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# A New Calculation Method for Neoclassical Flow and Transport of Impurities in Heliotron/Torsatron and Quasi-symmetric Configurations

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## Abstract

In this paper, we present a new neoclassical transport calculation method for general toroidal plasmas including quasi-symmetric configurations based on the moment approach with the DKES (Drift Kinetic Equation Solver) mono-energetic transport coefficients. The Onsager symmetric matrix, expressing parallel viscosity and the radial transports in terms of parallel flows and thermodynamic forces, is obtained from the numerical calculating results of the drift kinetic equation with the pitch angle scattering operator. And then, the radial transports and parallel flows are derived by combining this matrix, the friction-flow relation and the parallel momentum balance equations. To demonstrate the validity and the effectiveness of this method in which the momentum conservation is completely included and the treatment of multi-ion-species plasmas is easier, we present here how the intrinsic ambipolarity and the impurity accumulation in an axisymmetric limit, which are predicted by analytic theories, are obtained in this numerical calculation.

## Keywords:

neoclassical transport, non-symmetric configuration, quasi-symmetry, drift kinetics, moment approach, neoclassical ambipolarity condition, impurity transport

## 1. Introduction

In theoretical studies of the neoclassical transport in non-symmetric configurations, several numerical calculation methods based on Monte Carlo methods and/ or drift kinetic equations are developed to treat the complex magnetic field structures [1-6]. Many of these methods use the pitch angle scattering collision operator that does not satisfy the momentum conservation of binary Coulomb collisions, since the motivation of these methods is to treat the ripple induced non-ambipolar transport in low-collision-frequency regimes in conventional helical configurations where the strict treatment of the friction forces is not required.

However, in recently proposed quasi-symmetric configurations [7-8], in which the ripple induced non-ambipolar transport is strongly reduced and becomes comparable to or smaller than the banana-plateau transport, the strict treatment of the momentum conservation is indispensable. Even in conventional helical devices such as heliotron/torsatron type tori LHD (Large Helical Device) [9] and CHS (Compact Helical System) [10], the collisionality of impurity ions with high-Z values still corresponds to plateau and/or Pfirsch-Schlueter regimes and thus the neoclassical transport calculation including the behavior of the impurities should satisfy the momentum conservation. This problem is also important in the interpretation of the

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experimental results related to plasma flows and radial electric fields measured with the spectroscopic measurements of impurity ions [11]. Although some numerical calculation methods using collision operators conserving the momentum are proposed [12] and are applied to axisymmetric and quasi-symmetric tori [12,13], the treatment of multi-ion-species plasmas in these methods seems to be not so easy because of the increasing computation time.

Recently, we are developing a new neoclassical transport calculation method [14] based on the moment approach [15] with DKES (Drift Kinetic Equation Solver) [5-6] mono-energetic transport coefficients. In this paper, we present some examples of the calculation results in an imaginary axisymmetric limit in the quasi-axisymmetric stellarator CHS-qa [16] to demonstrate the validity and the effectiveness of this method.

## 2. Outline of the Theory

The DKES code [5,6] is one of the numerical calculation codes developed for the low-collision-frequency regimes of non-symmetric configurations based on a linearized drift kinetic equation with the pitch angle scattering (or Lorentz) collision operator [1-6]. This code calculates the mono-energetic transport coefficients $D_{11}$ (radial transports), $D_{13}$ (bootstrap flow and Ware pinch) and $D_{33}$ (parallel viscosity) at a specified magnetic flux surface (labeled by the normalize minor radius $\rho$ =constant) and at a specified test particle velocity $|\mathbf{v}|$. The energy integrated transport coefficients $L_{ij}$ given by the integration of these mono-energetic results with the Maxwellian distribution function are the elements of the $3 \times 3$ Onsager matrix determining the thermodynamic fluxes $\Gamma_a$, $Q_a$ and $\mathbf{u}_a \cdot \mathbf{B}$ of each particle species $a$ independently from the thermodynamic forces $n_a' \equiv \partial n_a/\partial\rho$, $T_a' \equiv \partial T_a/\partial\rho$, $e_a\phi' \equiv e_a\partial\phi/\partial\rho$ and $e_a\mathbf{E}\cdot\mathbf{B}$ of the particle species, where the notation in refs. [5-6] has been followed. This simplified procedure provides the convenience in calculating the ripple induced non-ambipolar transport in the low-collision-frequency regimes of non-symmetric configurations. However, we should note that the origin of the pitch angle scattering operator is the test particle portion $C_{ab}(f_{a1}, f_{bM})$ of the linearized Fokker-Planck collision operator [17] $C^L{}_a(f_{a1}) = \Sigma_b\, [C_{ab}(f_{a1}, f_{bM}) + C_{ab}(f_{aM}, f_{b1})]$, where $f_{aM}$ and $f_{bM}$ are the Maxwellian distribution functions of test particle species $a$ and field particle species $b$, respectively, and $f_{a1}$ and $f_{b1}$ are the deviations from the Maxwellian for each species. Neglecting the field particle portion $C_{ab}(f_{aM}, f_{b1})$ breaks the momentum conservation law $\Sigma_a\mathbf{F}_a = 0$ for the friction force $\mathbf{F}_a \equiv \int d^3\mathbf{v}\, m_a\mathbf{v}\, C^L{}_a(f_{a1})$ which has an important role in calculating the banana-plateau transport, the Pfirsch-Schlueter transport, and impurity behaviors such as the impurity accumulation.

To extend the application of this kind of numerical calculation codes to the symmetric limit and the high collisionality limit where the particle diffusion is intrinsically ambipolar [15], a new interpretation of the mono-energetic transport coefficients and a procedure to determine the friction force via the momentum conservation law are required. The basic idea of our theory [14] to interpret the mono-energetic transport coefficients is to separate the test particle velocity distribution function $f_{a1}$ into two parts; the $l = 1$ Legendre component $f_{a1}{}^{(l=1)}$ associated with the parallel flows and the remaining part $g_a \equiv f_{a1} - f_{a1}{}^{(l=1)}$ associated with the viscosity effects. Since the use of the pitch angle scattering operator in treating $g_a$ is better approximation than that in treating $f_{a1}$ from the point of view of the momentum conservation, so the numerical calculation results of the drift kinetic equation with the pitch angle scattering operator can be used to express the viscosity effects. Then the parallel particle and heat flows in the $f_{a1}{}^{(l=1)}$ can be determined by solving the parallel force balance equations with the viscosity term given by the drift kinetics. This idea is basically identical to that in so-called moment approach developed for tokamaks [15] and the relatively collisional regimes of non-symmetric configurations [18-21]. The advantage of our new method is that it has following features together; (1) the accurate treatments of 3-dimensional complex magnetic field structures, (2) the momentum conservation, (3) easiness in expanding to multi-ion-species problem.

In this theory, the parallel viscosity $\langle\mathbf{B}\cdot\nabla\cdot\pi_a\rangle$, $\langle\mathbf{B}\cdot\nabla\cdot\Theta_a\rangle$ and the non-ambipolar and banana-plateau components of radial particle and heat fluxes $\Gamma_a^{bn}$, $q_a^{bn}$ [21] are expressed in terms of the parallel particle and heat flows $\langle u_{//a}B\rangle$, $\langle q_{//a}B\rangle$ and the thermodynamic forces $X_{a1} \equiv -(1/n_a)p_a' - e_a\phi'$, $X_{a2} \equiv -T_a'$ as,

$$\begin{bmatrix} \langle\mathbf{B}\cdot\nabla\cdot\pi_a\rangle \\ \langle\mathbf{B}\cdot\nabla\cdot\Theta_a\rangle \\ \Gamma_a^{bn} \\ q_a^{bn}/T_a \end{bmatrix} = \begin{bmatrix} M_{a1} & M_{a2} & N_{a1} & N_{a2} \\ M_{a2} & M_{a3} & N_{a2} & N_{a3} \\ N_{a1} & N_{a2} & L_{a1} & L_{a2} \\ N_{a2} & N_{a3} & L_{a2} & L_{a3} \end{bmatrix} \begin{bmatrix} \langle u_{//a}B\rangle/\langle B^2\rangle \\ \dfrac{2}{5p_a}\langle q_{//a}B\rangle/\langle B^2\rangle \\ X_{a1} \\ X_{a2} \end{bmatrix} \quad (1)$$

where the all of matrix elements $M_{aj}$, $N_{aj}$, $L_{aj}$ are obtained from the mono-energetic transport coefficients

$D_{11}$, $D_{13}$, $D_{33}$ given by DKES code as follows ($K \equiv m_a v_a^2/2T_a$).

$$\begin{bmatrix} M_{a1} M_{a2} \\ M_{a2} M_{a3} \end{bmatrix} \equiv {}^t\mathrm{T} \begin{bmatrix} M_{a1}^{\ t} M_{a2}^{\ t} \\ M_{a2}^{\ t} M_{a3}^{\ t} \end{bmatrix} \mathrm{T} \quad \begin{bmatrix} N_{a1} N_{a2} \\ N_{a2} N_{a3} \end{bmatrix} \equiv {}^t\mathrm{T} \begin{bmatrix} N_{a1}^{\ t} N_{a2}^{\ t} \\ N_{a2}^{\ t} N_{a3}^{\ t} \end{bmatrix} \mathrm{T}$$
$$\begin{bmatrix} L_{a1} L_{a2} \\ L_{a2} L_{a3} \end{bmatrix} \equiv {}^t\mathrm{T} \begin{bmatrix} L_{a1}^{\ t} L_{a2}^{\ t} \\ L_{a2}^{\ t} L_{a3}^{\ t} \end{bmatrix} \mathrm{T} \qquad \mathrm{T} \equiv \begin{bmatrix} 1 & -5/2 \\ 0 & 1 \end{bmatrix} \tag{2}$$

$$M_{aj}^{\ t} \equiv \frac{n_a m_a^{\ 2}}{T_a} \frac{2}{\sqrt{\pi}} \int \mathrm{d}K\, \mathrm{e}^{-K} \left[ \nu_a(K) \right]^2 D_{33}(K) K^{j-1/2}$$
$$N_{aj}^{\ t} \equiv \frac{n_a m_a}{T_a} \frac{2}{\sqrt{\pi}} \int \mathrm{d}K\, \mathrm{e}^{-K} \nu_a(K) D_{13}(K) K^{j-1/2} \tag{3}$$
$$L_{aj}^{\ t} \equiv \frac{n_a}{T_a} \frac{2}{\sqrt{\pi}} \int \mathrm{d}K\, \mathrm{e}^{-K} D_{11}(K) K^{j-1/2}$$

In eq. (3), $\nu_a(K)$ is the energy-dependent pitch angle scattering collision frequency of the test particle $a$. By combining these results with parallel force balance equations $\langle \mathbf{B}\cdot\nabla\cdot \pi_a \rangle - n_a e_a \langle BE_{//} \rangle = \langle BF_{//a1} \rangle$, $\langle \mathbf{B}\cdot\nabla\cdot \Theta_a \rangle = \langle BF_{//a2} \rangle$ and the friction-flow relation that expresses $F_{//a1}$ and $F_{//a2}$ by the linear combinations of $u_{//b}$ and $q_{//b}$ as defined in refs. [15,18-21], we can express the parallel flows $\langle u_{//a}B \rangle$ and $\langle q_{//a}B \rangle$ for all particle species $a$ by the linear combination of the thermodynamic forces of all species defined as

$$\boldsymbol{A}_a \equiv \begin{bmatrix} A_{a1} \\ A_{a2} \end{bmatrix} \equiv -T_a \begin{bmatrix} \dfrac{n_a'}{n_a} - \dfrac{3}{2}\dfrac{T_a'}{T_a} - \dfrac{e_a \phi'}{T_a} \\ T_a'/T_a \end{bmatrix} \quad A_E \equiv \langle BE_{//} \rangle / \langle B^2 \rangle^{1/2} . \tag{4}$$

All of the combining coefficients are obtained from $M_{aj}^{\ t}$ and $N_{aj}^{\ t}$ defined in eq. (3) and the classical parallel friction coefficients $l_{jk}^{ab}$ defined in ref. [15]. It is noted that the friction-flow relation with these friction coefficients satisfies the momentum conservation by the symmetric relation $l_{jk}^{ab} = l_{kj}^{ba}$ and $\Sigma_a\, l_{1k}^{ab} = 0$. By substituting these flows $\langle u_{//a}B \rangle$ and $\langle q_{//a}B \rangle$ into eq. (1), expressions of the radial transport fluxes $\Gamma_a^{bn}$ and $q_a^{bn}$ in terms of thermodynamic forces are obtained. These expressions include completely the Onsager symmetric off-diagonal terms expressing inter-species interactions via the friction forces in the following form,

$$\begin{bmatrix} \Gamma^{bn}_{\ a} \\ Q^{bn}_{\ a}/T_a \end{bmatrix} = \begin{bmatrix} L_{a1}^{\ t} - L^{aa}_{\ 11} & L_{a2}^{\ t} - L^{aa}_{\ 12} \\ L_{a2}^{\ t} - L^{aa}_{\ 21} & L_{a3}^{\ t} - L^{aa}_{\ 22} \end{bmatrix} \boldsymbol{A}_a + \sum_{b \neq a} \begin{bmatrix} L^{ab}_{\ 11} & L^{ab}_{\ 12} \\ L^{ab}_{\ 21} & L^{ab}_{\ 22} \end{bmatrix} \boldsymbol{A}_b + \begin{bmatrix} L^{a}_{\ 1E} \\ L^{a}_{\ 2E} \end{bmatrix} A_E \tag{5}$$

$$J_E^{\ BS} = \sum_a \left[ L^{a}_{\ 1E} \ L^{a}_{\ 2E} \right] \boldsymbol{A}_a + L_{EE} A_E$$

where $J_E^{BS}$ is the bootstrap current, and $Q^{bn}_{\ a} \equiv q^{bn}_{\ a} + (5/2)\Gamma^{bn}_{\ a} T_a$ is the radial energy flux.

## 3. Numerical Examples

We present here the calculation results in the "imaginary axisymmetric limit" in CHS-qa [16] to demonstrate the validity and the effectiveness of this new method. Figure 1 shows the mono-energetic transport coefficients given by DKES code as the functions of CMUL $\equiv \nu(v)/v$ and EFIELD $\equiv E_r/v$ at the minor radial position of $r/a = 0.5$ in CHS-qa (so-called the "2b32" configuration ). The magnetic field strength is given to DKES in the expression by the Fourier expansion $B = \Sigma B_{mn}\cos(m\theta - nN\zeta)$ in the Boozer coordinates ($m$: poloidal mode, $n$: toroidal mode per toroidal period, $N$: toroidal period number). In the imaginary axisymmetric limit in which the non-axisymmetric components ($n \neq 0$) of this Fourier

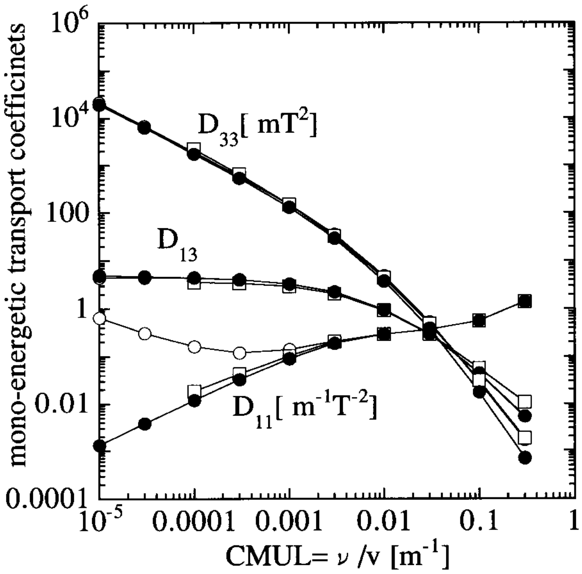


Fig. 1 The mono-energetic transport coefficients given by the DKES code at the minor radial position $r/a$ = 0.5 of CHS-qa. Open circles ○ indicate the case without radial electric fields ($E_r$=0) and open squares □ indicate the case with the radial electric field of $E_r/v$=0.01T. In the axisymmetric limit indicated by closed circle ● where the non-axisymmetric components of the magnetic field spectrum $B_{mn}(n \neq 0)$ are artificially set to be zero, dependence of the coefficients on the radial electric fields almost disappears.

expansion are artificially set to be zero, the results of the thermodynamic fluxes should coincide with the theory of axisymmetric tori [15], since neoclassical calculations based on the drift approximation need only magnetic fields expressed in magnetic flux coordinates and do not need the geometric shapes of magnetic surfaces.

Figure 2 shows the results on the particle diffusion in a fully ionized pure hydrogen plasma without the parallel electric field (causing Ware pinch). In the calculation of the diffusion coefficients shown in Fig. 2(a), (b), the electron and ion temperatures are assumed to be $T_e = T_i = 1$ keV at $r/a = 0.5$. The diagonal diffusion coefficients of proton $L_{ij}{}^t - L^{ii}{}_{lk}$ are strongly reduced from $L_{ij}{}^t$ calculated using only $D_{11}$ (eq. (3)) by adding the flow term in eq. (1) and become comparable to the off-diagonal diffusion coefficients $L^{ie}{}_{kl}$ and $L^{ei}{}_{kl}$ generated from $D_{13}$ and $D_{33}$ via the flow term in eq. (1), and to diagonal diffusion coefficients of electron $L_{ej}{}^t - L^{ee}{}_{lk}$. Therefore the dependence of the fluxes on the radial electric field in the thermodynamic forces is canceled, thus the well-known intrinsic ambipolarity is recovered as shown in Fig. 2(c) where the temperature and density profiles are assumed to be $T_e$, $T_i$, $n_e \propto [1-(r/a)^2]$ and $n_e = 5 \times 10^{18}$ m$^{-3}$ at $r/a = 0.5$. The energy integrated coefficients $L_{ij}{}^t$ calculated from $D_{11}$ of DKES including the Pfirsch-Schlueter flux cause an error even in the banana regime. In this axisymmetric limit case, by replacing $L_{ij}{}^t$ by $-cB_\zeta{}^{(\mathrm{Boozer})}/(e\chi')N_{ij}{}^t$ (indicated in Fig. 2 as "$L_{ij}{}^t$ (D13)") following the analytic theory of the banana-plateau transport in axisymmetric limit [14], this error can be removed. In general, Pfirsch-Schlueter components in $D_{11}$ should be removed before the energy integration in eq. (3) for this kind of calculation of the ambipolarity condition. The consistent treatment of the Pfirsch-Schlueter transport is a future theme.

Figure 3 shows the results on the particle diffusion in a fully ionized hydrogen plasma having fully ionized helium as an impurity. The ion density ratio, the temperatures and electron density are assumed to be $n_{He^{2+}}/(n_{H^+} + n_{He^{2+}}) = 10\%$, $T_e = T_i \propto [1-(r/a)^2]$, $T_e = T_i = 1$ keV and $n_e = 5 \times 10^{18}$ m$^{-3}$ at $r/a = 0.5$, and the radial and parallel electric fields are set to be zero. Under these assumption and the constraint of quasi-neutrality $n_e = n_{H^+} + 2n_{He^{2+}}$, the density profiles can be changed using the density gradient ratio of ions $(\partial \ln n_{He^{2+}}/\partial\rho)/(\partial \ln n_{H^+}/\partial\rho)$ as a free parameter. Although the diagonal diffusion coefficients of proton $L_{aj}{}^t - L^{aa}{}_{lk}$ (hereafter $a$ = H$^+$, $b$ = He$^{2+}$, $Z_a = 1$, $Z_b = 2$) are strongly increased due to the interaction with He$^{2+}$ compared with the pure plasma case in Fig. 2, the total ion charge diffusion flux $Z_a\Gamma_a$ +

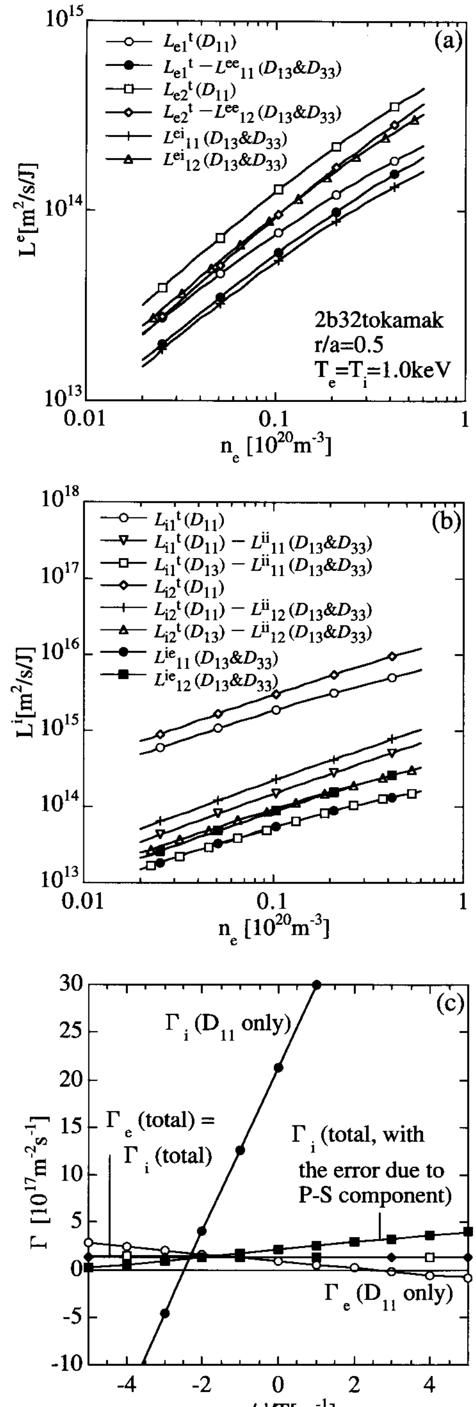


Fig. 2 (a) electron particle diffusion coefficients and (b) ion particle diffusion coefficients in the pure hydrogen plasma in the axisymmetric limit calculated with the assumed temperatures of $T_e = T_i = 1$ keV at $r/a = 0.5$. (c) shows the dependence of the particle diffusion fluxes on the radial electric field in the axisymmetric limit calculated with the assumed electron density of $n_e = 5 \times 10^{18}$ m$^{-3}$.

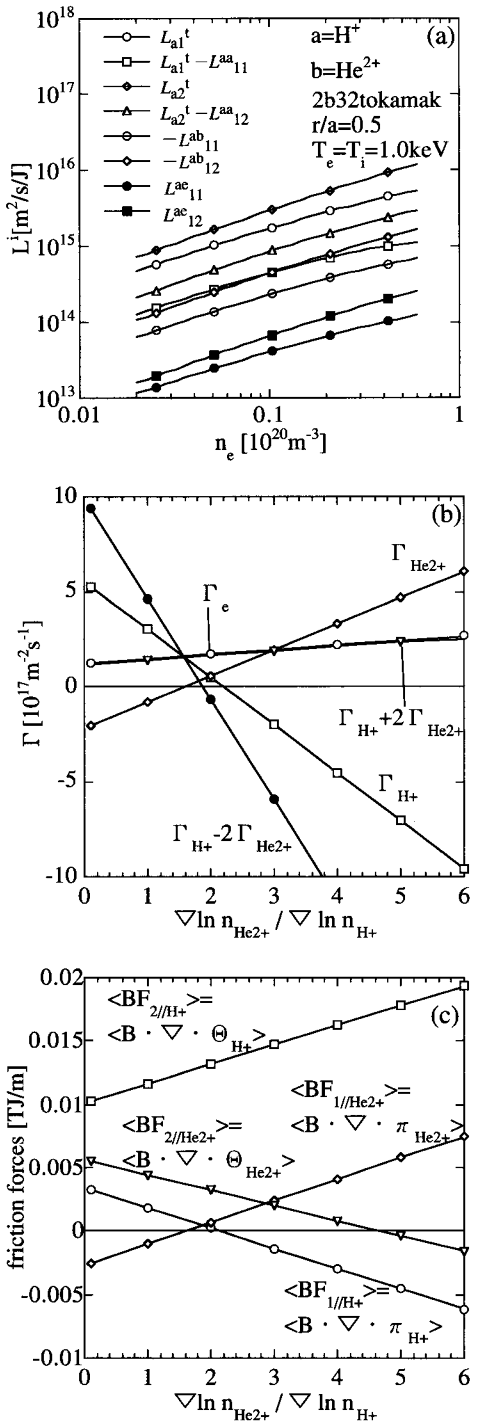

Fig. 3 (a) the diffusion coefficients of proton in a plasma having fully ionized helium as an impurity of 10% in the axisymmetric limit with the assumed temperatures of $T_e = T_i = 1$ keV at $r/a = 0.5$, and the dependence of (b) the particle diffusion fluxes and (c) ion friction forces balancing with the parallel viscosity, on the impurity-bulk density gradients ratio $(\partial \ln n_{He^{2+}}/\partial\rho)/(\partial \ln n_{H^+}/\partial\rho)$. The assumed electron density in (b) and (c) is $n_e = 5 \times 10^{18}\,\mathrm{m}^{-3}$.

$Z_b\Gamma_b$ is almost identical to that in the pure plasma case since the effective charge is only $Z_{\rm eff} = 1.18$. The ambipolarity condition is automatically attained. In this calculation, $L_{aj}{}^t$ and $L_{bj}{}^t$ do not contain the Pfirsch-Schlueter component. The strong dependence of the diffusion of $H^+$ and $He^{2+}$ on the density gradient ratio $(\partial \ln n_{He^{2+}}/\partial\rho)/(\partial \ln n_{H^+}/\partial\rho)$ indicates the well-known impurity accumulation minimizing the parallel friction forces $F_{//a1}$, $F_{//b1}$ between bulk ions and impurity ions. The quasi-steady state condition of the density profile $Z_a\Gamma_a - Z_b\Gamma_b \fallingdotseq 0$ is attained at the condition of $(\partial \ln n_{He^{2+}}/\partial\rho)/(\partial \ln n_{H^+}/\partial\rho) = Z_b/Z_a$.

## 4. Conclusion

A newly developed neoclassical transport calculation method and its numerical examples in the axisymmetric limit were presented. The results of numerical calculation codes based on the linearized drift kinetic equation with the pitch angle scattering operator are used to express the parallel viscosity and radial particle and heat transports in terms of the parallel particle and heat flows and the thermodynamic forces. The parallel particle and heat flows are determined by the parallel force balance equation satisfying the momentum conservation. It is a powerful method to calculate the neoclassical flows and transports of multi-ion-species plasmas in various collisionality regimes in general toroidal systems including quasi-symmetric configurations. In this paper, we presented how the intrinsic ambipolarity and the impurity accumulation in an axisymmetric limit are obtained, to demonstrate the validity of this method. Applications for non-symmetric configurations and actual quasi-symmetric configurations with residual ripples of a few % of magnetic field strength will be reported in future publications.

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## References

[1] A.H. Boozer and G. Kuo-Petravic, Phys. Fluids **24**, 851 (1981).

[2] R.H. Fowler, J.A. Rome and J.F. Lyon, Phys. Fluids **28**, 338 (1985).

[3] H.E. Mynick and W.N.G. Hitchon, Nucl. Fusion **26**, 425 (1986).

[4] C.D. Beidler, W.N.G. Hitchon, J.L. Shoet and J.

Comput. Phys. **72**, 220 (1987).
[5] S.P. Hirshman, K.C. Shaing, W.I. van Rij, *et al.*, Phys. Fluids **29**, 2951 (1986).
[6] W.I. van Rij and S.P. Hirshman, Phys. Fluids B**1**, 563 (1989).
[7] J. Nuehrenberg and R. Zille, Phys. Lett. A. **129**, 113 (1988).
[8] P. Garabedian and L-P. Ku, Phys. Plasmas **6**, 645 (1999).
[9] O. Motojima, *et al.*, Phys. Plasmas **6**, 1843 (1999).
[10] K. Matsuoka, *et al.*, Plasma Phys. Control. Fusion **42**, 1145 (2000).
[11] K. Ida, Plasma Phys. Control. Fusion **40**, 1429 (1998).
[12] Z. Lin, W.M. Tang and W.W. Lee, Phys. Plasmas 2, 2975 (1995).
[13] J.L.V. Lewandowski, J. Williams, A.H. Boozer and Z. Lin, Phys. Plasmas **8**, 2849 (2001).
[14] H. Sugama, S. Nishimura, "How to calculate the neoclassical viscosity, diffusion, and current coefficients in general toroidal plasmas", *submitted to* Phys. Plasmas
[15] S.P. Hirshman and D.J. Sigmar, Nucl. Fusion **21**, 1079 (1981).
[16] S. Okamura, K. Matsuoka and S. Nishimura, *et al.*, Nucl. Fusion **41**, 1865 (2001).
[17] F.L. Hinton and R.D. Hazeltine, Rev. Mod. Phys. **48**, 239 (1976).
[18] K.C. Shaing and J.D. Callen, Phys. Fluids 26, 3315 (1983).
[19] K.C. Shaing, S.P. Hirshman and J.D. Callen, Phys. Fluids **29**, 521 (1986).
[20] K.C. Shaing, S.P. Hirshman and J.S. Tolliver, Phys. Fluids **29**, 2548 (1986).
[21] H. Sugama and W. Horton, Phys. Plasmas **3**, 304 (1996).