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Numerical techniques used in Neutral Beam Injection modules [☆]

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Abstract

This paper describes and compares the numerical techniques for computing the Neutral Beam Injection (NBI) physics used in NBI modules in several integrated modeling codes. The Monte-Carlo NUBEAM module and the Fokker–Planck NBI ASTRA, DBEAMS, FPP, and NBEAMS neutral beam injection modules are considered. Physics included in these modules is discussed. Resulting electron and ion power heating profiles and particle source profiles for the TFTR discharge 66887 and the JET discharge 52009 are compared when computed with the NUBEAM, NBI ASTRA, DBEAMS and FPP modules.

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Keywords: Neutral Beam Injection; Tokamak; Fokker–Planck equation; Monte-Carlo

1. Introduction

This paper describes and compares the techniques that are used in the numerical simulations of neutral beam injection (NBI), which is one of the major methods for auxiliary heating of tokamak plasmas. Accurate simulation of the heating profiles is crucial for self-consistent integrated modeling of tokamak plasmas, which is used for the interpretation of existing experiments, testing theoretical hypothesis and planning future experiments.

Physical models, approximations and numerical techniques are different in each NBI module, but there are some physical processes that are included in all NBI modules—neutral beam deposition, fast ion orbiting, and slowing down of fast ions. Fast injected neutral particles are converted into fast ions within the plasma by impact ionizations and charge exchange processes. A large fraction of the resulting fast ions become trapped in the plasma confinement region, while the remainder leave the plasma region and hit the wall or the limiter. The process of following the fast ions in magnetically confined plasmas is referred as the fast ion orbiting. The fast ions slow down by transferring their energy and momentum to the thermal electrons and ions through collisions. Eventually, the fast ions become thermalized.

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Fast ion thermalization is described by the Fokker–Planck (FP) equation for the fast ion distribution function $f(\vec{r},\vec{v},t)$:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \mathcal{L}(f) + \mathcal{S} + L_{\mathrm{nc}}(f), \tag{1}$$

where $\mathcal{L}(f)$ is the Coulomb collision operator, $\mathcal{S}$ is the fast ion source, $L_{\mathrm{nc}}(f)$ is the operator that describes redistribution of the fast ions due to non-Coulomb processes such as interaction with rf waves, sawtooth oscillations, and magnetic ripple. The FP equation can be solved either by using a statistical Monte-Carlo (MC) method or by averaging the continuum equation over gyro and banana orbits in phase space. An advantage of the MC method is that the representation of complex physical processes is relatively straightforward. A disadvantage lies in the computational cost of reducing the statistical variance or "noise" in the model results. Generally, N^2 ions need to be followed in order to reduce the statistical variance by a factor of N.

Numerous approximations have been developed for the solution of the continuum FP equation in phase space. Some of them allow derivation of the analytical solution for the fast particle distribution function $f(\vec{r},\vec{v},t)$, while others require computer simulations. The nonlinear FP equation adequately describes NBI heating and current drive. However, when computational speed is more important than accuracy, a linearized version of the FP equation can be used. The linearized FP equation can be used for the cases when the fraction of fast ions is relatively small ($n_b/n_e \ll 1$) and when the rate of the radial diffusion is much smaller than the Coulomb slowing down, so that the fast ion distribution can be calculated on each magnetic surface separately.

There are other important physical processes, which are included in some NBI modules. Examples of such processes are charge exchange loss and recapture of slowing down fast ions, anomalous diffusion of fast ions, the effects of large scale instabilities, the effects of magnetic ripple, the effects of plasma rotation, and the effects of finite Larmor radius (FLR).

Five NBI modules are considered in this paper. The MC technique is used in the NUBEAM module [1], which is an essential element in the TRANSP code. Numerical solution of the continuum FP equation is used for the NBI heating module in the ASTRA code, the DBEAMS module in the BALDUR code, and in the FPP module in the TRANSP code. Finally, the NBEAMS module uses analytical solution of the FP equation.

2. Neutral Beam Injection NUBEAM module in the TRANSP code

The NUBEAM module from the TRANSP code [1,2] is a MC package for time dependent modeling of fast ion species in an axisymmetric tokamak. This MC package represents the fast ion slowing down distribution function as a discreet set of N weighted model ions. The NUBEAM module follows the fast ions until they slow down below $(3/2)T_i$, where T_i is the temperature of the thermal ions. At energies below $(3/2)T_i$ the ions are then considered to be "thermalized" ions and are described in terms of a thermalization source function provided as an output of the NUBEAM module.

The NUBEAM module takes into account multiple beamlines, each with its own beamline geometry and beam composition by isotope and energy fraction. The NUBEAM module computes the trajectory of neutral atoms and fast ion orbits. The evaluation of beam deposition takes into account the full range of atomic processes that affect beam stopping in a hot target plasma. The neutral beam stopping atomic physics includes collisions with partially slowed down fast ion species with an option for a neutral beam excitation correction. After deposition of fast ions in the plasma, the modeling associated with their slowing down includes anomalous diffusion of fast ions, the effects of large scale instabilities, and the effects of magnetic ripple. A FLR correction accounts for FLR displacement from a guiding center to the actual particle position. The model also includes charge exchange loss and recapture of slowing down fast ions. The effects of target plasma rotation on fast particle deposition, slowing down, and beam–target fusion rates are considered. The module accounts for multiple fast ion species that can be present, either due to beam injection of energetic neutral particles or as a result of the product of nuclear fusion reactions. The self-consistent treatment of the fusion product ions allows for the simulation of alpha particle effects, which can be potentially important for ‘next-step’ tokamaks, such as ITER.

The NUBEAM module has been recently extracted from the TRANSP code, using the standards of National Transport Code Collaboration (NTCC), and is available in the NTCC module library [3].

3. Neutral Beam Injection module in the ASTRA code

For the calculation of the beam deposition profiles within the magnetically confined plasma, the ASTRA NBI module [4] uses a multiple pencil-beamlet method for an appropriate computation of the continuous power distribution within the real NBI beamlets. For the neutral beam stopping cross section in the range of the high energies $E = 100 \div 10000$ keV/amu, the approximation in Ref. [5] is used. This approximation takes into account multistep processes (excitation and ionization) in the multispecies plasmas that are expected in a fusion reactor with negative-ion-based NBI. For the range of energies $E < 100$ keV/amu, which is typical for present day experiments, conventional neutral beam stopping cross sections [6] by ion and electron impact and charge exchange are used. The fast ion orbit analysis and gyro motion averaging are considered only in the “first orbit” approximation. The orbital losses and the losses of fast ions due to magnetic ripple are associated exclusively with direct trapping of the original fast ions in the loss cone or “banana” ion in the ripple loss cone. Ions with original orbits trapped within the plasma are considered as trapped on the same magnetic surfaces during the whole slowing down process. There are two versions of FP solver in the ASTRA NBI module. The first one uses an analytical solution of the steady state linearized FP equation, which takes into account only the drag force. This solver is very fast and gives reasonable results for plasmas with cold ions and a small fast ion fraction. The other version is a linearized time dependent 2D in velocity space FP solver. This solver uses linearization by direct subtraction of the thermalized ions from the fast-ion component at every time step. Thermalized ions are further considered as the thermal ion source. Note that the ASTRA code does not consider ionization of neutrals that are produced by charge exchange of fast ions as a source of electrons and ions. The later version of the FP solver takes into account charge exchange losses of fast ions and finite orbit width effects in the “first orbit” approximation. The linearized time dependent 2D FP solver is supposed to be more accurate for plasma with high ion temperature and small fast ion fraction. In this study, the ASTRA code version 5.3 with the NBI ASTRA module release 2 (August 2003) is used.

4. Neutral Beam Injection DBEAMS module in the BALDUR code

The DBEAMS module in the BALDUR code is based on the revised FREYA package [7]. The module accounts for realistic beamline geometry, including the focal length of the beams and the fractional energy components. The DBEAMS module calculates the source distribution function of the neutral beam particles at the pivot point. The beams are represented as a combination of individual beamlets, which propagate along straight lines without divergence. The tokamak plasma is divided into a fixed number of zones, with plasma parameters considered to be constant within each zone. Impact ionizations by electrons, charge-exchange collisions, and ion impact ionization from thermal and beam–beam ion interactions are considered during the calculation of the source distribution function for fast ions. The Coulomb scattering and slowing down of fast ions are described by a FP equation with a collision operator that includes the drag by electrons and ions and pitch angle scattering. Some effects related to the NBI heating are not in the DBEAMS module, but are implemented in other parts of the BALDUR code. For example, the redistribution of fast particles due to sawtooth crashes is in the sawtooth section of the code.

5. FPP module in the TRANSP code

The FPP module [8] in the TRANSP code is a module that solves the FP equation to simulate the fast ions produced by NBI or ICRF heating. In TRANSP, for example, the code calls the deposition subroutines of NUBEAM to calculate the fast ion source to be provided to FPP. FPP then uses this beam deposition source distribution in the solution of the FP equation in the small banana width limit. The FPP module calculates the fast ion distribution function $f(E,\mu,r,t)$ as a function of energy E, pitch angle μ, minor radius r, and time t. FPP includes the bounce-averaged quasilinear RF heating operator and radial transport models, as well as the collisional thermalization operator. The module utilizes a conservatively-differenced operator-splitting technique to solve the FP equation. The module makes use of more simplified assumptions than the NUBEAM module. In particular, the recapturing of fast ions is modeled by reducing charge-exchange cross-section by 50%. Charge exchange with newly injected beam neutrals is ignored. FPP also ignores the possibility of particles that are trapped in the inner magnetic well caused by indented plasmas. These assumptions are sufficient for many cases and they provide significant gain in computational time compared with the NUBEAM module.

6. Neutral Beam Injection NBEAMS module

The NBEAMS module [9] is a relatively simple and fast neutral beam heating and current drive module that was originally developed at Georgia Tech for the SuperCode. The neutral beam deposition model employed by the module uses pencil-beamlet techniques and takes into account the elongation of the flux surfaces. Geometry of the injection system such as beam focal length, beam divergence, and beamline aperture is included through appropriate selection of the Gaussian power distribution functions. An analytical solution [10] of the FP equation in the approximation of the uniform field is used to describe the thermalization of fast ions. This approach neglects the beam current density due to energy diffusion of the fast ions and possible trapping of the fast ions. The resulting fast distribution function $f(\vec{r},\vec{v},t)$ is used to calculate neutral beam power deposition to thermal electrons and ions, neutral beam current drive, fast ion density and pressure, and fusion reaction rates for beam–target interactions, which contribute to the total fusion power as well as neutron production. The NBEAMS module is a part of the NTCC module library [3].

7. Comparison of the modules for Neutral Beam Injection

The following criteria are used during the comparison of the NBI modules:

- *Total power absorption by electrons and ions, and current drive*. Figs. 1 and 2 compare power and particle density sources computed with the NUBEAM, ASTRA, DBEAMS, and FPP codes for supershot TFTR discharge 66887 [11] and ELMy H-mode JET discharge 52009 [12], respectively. All four modules produce similar profiles.
- *Physics that is included or missing from the module*. A summary of the physics included in the NUBEAM, ASTRA, DBEAMS, FPP, and NBEAMS modules is given in Table 1.[1] The physics that is included in each module and the applicability of approximations and numerical techniques that are used within each module define whether or not that module can be used for present and future tokamak discharges. There are some limitations which are inherent to the approximations that are used by the modules. For example, solutions of linearized FP equation are not accurate for discharge with large fractions of beam particles. Some NBI modules can compute cross-sections only for energies below 200 keV/amu, which limits their applicability to modeling only positive-ion-based NBI.
- *Computational speed of the module*. Fig. 3 shows the CPU time distribution between different physical modules during the simulation of the JET discharge 52009 using either the NUBEAM or FPP modules in the TRANSP code. This TRANSP simulation of 13 s of discharge time on a single processor Intel Pentium IV 2 GHz computer running under Redhat Linux 7.2 operation system with FPP module took about 2 h of CPU time, compared with 7 h of CPU time when the NUBEAM module was used.[2] A simulation of

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[1] Note that the FPP module uses deposition sources from the NUBEAM module.

[2] Note that since the FPP module requires deposition sources computed within the NUBEAM module, and the interface between the FPP and the new NUBEAM modules is not completely established yet, a version of the TRANSP code from January 2001 was used for this comparison within a single transport code.

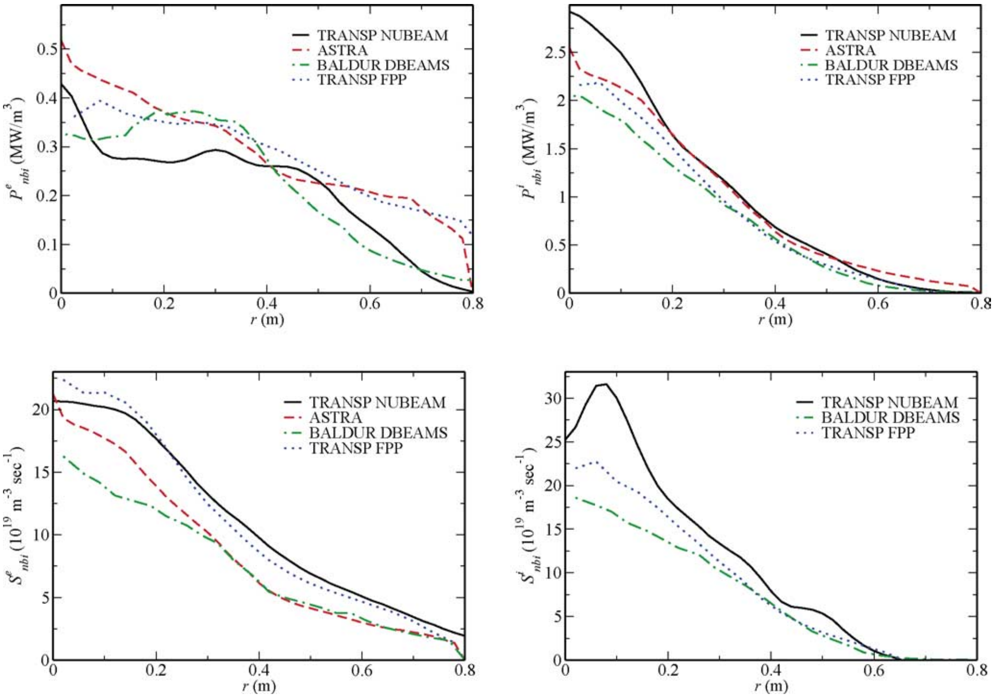

Fig. 1. NBI profiles of power and particle sources for the TFTR discharge 66887 at 3.9 s.

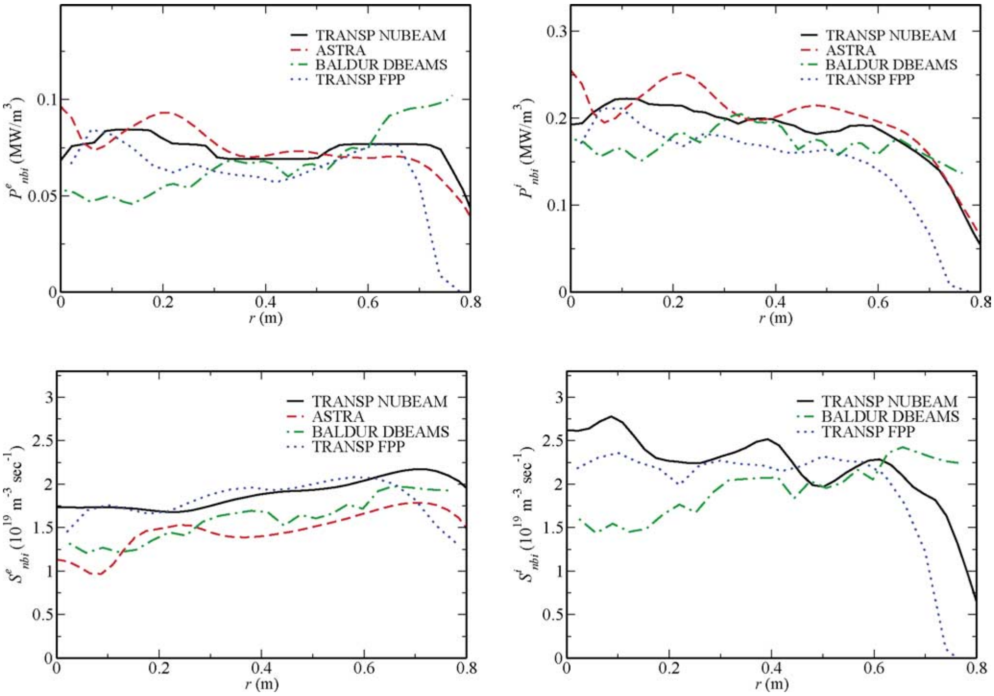

Fig. 2. NBI profiles of power and particle source for the JET discharge 52009 at 20 s.

Table 1
Physics included (+) or missing (−) in the NUBEAM, ASTRA NBI, DBEAMS, FPP, and NBEAMS modules

	NUBEAM	ASTRA	DBEAMS	FPP	NBEAMS
Beamline geometry	+	+	+	+	+
Beam composition	+	+	+	+	+
CX losses and recapture of fast ions	+	−	−	−	−
Losses of fast ions to the walls	+	+	+	+	+
Finite orbit width effects	+	−	−	−	−
Finite Larmor radius corrections	+	+	−	−	−
Effect of magnetic ripple	+	+	+	−	−
Effect of fishbone instabilities	+	−	−	+	−
Effect of sawtooth oscillations	+	−	+	+	−
Effect of plasma rotation	+	−	−	+	−
Heating rates	+	+	+	+	+
Momentum sources	+	+	−	+	−
Current source	+	+	+	+	+
Particle sources	+	+	+	+	+
Energy diffusion of fast ions	+	+	−	+	−
Anomalous diffusion of fast ions	+	−	+	+	−
ICRF resonant fast ions	−	−	−	+	−
Atomic reaction rates	+	+	+	+	+
Effect of excitation collisions	+	+	−	−	−
Beam stopping on beam ions	+	−	−	−	−
Multiple fast species supported	+	+	+	−	−
Fusion product ions	+	−	−	−	−
Beam–target fusion	+	+	+	+	+
Beam–beam fusion	+	−	−	−	−

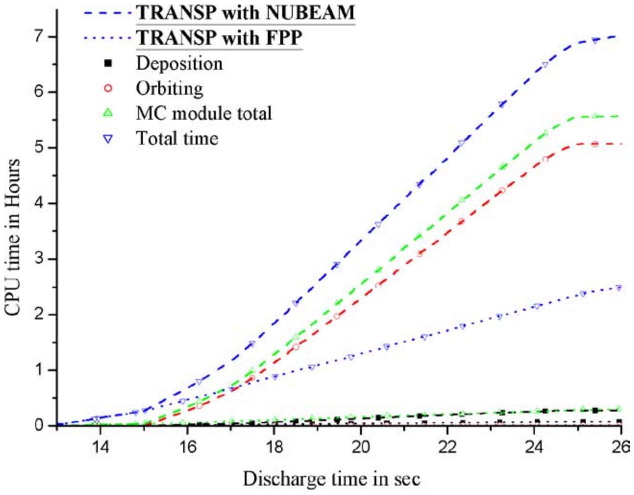

Fig. 3. CPU time distribution during simulation of the JET discharge 52009 with the NUBEAM and FPP NBI modules in the TRANSP code.

the NBI physics in the same JET discharge takes about 3 minutes of the CPU time when the NBI module is called every 250 ms in the ASTRA code.

– *Smoothness of the resulting power profiles and fast ion distributions; reproducibility of the resulting profiles*. These characteristics are important when MC algorithms are used for computing the NBI heating. For example, Fig. 4 shows several NB ion heating profiles computed with the NUBEAM module within the TRANSP code. Three profiles, N00, N01, and N02, are obtained

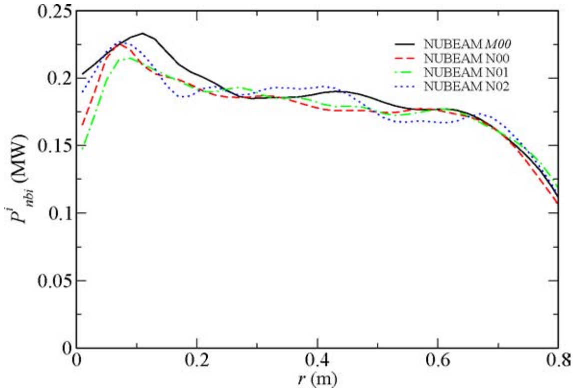

Fig. 4. Reproducibility of ion heating profiles for the JET discharge 52009 computed with the MC NUBEAM module in the TRANSP code.

with the same NUBEAM input. The average standard deviation is about 3% in these cases. The standard deviation is related exclusively with the characteristics of random number generator and number of MC particles used in each simulation. For the fourth profile M00, the number of MC particles is increased from default values used for the JET simulations. In particular, the number of MC particles per beam ion specie is increased from 5000 to 20000, number of MC particles per fusion product specie is increased from 100 to 500, and minimum number of deposition tracks per beam specie is increased from 500 to 1000.

References

[1] R.J. Goldston, et al., J. Comp. Phys. 43 (1981) 61.
[2] A. Pankin, D. McCune, R. Andre, G. Bateman, A. Kritz, Comput. Phys. Commun. 159 (2004) 157.
[3] NTCC module library, http://w3.pppl.gov/NTCC.
[4] S.E. Attenberger, W.A. Houlberg, S.P. Hirshman, J. Comp. Phys. 72 (1987) 435.
[5] R.K. Janev, C.D. Boley, D.E. Post, Nucl. Fusion 29 (1989) 2125.
[6] A.C. Riviere, Nucl. Fusion 11 (1971) 363;
R.E. Olson, A. Salop, Phys. Rev. A 16 (1977) 1811.
[7] C.G. Lister, D.E. Post, R. Goldston, in: Proc. 3rd Symp. on Plasma Heating in Toroidal Devices (Varenna, Italy – 1976), Euroatom, 1976, p. 303.
[8] G.W. Hammett, Fast ion studies of ion cyclotron heating in the PLT tokamak, Ph.D. Dissertation, Princeton, 1986.
[9] J. Mandrekas, Physics models and user's guide for the neutral beam module of the SuperCode, Tech. Rep. GTFR-102, Georgia Institute of Technology, 1992.
[10] J.D. Gaffey, J. Plasma Phys. 16 (1976) 149.
[11] R.V. Budny, Nucl. Fusion 34 (1994) 1247.
[12] G. Saibene, et al., Plasma Phys. Control. Fusion 44 (2002) 1769.