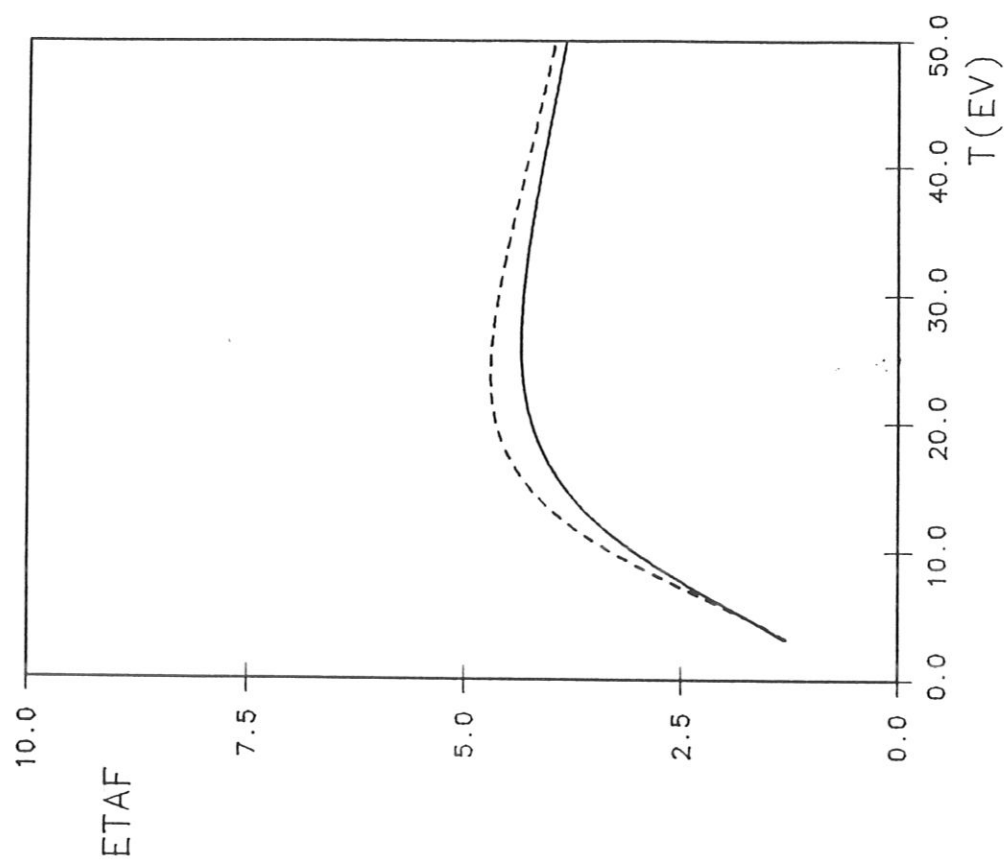
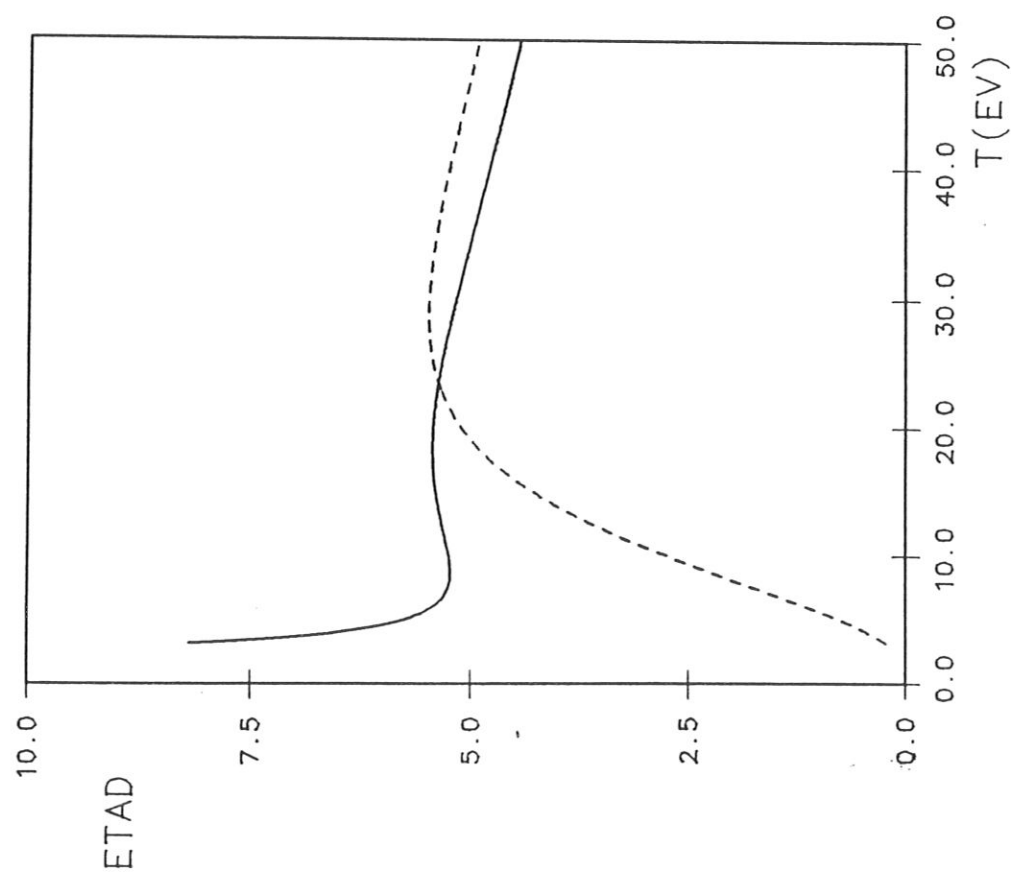


Fig. 6a,b. Analytic solutions for (a)  $\eta_d$  and (b)  $\eta_f$  for case (iii) (s. text).

UH=0.10 UHE=1.00 NEA=.20E+15 RDH=0.0 RDHE=0.0 NO EL. (— —)

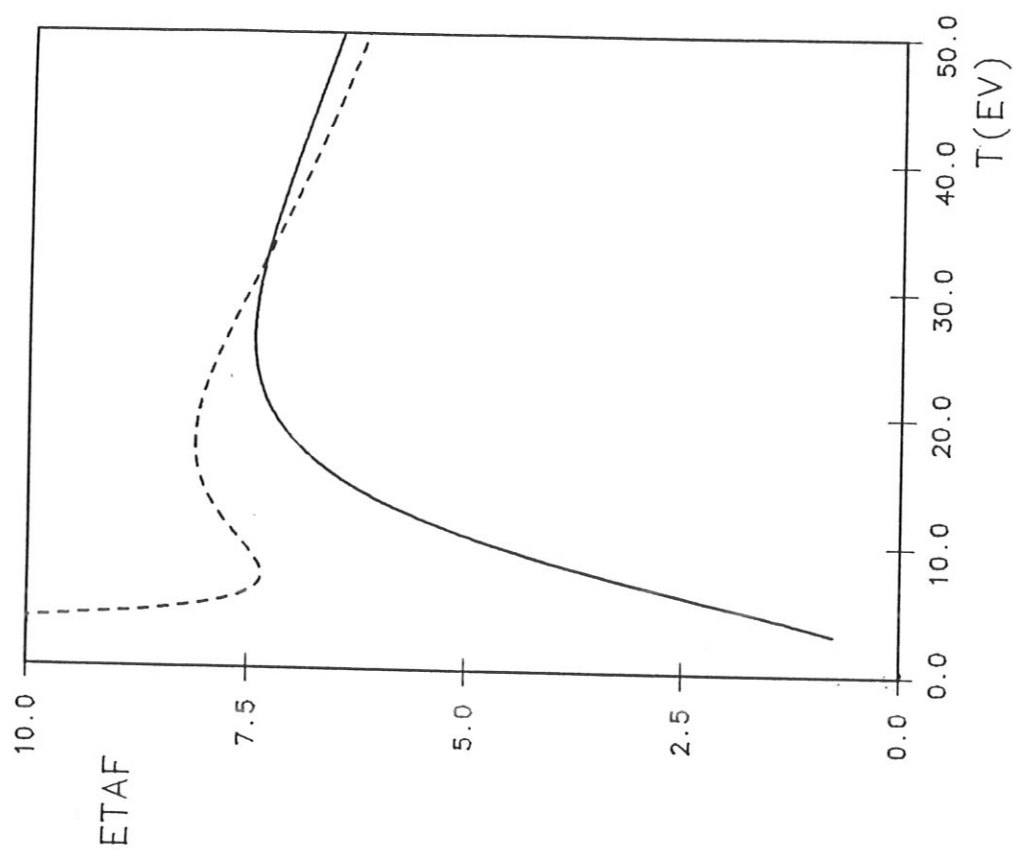
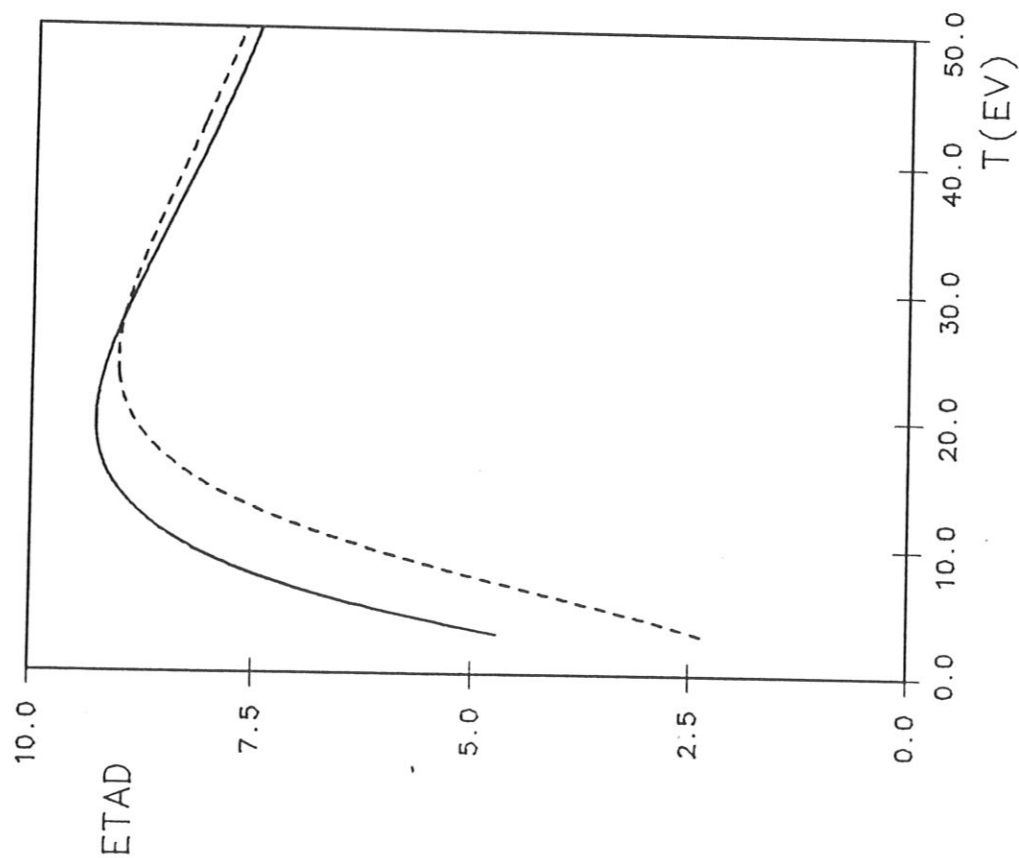


Fig. 7a,b. Analytic solutions for (a)  $\eta_d$  and (b)  $\eta_f$  for case (iv) (s. text).

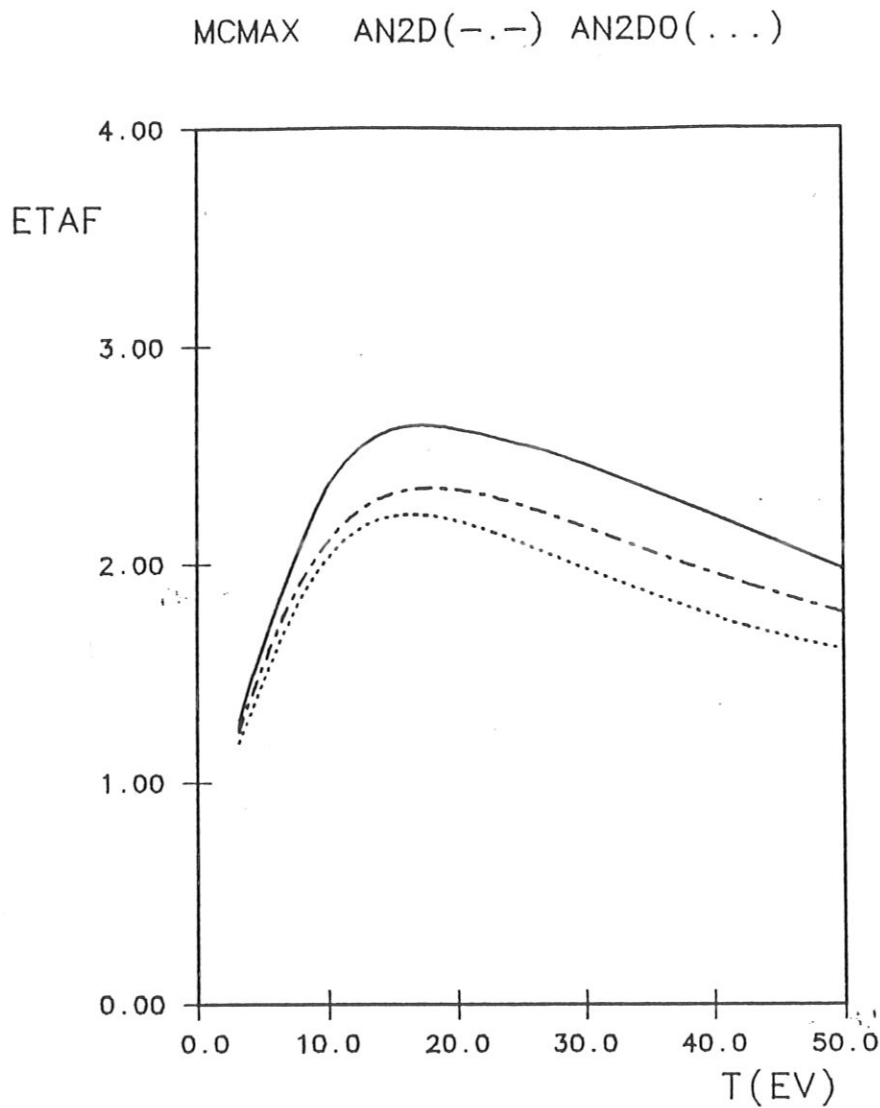


Fig. 8. Comparison of analytic with Monte Carlo calculations for helium enrichment  $\eta_f$  for case (i) (s. text): analytic (with (- • -), without (...) elastic interaction) for  $2\delta$  ion distribution and Monte Carlo for a fully Maxwellian ion distribution function (—).