ICNTS - Impact of Incompressible $\mathbf{E} \times \mathbf{B}$ Flow in Estimating Mono-Energetic Transport Coefficients

Craig D. BEIDLER[1)], Maxim Yu. ISAEV[1)], Sergei V. KASILOV[3,4)], Winfried KERNBICHLER[3)], Henning MAAßBERG[1)], Sadayoshi MURAKAMI[5)], Victor V. NEMOV[3,4)], Don A. SPONG[6)] and Victor TRIBALDOS[7)]

[1)] *Max-Planck Institut für Plasmaphysik, Assoc. EURATOM, Greifswald, Germany*
[2)] *Russian Research Center "Kurchatov Institute", Moscow, Russia*
[3)] *Institut für Theoretische Physik, Assoc. EURATOM-ÖAW, TU-Graz, Austria*
[4)] *Institute of Plasma Physics, NSC-KhIPT, Kharkov, Ukraine*
[5)] *Department of Nuclear Engineering, Kyoto University, Kyoto, Japan*
[6)] *Oak Ridge National Laboratory, U.S. Department of Energy, USA*
[7)] *Laboratorio Nacional de Fusion, CIEMAT, Assoc. EURATOM-CIEMAT, Madrid, Spain*

October 2, 2007

In the neoclassical ordering, an incompressible $\mathbf{E} \times \mathbf{B}$ drift is assumed in the 1^{st} order drift-kinetic equation (i.e. the approximation $\mathbf{E} \times \mathbf{B}/\langle B^2 \rangle$ is used). Then, the terms with $(\mathbf{E} \times \mathbf{B}) \cdot \nabla B$ disappear in both equations for $\dot{p}$ and $\dot{v}$ allowing for a monoenergetic treatment (with a conservative formulation of the equations of motions), as it is used e.g. in DKES. As a consequence, the magnetic moment is not an invariant in this approximation. For large radial electric fields, however, this ordering scheme is violated since the $(\mathbf{E} \times \mathbf{B}) \cdot \nabla B$ term in $\dot{p}$ becomes comparable with the mirror term ($\propto \mathbf{B} \cdot \nabla B$). The impact of this simplification is tested by strictly local δ-f Monte Carlo techniques (i.e. with $\dot{r} = 0$ for the equation of motion in 1^{st} order) where the $\mathbf{E} \times \mathbf{B}$ drift is treated in compressible and incompressible form (both completely conservative) for large radial electric fields.

1 Introduction

There is a subtle inconsistency in the way the effect of large radial electric fields are handled in obtaining neoclassical estimations of transport coefficients. Rather than being a limitation of the theory itself, the complication arises from some simplifying approximations used. The electric field enters the calculation through the $\mathbf{E} \times \mathbf{B}$ drift, $\mathbf{V}_E = \mathbf{E} \times \mathbf{B}/B^2$, and the *small gyroradius ordering* or *drift ordering* assumes that the ratio of this drift to the thermal speed of particles is of 1^{st} order, i.e. $V_E/v_{th} \sim \rho/L \sim \omega_{th}/\Omega = \delta << 1$, where ρ is the thermal gyroradius, L a characteristic plasma scale length and ω_{th} and Ω the transit frequency and gyrofrequency respectively. This approximation implies that the radial electric field is not so large as to distort gyration and varies slowly in time. The drift ordering is not very stringent, and is easily fulfilled even at the low-order electric field resonances (where the poloidal component of the drift speed vanishes) $E^{res} = \iota v B r/R$ since $V_{E^{res}}/v_{th} = \iota r/R$, where r/R is the inverse aspect ratio of the considered flux surface and ι its rotational transform.

In the drift ordering approximation particle motion is averaged over the the small gyro-scale and the resulting kinetic equation, now describing the distribution of guiding centers, is known as the *drift kinetic equation* (DKE) [1, 2]. Unfortunately, even with the drift ordering approximation solving the DKE is a daunting task. The inhomogeneity of the magnetic field along with the non-linearity of the collisional term makes the DKE a non-linear partial differential equation in a six dimensional space $f = f(\mathbf{r}, v, p, t)$, $\mathbf{r}$ being the guiding center position in 3D space, v and $p = \mathbf{v}\cdot\mathbf{B}/v$ its speed and pitch angle in velocity-space, and t the time. The central point of neoclassical theory is solving this equation to obtain different flux-surface-averaged moments of its solution. To this end the distribution of guiding centers is linearized around a local Maxwellian distribution and several approximations are made in the drift motion of guiding centers. In the drift ordering approximation, the total energy conservation, $E = mv^2/2 + q\Phi$ with $\mathbf{E} = -\nabla\Phi$, translates into an equation for the variation of the kinetic energy which is proportional to the divergence of the $\mathbf{E}\times\mathbf{B}$ drift, $\dot{v} = v(1 + p^2)/4\, \nabla \cdot \mathbf{V}_E$ (notice that drift ordering precludes rapid variation of the magnetic and electric fields. Whenever the $\mathbf{E}\times\mathbf{B}$ drift is incompressible, $\nabla\cdot\mathbf{V}_E = 0$, the total energy and the kinetic energy are conserved, which allows for quite some simplification in solving the DKE. Not only the speed of particles can be considered as a parameter, allowing for a mono-energetic treatment, but also the collision operator can be approximated by only its pitch angle scattering part. However, a direct calculation shows that $\nabla \cdot \mathbf{V}_E = -2V_E \nabla \ln B$ which in general is different from zero, thus to retain the benefits of incompressibility usually the exact drift $\mathbf{V}_E = \mathbf{E} \times \mathbf{B}/B^2$ is approximated by $\mathbf{V}_E = \mathbf{E} \times \mathbf{B}/\langle \mathbf{B}^2 \rangle$. Since the magnetic field gradient is de-

author's e-mail: V.Tribaldos@ciemat.es

termined by the device's configuration the incompressible approximation restricts the usual neoclassical treatment to *small* radial electric fields.

The purpose of this work is to shed some light on the effect of the incompressible $\mathbf{E}\times\mathbf{B}$ flow for a wide range of radial electric fields and its impact on the determination of the mono-energetic particle diffusion coefficient, D^*. In Sec. 2 the basic equations of motion are discussed and a local δf Monte Carlo [3, 4] (MC) technique capable of dealing with compressible and incompressible flows (both completely conservative) is presented. Results of the comparison between the DKES (Drift Kinetic Equation Solver) [5, 6] and the new δf MC codes for different configurations will be shown is Sec. 3. Finally, Sec. 4 contains some discussion of the results.

2 Basics

The starting point of neoclassical transport theory is the DKE, that can be formally written as [2]

$$\frac{df}{dt} = \dot{\mathbf{r}}_D \cdot \nabla f + \dot{p}\frac{\partial f}{\partial p} + \dot{v}\frac{\partial f}{\partial v} = C(f,f) \tag{1}$$

where $\dot{\mathbf{r}}_D = \mathbf{v}_D$, $\dot{p}$ and $\dot{v}$ are the drift speed and the time derivatives of the pitch (related to the conservation of the magnetic moment $\mu = mv_\perp^2/2B$) and the kinetic energy (derived from the conservation of the total energy $E = mv^2/2 + q\Phi$) given by:

$$\mathbf{v}_D = pv\frac{\mathbf{B}}{B} + \mathbf{V}_E + \frac{mv^2}{2qB^3}(1+p^2)\,\mathbf{B}\times\nabla B \tag{2}$$

$$\dot{p} = -\frac{v}{2B^2}(1-p^2)\,\mathbf{B}\cdot\nabla B - \frac{p}{2B}(1-p^2)\,\mathbf{V}_E\cdot\nabla B \tag{3}$$

$$\dot{v} = -\frac{v}{2B}(1+p^2)\,\mathbf{V}_E\cdot\nabla B \tag{4}$$

and $C(f,f)$ is a collision operator.

Since $\mathbf{V}_E\cdot\nabla B = -B/2\,\nabla\cdot\mathbf{V}_E$ the second term in the r.h.s. in Eq.3 and Eq.4 depend explicitly on the compressibility of the $\mathbf{E}\times\mathbf{B}$ flow. The procedure used to solve the DKE consists of linearising the distribution of guiding centers, f, in Eq. 1 with respect to the drift ordering small parameter $\delta = \rho/L << 1$ as $f = f_0 - \delta f_1(\partial f_0/\partial r_r)$. For stationary conditions, i.e. neglecting the explicit time dependence, $\partial f/\partial t$, the solution to the zero order, δ^0, equation is identically satisfied by the local Maxwellian $f_0 = f_M$. Therefore, the goal is to find the solution, f_1, to the first order DKE:

$$\mathbf{v}_D^s\cdot\nabla_{\mathbf{r}_s} f_1 + \dot{p}\,\frac{\partial f_1}{\partial p} + \dot{v}\,\frac{\partial f_1}{\partial v} - C(f_M, f_1) = v_D^r \tag{5}$$

Notice that the full first order distribution depends on the radial gradients of the zero order Maxwellian distribution, and that the inhomogeneous term is the radial drift of guiding centers v_D^r, thus the radial dependence enters the equation just like a parameter. Therefore, Eq. 5 describes a diffusion process in phase space rather than in real space. Different methods are usually applied to solve the Eq. 5, each with its strengths and drawbacks: i) analytical calculations [1]; ii) explicit spectral procedures, expanding f_1 in a base of eigenfunctions (like the DKES code [5, 6]) and iii) Monte Carlo techniques [7]. Analytical solutions are usually restricted to simplified magnetic fields and collisionality regimes, on the other hand explicit and MC numerical methods can deal with realistic configurations for broad collisionality ranges, but are extremely time consuming and sometimes not very accurate (e.g. non diagonal transport matrix elements in MC.

The usual approximation, as for example is done in DKES code, for computing the diffusion transport coefficients consists in neglecting $\nabla\cdot\mathbf{V}_E$ in equations 3 and 4, i.e. considering the $\mathbf{E}\times\mathbf{B}$ flow incompressible. Since $\dot{v} = 0$, the energy in Eq. 5 enters only as a parameter, once the collision operator is approximated by just its pitch-angle scattering part, and the coefficients are obtained by the convolution of mono-energetic solutions with the Maxwellian distribution. The price to pay in this approximation is that the radial electric field cannot be very large, and that the magnetic moment μ is not conserved (see Eq. 3). To check the approximation made by DKES for the mono-energetic diffusion coefficient for large radial electric fields it would be desirable to benchmark it against a MC type calculation with and without assuming $\nabla\cdot\mathbf{V}_E = 0$. In usual *full* f [7] MC calculations, based on fitting the slope of the time dependence of the radial broadening of a test particle ensemble (diffusion in real space), it is easy to include the full set of equations (conserving μ and E. However, when the radial electric field becomes *large* particles can win or lose kinetic energy as they move radially because of their drifts, thus making the calculation non-mono-energetic. The method proposed here to make such comparison is using the method of characteristic to solve partial differential equations like Eq. 5, which is at the base of the δf MC technique.

Formally, the solution to an equation of the type $a(x,y,...)\partial f/\partial x + b(x,y,...)\partial f/\partial y + ... = g(x,y,...,f)$ is a surface S such that at each point $(x,y,...)$ on S, the vector $\mathbf{V} = (a(x,y,..), b(x,y,...),...,g(x,y,..,f))$ lies in the tangent plane. Such surface can be constructed by the union of curves C parametrized by s such that at each point on the curve, the vector $\mathbf{V}$ is tangent to the curve. In particular $C = \{(x(s), y(s),...,g(s))\}$ will satisfy the following system of ordinary differential equations:$dx/ds = a(x,y,...); dy/ds = b(x,y,...); ...; du/ds = g(x,y,...,f)$, called characteristic curves, and the solution is $f(x,y,...) = u(x,y,...)$. Rephrasing this method for the collisionless DKE means solving the system of equations:

$$\frac{d\mathbf{r}_D^s}{dt} = \mathbf{v}_D^s\,; \quad \frac{dp}{dt} = \dot{p}\,; \quad \frac{dv}{dt} = \dot{v}\,; \quad \frac{du}{dt} = v_D^r \tag{6}$$

$f_1 = u$ being its solution. Please notice that even though the system of equations 6 are the equations of motion of the guiding center, and the characteristic curves are the trajectories, thus clarifying the link with a MC particle simulation view, there is no equation for the radial drift r^r_D. Particles cannot escape the birth flux surface and no radial broadening calculation can be done. However, the solution $f_1 = u \sim \int v^r_D dt$ directly depends on the bounce-average of the radial drift speed along the parallel motion. The MC implementation is straightforward; the system of equations is integrated (taking care to retain the conservative nature of the motion) for an ensemble of markers (since no radial motion is included they cannot be regarded as particles anymore), all sharing the same energy and flux surface but with random toroidal and poloidal position and pitch. The effect of collisions in the DKE is simulated by applying a pitch angle collision operator [7].

3 Results

Three different magnetic configurations were studied with quite different B structures, namely: a tokamak with the same aspect ratio and rotational transform as the W7-AS stellarator, the LHD heliotron configuration with major radius $R_{axis} = 3.75$ m, and the W7-X standard configuration. The impact of the incompressibility of the $\mathbf{E} \times \mathbf{B}$ flow was studied by evaluating the diffusion coefficient for a wide range of radial electric fields. For each case two different collisionalities were chosen corresponding to the beginning of the ripple regime, $\nu/v = 10^{-3}\mathrm{m}^{-1}$, and one at the beginning of the *lmfp*, $\nu/v = 10^{-4}\mathrm{m}^{-1}$. The δf MC integrates 1024 markers for three collisional times divided in eight groups of 128 markers each. The error bar is obtained with the standard error from the eight estimations.

As was noted long ago, e.g. [8] Eq. 5 has a singularity when the poloidal component of the drift speed vanishes, which corresponds to resonant radial electric field values. In the following the radial electric field has been normalized to the first toroidal resonance $E_{res} = \iota v B r/R$.

In Fig. 1 the diffusion coefficient at half radius, $r/a = 0.5$, for an ideal tokamak configuration, with $B(r,\theta) = B_0(1 + r/R\cos\theta)$, $R = 2$m, $a = 0.2$m, and $\iota = 0.51$. This was selected because radial excursions from the flux surfaces are small and only one electric field resonance exists. There is a good agreement between DKES code results and the δf MC incompressible calculation; both displaying a peaked feature around the resonance followed by a strong decrease because of the disappearance of *banana* orbits. When compressible effects are included in the calculation the resonance is smoothed as well as the later sharp diffusion decrease flattened. The reason being the variation in the kinetic energy of the particles, $\dot{v}$ in Eq. 4, as can be seen in Fig. 2. The broadening of the kinetic energy spectra, due to $\dot{v}$, reduces the number of particles at the resonant field, $E_r/E_{res} = 1$ but also pushes some particles to energies that resonate at larger values of E_r/E_{res}. At very large radial electric fields there is a systematic difference between the DKES and MC results which is attributed to numerical diffusion. Nevertheless, please notice the rather small values of the diffusion coefficient

The results for the other two devices (see Figs. 3 and 4) are similar to the tokamak result, apart from the different resonance structure due to their broader magnetic field spectra. The helical resonance peak at $E_{res} = (N_{periods} - m\iota)vBr/R$ can be clearly identified. As in the tokamak case the flattening is more pronounced at smaller collisionalities, pitch angle scattering is less efficient in moving particles out of the resonance. The incompressible approach is rather good for small E_r, but unexpectedly it is also working at large radial electric fields, provided that there is no resonance overlapping; see the almost mono-energetic structure of the PDF in Fig. 2 at $E_r/E_{res} = 4$. Finally, there is an inconsistency in comparing the mono-energetic diffusion coefficients of the DKES and incompressible δf codes with the compressible result since the latter, as has been shown, is not really mono-energetic. Moreover, considering only the pitch-angle part of the collision operator close to the resonance is not justified [8, 7].

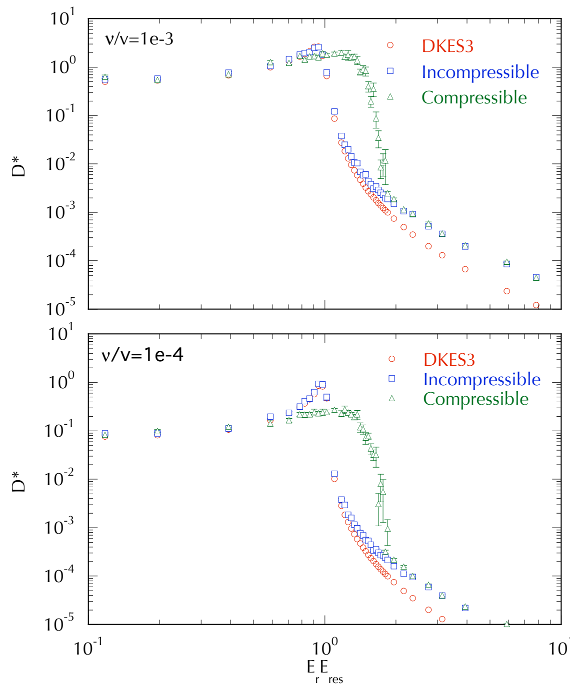

Fig. 1 Diffusion coefficient for the tokamak configuration for $\nu/v = 10^{-3}\mathrm{m}^{-1}$ (top) and $\nu/v = 10^{-4}\mathrm{m}^{-1}$ (bottom) obtained with the DKES code (circles) and the δf MC incompressible (squares) and compressible (triangles) approaches.

4 Discussion

The aim of this work was to check the accuracy of local mono-energetic transport coefficient calculations for large radial electric fields. On the one hand DKES estimations

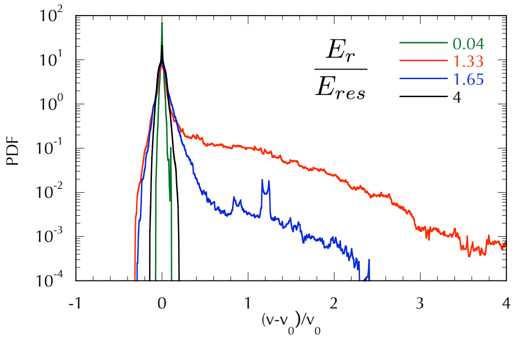

Fig. 2 Probability distribution function of velocities for several values of E_r/E_{res} and $\nu/v = 10^{-3}\mathrm{m}^{-1}$ of Fig. 1 in the compressible approach.

are mono-energetic and local and transport is due to a pitch-angle diffusion process in phase space. But, the $\mathbf{E}\times\mathbf{B}$ term is treated as incompressible, $\nabla \cdot \mathbf{V}_E = 0$, to keep the kinetic energy constant. On the other hand, common full-f MC based calculations are not exactly local, because radial space broadening is used to describe the diffusion process. And, again their applicability is limited to consider small radial electric fields to keep particles' kinetic energy almost constant during their radial drifts. Here, a fully conservative δf MC code was introduced where local diffusion is computed in phase-space with particles (*markers*) remaining indefinitely on their birth flux surface (solving a general MC problem with particle losses).

The impact of the incompressible $\mathbf{E}\times\mathbf{B}$ flow approximation was tested comparing DKES results with the strictly local δf MC where the $\mathbf{E}\times\mathbf{B}$ drift is treated in compressible and incompressible form for large radial electric fields and several magnetic field configurations.

It was found that considering $\nabla \cdot \mathbf{V}_E = 0$ is indeed a good approximation for small radial electric fields, as expected, but also for large E_r far from the resonances. This also serves as a benchmark between DKES and the δf MC. The discrepancy between the results with and without $\nabla \cdot \mathbf{V}_E = 0$ close to the resonance is due to the variation of the kinetic energy. This results calls into question the *usual* mono-energetic calculations, which, to be safe, should be restricted to $E_r < 0.5 - 0.7\, E_{res}$.

[1] A.A. Galeev and R.Z. Sagdeev, Sov. Phys. JETP **26**, 233 (1968).
[2] R.D. Hazeltine, Phys. Fluids **15**, 77 (1973).
[3] M. Sasinowsky and A. Boozer, Phys. Plasmas **2**, 610 (1995).
[4] A.M. Dimits and W.W. Lee, J. Comput. Phys. **107**, 309 (1993).
[5] S.P. Hirshman *et al.*, Phys. Fluids **29**, 2951 (1986).
[6] W.I. van Rij and S.P. Hirshman, Phys. Fluids B **1**, 563 (1989).
[7] A. Boozer and G. Kuo Petravic, Phys. Fluids **24**, 851 (1981).
[8] E.F. Jaeger, C.L. Hedrik and D.A. Spong, Nuc. Fusion **19** Vol. 12, 1627 (1979).

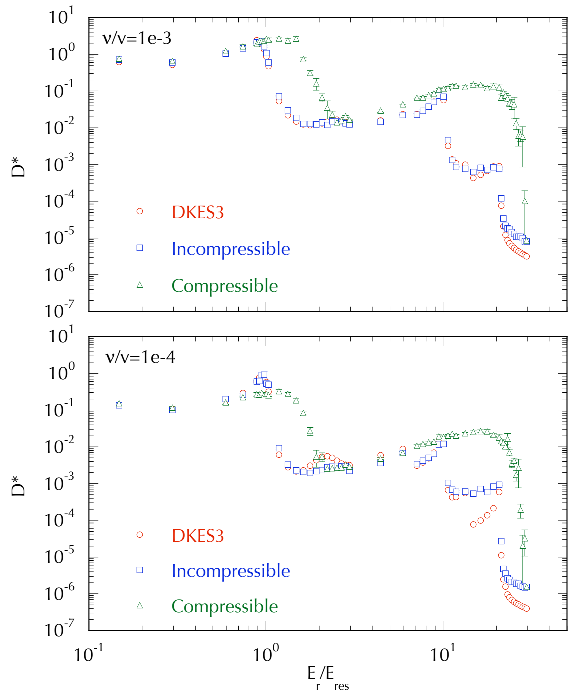

Fig. 3 Diffusion coefficient for the LHD configuration with $R_{axis} = 3.75$m for $\nu/v = 10^{-3}\mathrm{m}^{-1}$ (top) and $\nu/v = 10^{-4}\mathrm{m}^{-1}$ (bottom) obtained with the DKES code (circles) and the δf MC incompressible (squares) and compressible (triangles) approaches.

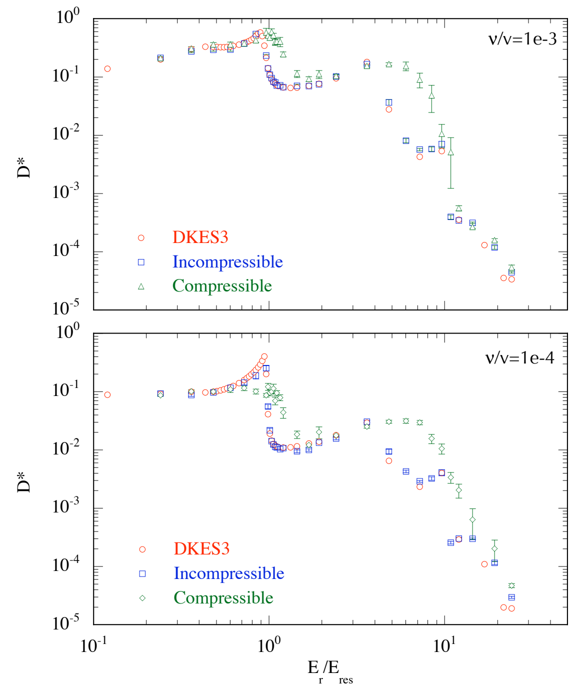

Fig. 4 Diffusion coefficient for the W7-X standard configuration for $\nu/v = 10^{-3}\mathrm{m}^{-1}$ (top) and $\nu/v = 10^{-4}\mathrm{m}^{-1}$ (bottom) obtained with the DKES code (circles) and the δf MC incompressible (squares) and compressible (triangles) approaches.