# Development of a Neoclassical Transport Database by Neural Network Fitting in LHD

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## Abstract

A database of neoclassical transport coefficients for the Large Helical Device is developed using normalized mono-energetic diffusion coefficients evaluated by Monte Carlo simulation code; DCOM. A neural network fitting method is applied to take energy convolutions with the given distribution function, e.g. Maxwellian. The database gives the diffusion coefficients as a function of the collision frequency, the radial electric field and the minor radius position.

#### Keywords:

LHD, neoclasiscal transport, neural network, Monte Carlo method

## 1. Introduction

Because of the radial drift motions of helical trapped particles, the neoclassical transport increases as the collision frequency decreases (1/v regime) in the long-mean-free-path (LMFP) regime in heliotrons. The neoclassical transport would play an important role as well as the anomalous transport in fusion plasma, where the confinement of high temperature plasma is required. Also, recent LHD experiment results suggest a key role of the neoclassical transport in the electron internal transport barrier [1] formation to determine radial electric field.

The estimate of the neoclassical transport coefficient is an important issue, and many studies have been done to evaluate the neoclassical transport coefficient analytically and numerically in helical systems. Among them the DKES (Drift Kinetic Equation Solver) code [2,3] has been commonly used for the experimental data analysis [4,5] and for theoretical predictions [6,7]. However, in the LMFP regime, a large number of Fourier modes must be used for the distribution function and a convergence problem can be seen.

Monte Carlo method is also used to evaluate the neoclassical transport coefficient, where the diffusion coefficients are estimated by the radial diffusion of test particles. This method does not have a convergence problem and is more applicable in the LMFP regime. Owing to above, we have developed the DCOM (Diffusion COeficient calculator by Monte carlo method) code [8].

The calculation of the mono-energetic diffusion coefficient using the Monte Carlo method, however, takes very long time. Since the neoclassical diffusion coefficient depends on the radial position, the radial electric field, and the collision frequency, it is difficult to calculate whenever those parameters change.

All the elements of the transport matrix can be obtained from the convolution of Maxwellian distribution function with three different mono-energetic coefficients [9];

$$D_j^k = \frac{4}{\sqrt{\pi}} \int D^k(v) \left(\frac{v}{v_{th}}\right)^{2j} \exp\left[-\left(\frac{v}{v_{th}}\right)^2\right] \frac{\mathrm{d}v}{v_{th}},$$
$$D^k(v) = D_p^k D^* (v^*, G) \left(\frac{v}{v_{th}}\right)^3,$$

where k = e, *i* (for electrons or ions) and j = 1, 2, 3 (related to the diffusion, the bootstrap current and parallel resistivity),  $D_P$  is the tokamak plateau value of mono-energetic case,  $D_P$  $= (\pi/16)(v^3/tR\omega_c^2)$ , *R* is the major magnetic radius, *v* is the velocity of test particles, *t* is the rotational transform normalized by  $2\pi$ ,  $\omega_c$  is cyclotron frequency of test particles,

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 $v^*$  is the collision frequency normalized by vt/R,  $v_{th}$  is the thermal velocity,  $D^*$  is the diffusion mono-energetic coefficient normalized by  $D_p$ , G is the normalized radial electric field,  $G = (R/tr)(E_r/vB)$ , which measures the effect of the poloidal rotation induced by the radial electric field to the poloidal rotation of circulating particles, r is the minor radial position,  $E_r$  is the radial electric field and B is the magnetic field strength. In order to calculate the transport coefficient for Maxwellian distribution, it is necessary to interpolate the mono-energetic diffusion coefficient calculated by DCOM code. A conventional fitting method assuming the common analytical relations depending on each collisionality regimes with their matching conditions, has been used so far. However, this technique can't describe accurately the overlapping of the each collisionality regimes.

Recently, the technique of neural networks (NNW) [10], that has strong nonlinear and has high fitting abilities have become a center of attraction. The NNW has their origins in studies of the brain, and has been the subject of active research since the mid 1940's. In the last few years in particular, the NNW has been used to solve a large range of practical problems in many areas of physics and engineering. It is appropriate to use the NNW for the interpolation of the diffusion coefficient in LHD.

In this paper, we show the neoclassical transport database for LHD using NNW fitting method. The evaluation of the mono-energetic diffusion coefficients by DCOM code is explained for the LHD standard configuration ( $R_{ax} = 3.75$  m) in Sec. 2. In Sec. 3, we have constructed the data base containing the normalized mono-energetic diffusion coefficients for several radial points, radial electric field and collisionalities by using the NNW.

# 2. Calculation of the monoenergetic coefficients by Monte Carlo method

The neoclassical transport coefficient has been evaluated using Monte Carlo technique directly following the particle orbits. We evaluate a mono-energetic local diffusion coefficient, D. In the simulation the N monoenergetic particles are released at an initial minor radial position,  $r_0$ , where the particles are randomly distributed in the poloidal, toroidal coordinates, and in the pitch angle space. The test particle orbits are followed solving the guiding-center equations in the Boozer coordinates with 50 Fourier modes of the magnetic field. The magnetic field in the Boozer coordinates is constructed from the magnetohydrodynamics (MHD) equilibrium obtained by the VMEC code. The pitch angle scatterings are taken into account in the Monte Carlo collision operator based on the binominal distribution [10]. The pitch angle scattering after the time interval  $\Delta t$  is given in terms of  $\lambda (= v_{\parallel}/v)$  by

$$\lambda_{n+1} = \lambda_n \left(1 - v\Delta t\right) + \sigma \left[ \left(1 - \lambda_n^2 \right) v\Delta t \right]^{\frac{1}{2}}$$

where  $\sigma$  takes +1 or -1 with equal probabilities, v is the deflection collision frequency. After several characteristic



Fig. 1 The monoenergetic diffusion coefficient,  $D^*$  vs the normalized collision frequency,  $v^*$  in standard LHD configuration,  $R_{ax} = 3.75$  m for different values of electric potential corresponding to G = 0,  $1 \times 10^{-3}$ ,  $3 \times 10^{-3}$ ,  $1 \times 10^{-2}$ ,  $3 \times 10^{-2}$ ,  $1 \times 10^{-1}$  and  $3 \times 10^{-1}$  (crosses, squares, circles, triangles, down triangles, diamonds and pentagons, respectively; closed signs are calculating by DCOM and opened signs are by DKES).

times,  $\tau$ , the diffusion coefficient can be evaluated by taking the mean square displacement of *N* particles as

$$D = \frac{1}{2N\tau} \sum_{i=1}^{N} \left( r_i - \left\langle r \right\rangle \right)^2,$$

where  $r_i$  stands for the radial position of *i*-th particle, and

$$\langle r \rangle = (1/N) \sum_{i=1}^{N} r_i.$$

In order to obtain mono-energetic diffusion coefficients, we have chosen N = 1000 with the energy of  $1.0 \times 10^{-3}$  eV. The magnetic field is set to be 3 T at the magnetic axis. The test particles are followed for several collisional times until the evaluated diffusion coefficient is converged.

In this work, we calculated the normalized monoenergetic diffusion coefficients; standard LHD configurations,  $R_{ax} = 3.75$  m, 5 radial positions normalized the minor radius,  $\rho = 0.1, 0.25, 0.5, 0.75, 0.9, 14$  normalized collisionalities,  $3.16 \times 10^{-2} < v^* < 1.00 \times 10^6$  and 7 electric fields, 0.00 < G < 0.03.

The calculation results obtained by DCOM code without  $E_r$  are shown by the diagonal cross sign in Fig. 1. The normalized diffusion coefficients  $D^*$  as a function of  $v^*$  at  $\rho = 0.5$  in the standard configuration are shown. Shown in Fig. 1 are also the DKES results (cross sign) and analytical results (dashed line). The results of DCOM and DKES agree well from Pfirsch-Schlüter (P-S) regime to 1/v regime for both configuration cases. The dashed lines represent analytical result of diffusion coefficient  $D_{ana}$  (=  $D_a + D_{1/v}$ ) which is the sum of non-axisymmetric contribution  $D_{1/v}$  given by a multihelicity model [11] and the axisymmetric contribution  $D_a$ 

given by

$$D_a = \left(D_{bp}^{3/2} + D_{PS}^{3/2}\right)^{2/3}$$

where

$$D_{bp} = D_b D_p / (D_b + D_p),$$
  

$$D_b = (B_{1,0}^{1/2} / \varepsilon_t^2) (v_d R / \omega_c t^2) v,$$
  

$$D_p = (2/5) (B_{1,0} / \varepsilon_t) (v_d v / \omega_c t)$$

and

$$D_{PS} = \left(7/5\right) \left(B_{1,0}/\varepsilon_{t}\right) \left(v_{d}R/\omega_{c}t^{2}\right) v,$$

where  $v_d = v^2/RB^2$  is the drift velocity of the test particles. As shown Fig. 1, the correct diffusion coefficient using analytical results in plateau regime can not be obtained.

Next, we considered the effect of the radial electric field,  $E_r$ . In Fig. 1, the diffusion coefficients at  $\rho = 0.5$  are shown for different amplitude of radial electric field. The open signs represent the computational results by DKES and the closed signs represent by DCOM. The strong reductions in the diffusion coefficients as the radial electric field strengthens are observed in the  $1/\nu$  regime.

# 3. Construction of the database of the diffusion coefficient using Neural Net Work

The diffusion coefficient of LHD has a strong nonlinearity and is a function of several parameters;  $v^*$ ,  $E_r$ ,  $\rho$ ,  $R_{ax}$ ,  $\beta$ , and etc. The NNW is suitable for the interpolation of the nonlinear function which depends on the several parameters. We consider the most widely used NNW, known as a multilayer perceptron (MLP), with only one hidden layer, MLP1 to construct the database of the neoclassical transport. The outputs of this network  $y_n(n = 1, 2, ...N)$  can be written as a function of its inputs  $x_m(m = 1, 2, ...M)$  through a set of coefficients, or weights,  $\{\omega_{hm}^1, b_{h}^1, \omega_{hm}^2, b_{n}^2\}(h = 1, 2, ...H)$ , as

$$y_n(x_1, x_2, ..., x_M) = f\left(\sum_{h=1}^H \omega_{hn}^2 f\left(\sum_{m=1}^M \omega_{hm}^1 x_m + b_n^1\right) + b_n^2\right)$$

with a sigmoid function  $f(x) \equiv \tanh(x)$ . In this work, the NNW was constructed as in Fig. 2. The inputs are  $v^*$ , G and  $\rho$  and the output is  $D^*$ . To equate the computational result of DCOM and output of the NNW, the weights  $\omega$  have been corrected. The BFGS (Broyden-Fletcher-Goldfarb-Shanno) method [12] of the quasi-Newton method was used for this minimum value search in this study.

The accuracy of the NNW depends on the number of the hidden unit. The error margin decreases as a number of the hidden unit increases. However, if the order of the hidden unit is increased too far, the phenomenon of the overfitting occurs which gives a very small error with respect to the training data, but which again gives a poor representation of



Fig. 2 Schematic view of the MLP1 neural network used in the calculations of the normalized *D*\*.



Fig. 3 A plot of the averaged relative error versus the number of the hidden unit.

the underlying trend in the data and which therefore gives poor predictions for a new data. Figure 3 shows a plot of the averaged relative error versus the order of the hidden units. The results in Fig. 3 decided a number of the hidden unit was 14.

We can obtain  $D^*$  by using the NNW for arbitrary  $v^*$ , G and  $\rho$ . The NNW results at  $\rho = 0.5$  for  $R_{ax} = 3.75$  m are shown in Fig. 4. The square symbols represent the computational results by DCOM with the training of the NNW and the solid lines represent the outputs from NNW. The NNW results agree well with DCOM results in each region of 1/v, plateau, and P-S, and smooth fitting is done in the joint of each region. The triangle symbols show the DCOM results without the training of NNW and the dashed lines show the results with NNW. It should be noted that the accuracy of the NNW interpolation with respect to the electric field is also good.

Figure 5(a) shows contour plot of  $D^*$ , obtained by the NNW, at  $\rho = 0.5$ . The horizontal axis indicates  $v^*$  and the vertical axis is G. We found that  $D^*$  does not depend on the electric field in P-S regime and  $D^*$  is improved in 1/v region

as the electric field strengthens. Figure. 5(b) shows the contour plot of  $D^*$  as a function of  $v^*$  (horizontal axis) and  $\rho$  (vertical axis). It is seen that the plateau regime has narrowed as the radial position goes toward outside of the plasma in each configuration.

## 4. Summary

We have constructed the database of the neoclassical transport in LHD. The mono-energetic neoclassical diffusion coefficients are evaluated numerically using Monte Carlo technique. We have used a Monte Carlo simulation code, DCOM, in which the neoclassical diffusion coefficients are estimated by the radial diffusion of test particles in Boozer co-ordinates.

In order to take the convolution of mono-energetic coefficients,  $D^*$ , with a Maxwellian energy distribution it is



Fig. 4 The normalized diffusion coefficient  $D^*$  vs the normalized collision frequency  $v^*$  at  $\rho = 0.5$ . The square symbols represent the results by DCOM with the training of the NNW and the solid lines represent the outputs from NNW. The triangle symbols represent the DCOM results without the training of NNW and the dashed lines represent the results with NNW.

necessary to interpolate the values of  $D^*$  as a function of the collision frequency, the radial electric field, the minor radius and etc. The neural network (NNW) is applied to fit the diffusion coefficient of LHD, which shows complex behavior in the several collisional regimes; i.e. v,  $\sqrt{v}$ , 1/v, plateau, and P-S regimes. A multilayer perceptron NNW with only one hidden layer, usually known as MLP1, was used. Input parameters are  $\rho$ ,  $v^*$  and G, and  $D^*$  can be obtained as an output of the NNW.

A single set of  $D^*$  database can be applicable to the evaluation of the transport coefficients of one configuration in any density and temperature parameter plasma. Also, the NNW database can evaluate the mono-energetic diffusion coefficient in a very short time and we can evaluate the neoclassical transport including the ambipolar radial electric field in a minute using a present PC. On the other hand, the configuration changes significantly in a finite beta plasma of LHD and, thus, the construction of  $D^*$  database in the finite beta is necessary for accurate evaluation of neoclassical transport. The database construction in a finite beta is in progress.

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Fig. 5 The normalized monoenergetic coefficients,  $D^*$  as a function  $D^*(v^*, \rho, G)$ . (a)  $\rho$  is constant ( $\rho = 0.5$ ) and (b) G is constant (G = 0.0).