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# Monte Carlo Simulation of Transport

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This paper is concerned with the problem of transport in controlled nuclear fusion as it applies to confinement in a tokamak or stellarator. Numerical experiments validate a mathematical model of Paul R. Garabedian in which the electric potential is determined by quasineutrality because of singular perturbation of the Poisson equation. The Monte Carlo method is used to solve a test particle drift kinetic equation. The collision operator drives the distribution function in velocity space towards the normal distribution, or Maxwellian, as suggested by the central limit theorem. The detailed structure of the collision operator and the role of conservation of momentum are investigated. Exponential decay of expected values allows the computation of the confinement times of both ions and electrons. Three-dimensional perturbations in the electromagnetic field model the anomalous transport of electrons and simulate the turbulent behavior that is presumably triggered by the displacement current. Comparison with experimental data and derivation of scaling laws are presented. 

## 1. INTRODUCTION

The preferred approach in fusion experiments is to use a strong magnetic field with toroidal geometry to confine the plasma. The two standard configurations for confinement are tokamaks and stellarators, and we model both of them in a common framework so that comparison with the experimental data available for tokamaks can be used in making reactor studies of a stellarator. Our methodology is that of computational physics, which means that differential equations are solved numerically, providing results to validate theory through comparisons with experimental data.

A basic tool in the study of transport is to track particle orbits, for the mean free path is large compared to the dimensions of the device. Since the confining magnetic field is strong, these orbits are approximately described by the differential equations of the guiding center. They are obtained from the equations of motion by an asymptotic expansion in the dimensionless gyroradius, with the rapid gyration around the magnetic lines averaged out. A rigorous mathematical proof can be found in [1].

We use a test particle model from kinetic theory to evaluate confinement time [2, 3]. This consists in a mathematical idealization of the process of inserting a particle in the plasma and seeing how long it takes to leave. Since the effect of a single particle on macroscopic quantities is negligible, the background electromagnetic and flow fields and their profiles remain fixed. Collisions generate a random process, and therefore we study the test particles statistically. Their distribution function satisfies a partial differential equation called the test particle drift kinetic equation. The collision operator is modeled in this equation by a second-order elliptic partial differential operator acting in the velocity coordinates, as in a Fokker–Planck equation. Solutions of the associated diffusion equation in velocity space decay to the normal distribution, or Maxwellian, as suggested by the central limit theorem. In the absence of the collision operator, the test particle drift kinetic equation reduces to a first-order partial differential equation whose characteristics are the guiding center orbits. The mathematics of this approach should not be confused with the statistical mechanics occurring in more conventional plasma theory [4].

The test particle model is implemented in a natural way by the Monte Carlo method. The test particles move on drift surfaces and jump back and forth between these surfaces following a random walk that models collisions. When a particle reaches the boundary of the plasma it escapes, and therefore the particle distribution function necessarily decays. We are led to impose a corresponding Dirichlet boundary condition on the distribution function. The inverse of the particle confinement time defines a rate of decay which is equal to the lowest eigenvalue of the time-independent part of the linear operator defining the drift kinetic equation. A Rayleigh quotient of the corresponding eigenfunction is analogous to the standard expression for the energy confinement time measured in experiments.

In this theory we assert that the electric potential should be determined by the requirement of charge neutrality rather than from equations of motion represented by Ohm's law because of the singular perturbation of Poisson's equation associated with small Debye length [5]. The resulting perturbations of the electric field from radial symmetry serve in our model to explain the anomalous transport of electrons. Numerical simulations for tokamaks with only a radial electric field give a confinement time for the electrons much higher than the confinement time for the



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ions. This requires different rates of decay and hence different sources for ions and electrons to maintain a steady state. The impossibility of producing these different sources in practice seems to explain the origin of turbulence in tokamaks, triggered presumably by the displacement current in an attempt to enforce quasineutrality.

We perform our simulations with the Monte Carlo code TRAN [5, 6]. Exponential rates of decay of expected values of carefully selected integrals of the solution of the drift kinetic equation provide estimates of the confinement time for both ions and electrons. This code is one of the few tools available to study the electron case efficiently. The importance of such a capability lies in the good agreement with experimental data that can be achieved by running both the ion and the electron cases, together with a mechanism to enforce charge neutrality and evaluate the electric field.

We use the equations of magnetohydrodynamics to determine the structure of the magnetic field in the plasma. In a time-averaged model with the plasma velocity set equal to zero, the magnetostatic equations are

$$\mathbf{J} \times \mathbf{B} = \nabla p, \quad \nabla \cdot \mathbf{B} = 0.$$

Here $\mathbf{B}$ is the magnetic field, $p$ is the scalar pressure, and the current density $\mathbf{J}$ is related to $\mathbf{B}$ by Ampere's law $\mathbf{J} = \nabla \times \mathbf{B}$. The magnetic field lines, which are the integral curves of the vector field $\mathbf{B}$, are assumed to form a nested family of toroidal flux surfaces, labeled by $s$. Because of the KAM theory, only weak solutions of the equations are expected to exist [6, 7]. The theory of Clebsch potentials yields the representation

$$\mathbf{B} = \nabla s \times \nabla \theta = \nabla \phi + \zeta \nabla s,$$

which enables us to express the guiding center differential equations in terms of invariant flux coordinates $s$, $\theta$, and $\phi$. A suitable linear transformation maps the Clebsch potentials onto poloidal and toroidal angles on each flux surface, from now on denoted by $\theta$ and $\phi$ in the text. All we need to integrate the equations is a knowledge of the Fourier representation

$$\frac{1}{B^2} = \sum b_{mn}(s) \cos(m\theta - n\phi),$$

where a stellarator symmetry is assumed that eliminates the sine contributions [2].

## 2. CHARGE NEUTRALITY

### 2.1 *Displacement Current and Quasineutrality*

The addition of the displacement current to Ampere's law makes the equations for the electric and magnetic fields consistent with conservation of charge. This relativistic equation is of crucial importance for rapidly fluctuating fields. We write it in the form

$$\lambda^2 \mathbf{E}_t = \nabla \times \mathbf{B} - \mathbf{J},$$

where $\lambda$ is the Debye length and $\mathbf{E}$ is the electric field. In a plasma, the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ act on both electrons and ions to produce dynamical effects including mass motion, which in turn produces modifications in the electromagnetic fields. Consequently we are dealing with a coupled system of matter and fields. In this context the equation for the displacement current is a relation between the electromagnetic fields and the current density

$$\mathbf{J} = q n_{\mathrm{i}} \mathbf{u}_{\mathrm{i}} - q n_{\mathrm{e}} \mathbf{u}_{\mathrm{e}}$$

expressed in terms of the number densities $n_{\mathrm{i}}$ and $n_{\mathrm{e}}$ and velocities $\mathbf{u}_{\mathrm{i}}$ and $\mathbf{u}_{\mathrm{e}}$ of the ions and the electrons.

Since the Debye length is small, it is usual in plasma physics to neglect the displacement current. The three components of the magnetic field then must solve the four scalar equations

$$\nabla \times \mathbf{B} = \mathbf{J}, \quad \nabla \cdot \mathbf{B} = 0.$$

A solution cannot exist unless the compatibility requirement of quasineutrality

$$\nabla \cdot \mathbf{J} = 0$$

is imposed. Hence in any argument involving $\mathbf{B}$ the plasma is constrained to satisfy this condition.

We neglect the displacement current because the factor $\lambda^2$ is small, not because $\mathbf{E}_t$ is zero. When the displacement current is retained in Maxwell's equations, coupled to quasineutrality, it can be expected to introduce fluctuations of the electric potential $\Phi$ along the magnetic lines in three dimensions. These fluctuations are associated with plasma oscillations and turbulence that lead to significant transport. This more complicated time-dependent behavior must somehow be taken into account in any model based on static fields. We also need a new rule to determine the electric field when it is suppressed in Maxwell's equations. Thus it is natural to consider quasineutrality as a static equation for the electric potential because of the way it is obtained by dropping higher derivatives in Poisson's equation

$$\lambda^2 \, \Delta \Phi = n_{\mathrm{e}} - n_{\mathrm{i}}$$

for the electric potential $\Phi$, which is measured in units

of the temperature. The theory of singular perturbations suggests that when the left side is neglected, the resulting requirement of quasineutrality

$$n_e(\Phi) - n_i(\Phi) = 0$$

must be what determines the electric field, even though $\Phi$ no longer appears explicitly.

It is more customary in the fusion community to find the electric field from Ohm's law

$$\mathbf{E} + \mathbf{u} \times \mathbf{B} = \eta \mathbf{J}.$$

Its derivation from kinetic theory involves subtractions, making it questionable to neglect small terms. But this law is used to establish the radial character of the electric field. If the resistivity vanishes, the partial differential equation $\mathbf{B} \cdot \nabla\Phi = 0$ leads to the conclusion that $\Phi$ is a function of the toroidal flux $s$ alone. This conclusion is based on an ill-posed problem in which the right-hand side may not even vanish, and it appears to be responsible for anomalies in the conventional theory of electron transport.

The electric field is indeed dominated by a radial term, but small three-dimensional oscillations of the electrostatic potential seem to have the same effect as observed fluctuations in density and potential to which anomalous transport is usually attributed. A sensible mechanism to enforce the quasineutrality requirement $n_e = n_i$ naturally introduces such oscillations and provides a time-averaged simulation of the more complex physical behavior.

Based on these considerations, we reject Ohm's law in favor of quasineutrality as the rule to obtain the electric field. Quasineutrality is assumed in the derivation of Ohm's law, so using that law to determine the fine structure of the electric field is a dubious procedure.

### 2.2. *A Mechanism to Achieve Quasineutrality*

We believe that the oscillations in the particle densities and in the fields introduced by the term $\mathbf{E}_t$ are responsible for bringing the confinement time of electrons down to the confinement time of ions. We simulate this behavior in our model with static fields by solving the quasineutrality and ambipolarity equations

$$n_e = n_i, \quad \tau_e = \tau_i.$$

The mechanism implemented in the TRAN code solves the quasineutrality equation by requiring that the Fourier coefficients of the densities $n_i$ and $n_e$ of ions and electrons coincide. The electric potential $\Phi$ is expanded as a Fourier series,

$$\Phi = \sum P_{mn} \cos(m\theta - n\phi),$$

in the invariant poloidal and toroidal angles $\theta$ and $\phi$ with coefficients $P_{mn}$, measured in units of temperature, that depend on the flux $s$. Other trigonometric functions are neglected because stellarator symmetry is assumed.

The charge separation is expanded in a similar Fourier series,

$$n_e - n_i = \sum C_{mn} \cos(m\theta - n\phi),$$

after dividing out the total number of electrons or ions. Calculation of the Fourier coefficients $C_{mn}$ is accomplished by using the Monte Carlo method to estimate the expected values of trigonometric functions. Convergence has been tested to establish that the results are statistically significant.

The aim is to determine the coefficients $P_{mn}$ so that $C_{mn} = 0$. Charge separation gives rise to strong electrostatic restoring forces, and thus it is reasonable to expect wells and hills in the electric potential to correct for similar oscillations in the charge separation $n_e - n_i$. This suggests that the relationship between the two matrices $P_{mn}$ and $C_{mn}$ might be diagonally dominant, and in practice we get a numerical solution by truncating both of the series for $\Phi$ and $n_e - n_i$ in the same way.

A successful iteration driving the $C_{mn}$ towards zero can be based on the hypothesis that the Jacobian matrix relating $C_{mn}$ to $P_{mn}$ is well approximated by the identity [5], so with a suitable relaxation factor $\varepsilon$ we can put

$$P_{mn}^{l+1} = P_{mn}^{l} + \varepsilon C_{mn}^{l}. \tag{1}$$

Numerical calculations with the algorithm (1) show that resonant coefficients $P_{mn}$ with rotational transform $\iota = n/m$ inside the plasma can be found so that $C_{mn} = 0$ even when they are less than 2% of the temperature. These relatively small terms in $\Phi$ that depend on the poloidal and toroidal angles $\theta$ and $\phi$ explain the anomalous transport of electrons in this model of transport because they reduce $\tau_e$ much more than $\tau_i$.

The algorithm described up to this point provides a one parameter family of solutions because $P_{00}$ is not yet determined, since the average value of $C_{00}$ is normalized to be zero. One of the advantages of the TRAN code is its capability to compute both the ion and the electron confinement times, so we can solve the ambipolarity equation $\tau_e = \tau_i$ simultaneously with the quasineutrality equation to obtain a physically relevant solution $P_{00}$. Numerical simulations with stellarators have shown that an increase of $P_{00}$ increases the ion confinement time while leaving the electron confinement time practically unchanged. The iteration

$$P_{00}^{l+1} = \left(1 - \varepsilon \log \frac{\tau_i}{\tau_e}\right) P_{00}^{l}$$

yields good results when coupled with (1) to solve for quasineutrality and ambipolarity in stellarators.

For tokamaks the dependence of the ion confinement time on $P_{00}$ is less pronounced when the device is nearly axisymmetric, so we simply fix it at a plausible value. On the other hand, it has been observed from simulations with three-dimensional bifurcated tokamak equilibria that an increase in the helical excursion $\Delta_{11}$ of the magnetic axis can reduce the electron confinement time without significantly affecting the ion confinement time. A similar result can be achieved by increasing the magnitudes of other three-dimensional modes of perturbation. Hence to study tokamak transport, the axisymmetric coefficients $b_{m0}$ in the expansion of $1/B^2$ are obtained from an equilibrium calculation, but small three-dimensional terms $b_{mn}$ with $n \neq 0$ are allowed to appear, too. It seems appropriate to input these coefficients with values having the same order of magnitude, so we produce a family of solutions parametrized by the size of the three-dimensional perturbation. This is to be determined by solving the ambipolarity equation $\tau_e = \tau_i$. Increasing the magnitude of the perturbation reduces $\tau_e$ without changing $\tau_i$ significantly, but decreasing it has the opposite effect. Thus we are led to couple the iteration

$$b_{mn}^{l+1} = \left(1 - \varepsilon \log \frac{\tau_i}{\tau_e}\right) b_{mn}^{l}$$

with (1) in order to solve the quasineutrality and ambipolarity equations for tokamaks. The iteration converges well in practice and gives results in agreement with experiment.

Our algorithm introduces perturbations in the electric potential through the iterations on $P_{mn}$ and modulates the perturbations of the magnetic field. These asymmetries avoid the anomalous behavior of two-dimensional models of transport and provide a three-dimensional simulation of the turbulence associated with microinstabilities and drift waves. We demonstrate that the algorithm does simulate turbulence by showing that the confinement time is relatively insensitive to the choice of a three-dimensional mode of perturbation $b_{mn}$. To do so we choose a set of modes to work with and initialize them with values having the same magnitude, but in each experiment we change the signs of the terms. We compute the confinement times for all combinations of signs. Calculations of this kind have been run for the ITER tokamak [8]. Usually the magnitude of the perturbations converges to approximately 1% of the average magnetic field strength $B$ and the confinement time does not vary significantly with the details of the node (see Fig. 1).

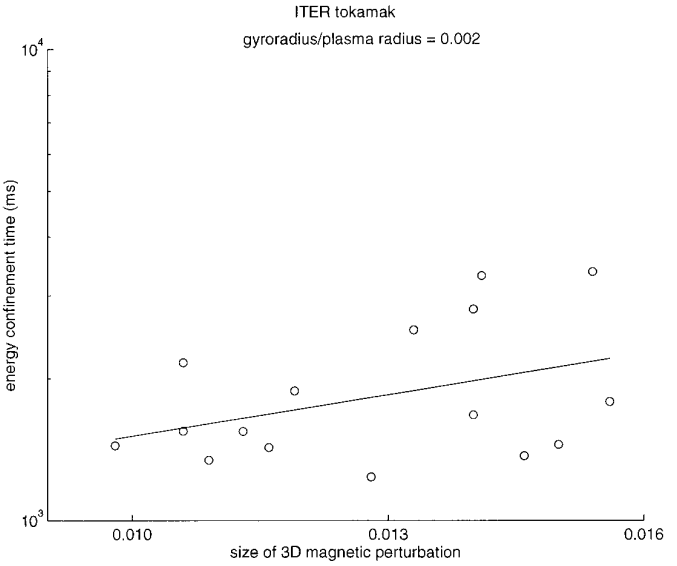


**FIG. 1.** Insensitivity of transport to the choice of a particular three-dimensional mode of perturbation in the spectrum of the magnetic field. Each point represents a different choice of the perturbation. Typically the size of the perturbation is a small percentage of the average magnetic field strength, and the confinement time does not vary significantly with the details of the mode.

## 3. DRIFT KINETIC EQUATION

### 3.1. *Test Particle Model and Collision Operator*

At the experimental conditions for plasma confinement, the mean free paths of ions and electrons are many times larger than the dimensions of the experimental apparatus. The particle motion is given approximately by rapid gyration around a guiding center which drifts slowly across the magnetic field lines. The gyroradius $\rho_L = mv_\perp/qB$ is assumed small, compared with the plasma radius. The rapid particle gyration is averaged out, leaving equations for the guiding center of the form

$$\dot{\mathbf{x}} = \rho_\parallel[\mathbf{B} + \nabla \times \rho_\parallel \mathbf{B}].$$

Here $\rho_\parallel = mv_\parallel/qB$ is the parallel gyroradius, which is of the same order of magnitude as the gyroradius. It is determined from the conservation of energy

$$W = \frac{q^2 B^2 \rho_\parallel^2}{2m} + \mu B + q\Phi,$$

where $\Phi$ is the electric potential, and the magnetic moment $\mu = mv_\perp^2/2B$ is an adiabatic invariant that is held constant along trajectories. An advantage of these equations is that they can be transformed into a simple system of ordinary differential equations in terms of the flux coordinates $s$, $\theta$, $\phi$ involving only knowledge of $1/B^2$ [2].

Motivated by the problem of tracking particles in plasma physics, we adopt the test particle model of kinetic theory [3] to estimate confinement times. The model consists in a mathematical idealization of the process of inserting a particle in the plasma and seeing how long it takes to leave. The particle interacts with a fixed background in which the electromagnetic and flow fields are specified.

We introduce a test particle distribution function $f$ to study the statistics due to collisions. Test particles collide only with the background plasma particles and therefore the collision operator becomes linearized. As in a Fokker–Planck model, the collision operator is described by a second-order elliptic partial differential operator in conservation form that acts on velocity coordinates. The central limit theorem suggests that solutions of the associated diffusion equation in velocity space should decay to the normal distribution or Maxwellian, shifted by the flow velocity $\mathbf{u}$.

We write the drift kinetic equation for the distribution function $f$ of the test particles in the form

$$\frac{\partial f}{\partial t} + \rho_{\|}[\mathbf{B} + \nabla \times \rho_{\|}\mathbf{B}] \cdot \nabla f = \nabla \cdot [\nu\, e^{-m(\mathbf{v}-\mathbf{u})^2/2T}\, \nabla e^{m(\mathbf{v}-\mathbf{u})^2/2T} f]. \tag{2}$$

The operator $\nabla$ acts on spatial coordinates on the left, but on velocity coordinates on the right. The collision frequency $\nu$ and the temperature $T$ are known functions of $|\mathbf{v} - \mathbf{u}|$ and the flux $s$, respectively. The term in square brackets on the left is the guiding center velocity, and the term on the right is the collision operator. There are actually two separate equations to solve, one for the ions and one for the electrons, distinguished by the respective guiding center equations, collision frequencies, and temperatures. The normal distribution shifted by $\mathbf{u}$ accounts for conservation of momentum in the test particle model.

We shall refer to (2) as the drift kinetic equation. Absence of explicit dependence on the time $t$ suggests exponential decay to the normal distribution in velocity space, and the dependence of the collision operator on the collision frequency and temperature are exhibited. But there are other factors that must be taken into account. The sign of $\rho_{\|}$ is not determined by the energy equation and therefore besides $s$, $\theta$, $\phi$, $W$, and $\mu$ the distribution function depends also on the sign of $\rho_{\|}$. The problem with the sign of the parallel gyroradius is dealt with by adding an ordinary differential equation for $\rho_{\|}$. The most relevant features of the collision operator are its dependence on the temperature and collision frequency, and small modifications preserving these properties do not seem to affect transport.

If we differentiate products on the right-hand side in the drift kinetic equation, it assumes the more standard form

$$\frac{\partial f}{\partial t} + \rho_{\|}[\mathbf{B} + \nabla \times \rho_{\|}\mathbf{B}] \cdot \nabla f = \nabla \cdot \left[ \nu \left( \frac{m(\mathbf{v}-\mathbf{u})}{T} + \nabla f \right) \right] = \frac{\nu}{2} \Delta f + \frac{1}{c^2} \frac{\partial}{\partial c} \left[ c^2\, \nu \left( cf + \frac{T}{m} \frac{\partial f}{\partial c} \right) \right]$$

exhibiting a friction term, where $c = |\mathbf{v} - \mathbf{u}|$ and $\Delta$ is the Laplacian on the unit sphere in velocity space. For the collision frequency we use formulas appearing in the literature that distinguish between pitch angle scattering and energy scattering [2, 3].

### 3.2. *Exponential Decay and Confinement Time*

We describe next how it is possible for us to compute not only the ion confinement time, but also the electron confinement time. The problem of computing the electron confinement time requires an efficient technique because of the very slow drift of the electrons across magnetic surfaces. The importance of computing both confinement times is that they allow us to extract a physically relevant answer from a parametrized family of solutions of the transport problem by taking into account quasineutrality.

Exponential decay of $f$ is suggested naturally by the method of separation of variables because $t$ does not appear explicitly in the drift kinetic equation. We look for solutions of the form

$$f = e^{-\lambda t} F,$$

where $F$ does not depend on time. Substitution of this identity into the drift kinetic equation leads to the eigenvalue problem

$$\rho_{\|}[\mathbf{B} + \nabla \times \rho_{\|}\mathbf{B}] \cdot \nabla F = \nabla \cdot \left[ \nu \left( \frac{m(\mathbf{v}-\mathbf{u})}{T} + \nabla f \right) \right] + \lambda F.$$

If the smallest eigenvalue is positive, then solutions of the drift kinetic equation decay exponentially, and the rate of decay is dominated by this eigenvalue. The particle confinement time

$$\tau = 1/\lambda$$

is defined as the inverse of the smallest eigenvalue $\lambda$ and is a measure of how long it takes for the test particles to leave the plasma.

If we identify the term $\lambda F$ on the righ-hand side of the eigenvalue equation as a source $S$, then for the lowest eigenvalue we have

$$S = \frac{1}{\tau} F.$$

The source is related to the rate at which particles must be injected into the plasma to maintain a steady state. For a reasonable definition of the norm, the Rayleigh quotient

$$\tau = \frac{\|F\|}{\|S\|}$$

gives a suggestive representation for the confinement time.

Note that there are two distinct sources, one for the ions and one for the electrons, so that when the confinement times are different the sources must be, too. This situation causes trouble in two-dimensional models of transport where the electron confinement time is an order of magnitude larger than the ion confinement time. The necessity of producing two different sources makes it impossible to maintain a steady state in tokamaks and induces oscillations of the electric field that are associated with turbulence.

The TRAN code computes the particle confinement time $\tau$ rather than the energy confinement time $\tau_E$. For comparison with experiments and in reactor studies we need a relationship between these confinement times. The semiempirical formula

$$\tau_E = \tau/3B$$

has worked well in practice, where the division by $B$ comes from normalization of time by the ion gyrofrequency.

In the TRAN code the particle confinement time is evaluated by estimating the exponential rate of decay of functionals using the Monte Carlo method [6]. Numerical experiments have shown that good estimates for both the ion and electron confinement times are obtained from the functional

$$\sum\sum \cos\left(\frac{s_{jk} - \sigma_k}{1 - \sigma_k s_{jk}} \frac{\pi}{2}\right) = Ae^{-t/\tau} + \cdots,$$

where $s_{jk}$ stands for the coordinate $s$ of the $j$th particle launched from the flux surface $s = \sigma_k$. We remark that at low collisionality one can obtain the exponential rate of decay of the expected value $N(t)$ of the number of particles remaining in the plasma by approximating the distribution of arrival times by a Poisson process. But this argument is not valid at higher collisionality and, moreover, the use of $N(t)$ to estimate the electron confinement time would require an excessive amount of computation. The success of our method of calculation of particle confinement times is due to the exponential decay of the principal eigenfunction, which also occurs in more general situations.

## 4. MONTE CARLO METHOD

### 4.1. *A Random Walk for the Collision Operator*

The evaluation of confinement time and the Fourier coefficients of the charge separation involves multiple integrals in a five-dimensional space described by the variables $s$, $\theta$, $\phi$, $W$, and $\mu$. To do these integrations we must solve the drift kinetic equation for the particle distribution function $f$, which depends on the five variables above, the time $t$, and the sign $\pm$ of the parallel velocity. The Monte Carlo method is an appropriate tool for these computations in a space of high dimension.

An algorithm to solve the drift kinetic equation has been implemented in the TRAN code. It is a split time method consisting alternately of numerical integrations of guiding center orbits in flux coordinates and applications of a random walk in velocity space that models the collision operator.

We now apply the ideas of the last section to derive a random walk modeling the collision operator that is implemented in the TRAN code. This operator is expressed in a spherical coordinate system whose origin has been translated by $\mathbf{u}$. Moreover, the collision frequency is itself a function of $c = |\mathbf{v} - \mathbf{u}|$, so it is convenient to translate the coordinate system by $\mathbf{u}$ before we apply the random walk. The formulas for the change of coordinates show that when $\mathbf{u}$ is small compared with the ion thermal speed the changes made in the energy $W$ and in the magnetic moment $\mu$ by the random walk are small, indicating that conservation of momentum should not play a major role in transport.

In the guiding center approximation the energy $W$ and the cosine $\eta$ of the pitch angle suffice to specify the velocity. After $W$ and $\eta$ are changed by a random walk the magnetic moment $\mu$ is updated accordingly. The presence of the flow velocity $\mathbf{u}$ in the collision operator makes it necessary to use a third coordinate for the particle velocity in order to apply the random walk. At low collisionality, the case we are most interested in, it is reasonable to sample the angle $\alpha$ defined by

$$\mathbf{v}_\perp \cdot \mathbf{u}_\perp = v_\perp u_\perp \cos\alpha$$

from a uniform distribution just before collisions. Here $\mathbf{v}_\perp$ and $\mathbf{u}_\perp$ are the components of $\mathbf{v}$ and $\mathbf{u}$ perpendicular to $\mathbf{B}$.

The collision operator is to be written in a coordinate system translated by $\mathbf{u}$ and therefore we transform the variables $W$, $\eta$, and $\alpha$ to new variables $\tilde{W}$, $\tilde{\eta}$, and $\tilde{\alpha}$ using the formulas

$$\tilde{W} = W + u_\parallel^2 + u_\perp^2 - 2\sqrt{W}\,(u_\parallel \eta + u_\perp \sqrt{1 - \eta^2}\cos\alpha)$$

$$\tilde{\eta} = \frac{\sqrt{W}\,\eta - u_\parallel}{\sqrt{\tilde{W}}}$$

$$\tan \tilde{\alpha} = \frac{\sqrt{W(1-\eta^2)}\sin\alpha}{\sqrt{W(1-\eta^2)}\cos\alpha - u_\perp}.$$

If we write the formal adjoint of the collision operator in these coordinates, then a split time argument leads to the random walk

$$\tilde{\alpha}_{n+1} = \tilde{\alpha}_n \pm \sqrt{\frac{\nu\,\Delta t}{(1-\tilde{\eta}_n^2)}}$$

$$\tilde{\eta}_{n+1} = (1-\nu\,\Delta t)\tilde{\eta}_n \pm \sqrt{\nu\,\Delta t(1-\tilde{\eta}_n^2)}$$

$$\tilde{W}_{n+1} = \tilde{W}_n + 2\nu\,\Delta t\left[\left(\frac{3}{2} + \frac{\tilde{W}_n \nu'}{\nu}\right) T - \tilde{W}_n\right] \pm 2\sqrt{T\tilde{W}_n \nu\,\Delta t}.$$

This can be derived from one-dimensional diffusion by the following argument. Consider a linear second-order elliptic operator $L$ whose formal adjoint is $L^* = a(x)\partial_x^2 + b(x)\partial_x$. For a probability density function $f(t, x)$ satisfying $f_t = L[f]$, the random walk $x_{n+1} = x_n + b(x_n)\,\Delta t \pm \sqrt{2a(x_n)\,\Delta t}$ models the associated diffusion.

New values for $W$ and $\eta$ are obtained by translating the coordinate system back again. The algorithm implemented in TRAN to solve the drift kinetic equation consists in alternating between numerical integrations of the guiding center equations in flux coordinates and changes in $W$ and $\eta$ defined by the random walk.

### 4.2. *Detailed Structure of the Collision Operator*

The principal parameters in the collision operator are the temperature and the collision frequency. Runs of TRAN provide numerical evidence that other details of the collision operator matter little for transport. In order to study this property systematically we modify the collision operator by introducing anisotropy in the Maxwellian and then observe the effect on transport. Our numerical results show that there is little change in the confinement time, corroborating our claim that details of the collision operator other than its dependence on the temperature and the collision frequency have a negligible effect on transport.

The modified collision operator is given by

$$L[f] = \nabla \cdot \left[\nu A e^{-m(\mathbf{v}-\mathbf{u})^2/2T}\nabla\left(\frac{e^{m(\mathbf{v}-\mathbf{u})^2/2T}}{A} f\right)\right],$$

where $A$ depends on the angle between $\mathbf{v}$ and $\mathbf{B}$. It has the property that the associated diffusion equation in velocity space admits as a solution the normal distribution multiplied by the anisotropy factor $A$. This choice for $L[f]$ is motivated by the possibility of the magnetic field $\mathbf{B}$ introducing anisotropies in the distribution function. A natural representation for $A$ is given by a superposition of

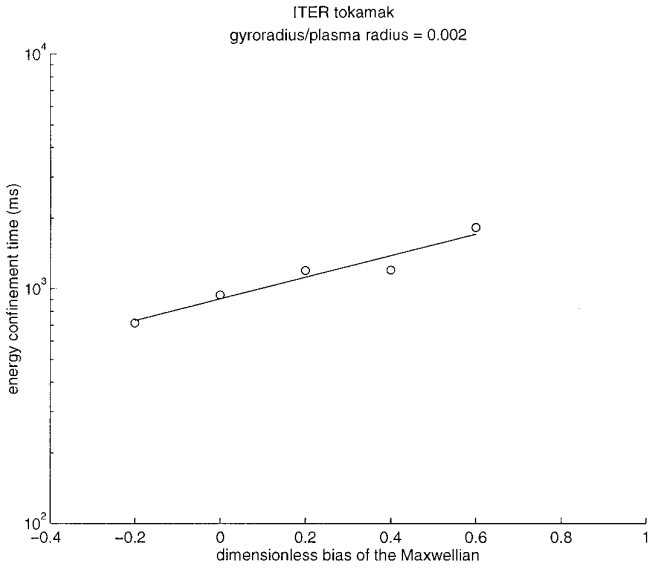


**FIG. 2.** Dependence of confinement time on the detailed structure of the collision operator. The horizontal coordinate measures deviation of the distribution function from a Maxwellian. The resulting changes in the confinement time are not large enough to compensate for failure of quasineutrality.

Legendere polynomials $P_n(\eta)$. For reasons of symmetry we restrict ourselves to even polynomials and make the choice

$$A(\eta) = P_0(\eta) + b\,P_2(\eta),$$

where $P_0$ and $P_2$ are the Legendre polynomials of degrees zero and two, respectively, divided by their norms. The coefficient $b$ specifies a dimensionless bias of the Maxwellian.

A similar modification of the random walk can be made in order to introduce anisotropy. In the coordinates $W$, $\eta$, with the flow $\mathbf{u}$ set to zero, we obtain a random walk for $W$ equal to the random walk for $\tilde{W}$ of the last section, and for $\eta$ the random walk

$$\eta_{n+1} = (1-\nu\,\Delta t)\eta_n \pm \sqrt{\nu\,\Delta t(1-\eta_n^2)} + \frac{1}{2}\frac{A'}{A}\nu\,\Delta t(1-\eta_n^2)$$

prevails, where $A'$ and $A$ are evaluated at $\eta_n$, and $\nu$ at $W_n$. Each sign in front of the square root has probability $\frac{1}{2}$.

We have run the TRAN code to assess the theory just described for the example of the ITER tokamak. The results show that there is only secondary variation of the confinement times of the ions and electrons with changes of the bias in the collision operator (see Fig. 2). Such an effect could not compensate for the failure of quasineutrality in practice. The calculations also suggest that the perturbation from constant magnetic moment $\mu$ associated with

any deviation of exact orbits from the guiding center approximation can be neglected.

### 4.3. *Decay to a Flow and Conservation of Momentum*

For two-dimensionally symmetric devices, there exists an argument showing that conservation of momentum implies ambipolarity [4]. This result can be interpreted as a consistency of quasineutrality with the equations of motion because the proof uses the magnetic field, which constrains the plasma to satisfy $\nabla \cdot \mathbf{J} = 0$. Elsewhere we have shown that a two-dimensionally symmetric quasineutral solution for transport that decays exponentially cannot exist [9]. We are thus led to investigate the effect of momentum conservation on the confinement time.

Note that for test particles the integral in velocity space of the collision operator times $\mathbf{v}$, which measures the rate of change of momentum, is not necessarily zero, because this would imply

$$\mathbf{u} = \int \mathbf{v} f \, d\mathbf{v} \Big/ \int f \, d\mathbf{v}$$

when we make the simplifying assumption that $\nu$ is independent of velocity. But $f$ is the distribution function of the test particles and not of the background particles. Even if we wanted to implement such a flow $\mathbf{u}$, it would require a large number of particles to compute a statistically significant answer, making the calculation prohibitive. That we would obtain little new information is shown below by our results with an arbitrary flow.

In the test particle model the electromagnetic field and the flow velocity $\mathbf{u}(\mathbf{x})$ are assigned. The test particles scatter against a fixed background and therefore conservation of momentum is to be understood as a decay to the flow. In other words, the first moment

$$I_c = \int \mathbf{c} f \, d\mathbf{c}$$

of the random velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}$ must converge to zero as $t$ goes to infinity. We give here a formal proof showing that our collision operator conserves momentum in this sense.

Consider the associated diffusion equation

$$\frac{\partial f}{\partial t} = \nabla \cdot [\nu e^{-m(\mathbf{v}-\mathbf{u})^2/2T} \nabla e^{m(\mathbf{v}-\mathbf{u})^2/2T} f]$$

in velocity space. Since the collision frequency is a function of $|\mathbf{c}|$ only, we can separate variables in the form

$$f = \sum f_n(t, |\mathbf{c}|) P_n(\mathbf{c}/|\mathbf{c}|),$$

where the $P_n$'s are spherical harmonics. When we compute the expected value $I_c$ of $\mathbf{c}$, all terms in the expansion drop out except for those multiplying the spherical harmonics obtained from homogeneous polynomials of degree one. We use the subscript 1 for such a term and further separate the time variable in the form

$$f_1 = e^{-kt} F(|\mathbf{c}|)$$

to arrive at the eigenvalue problem

$$-kF = \frac{-\lambda_1 \nu}{c^2} F + \frac{1}{c^2} \frac{\partial}{\partial c} \left( c^2 \, \nu e^{-mc^2/2T} \frac{\partial}{\partial c} e^{mc^2/2T} F \right),$$

where $c = |\mathbf{c}|$ and $-\lambda_1$ is the eigenvalue of the Laplacian on the unit sphere having the first degree spherical harmonics as eigenfunctions. What we need to show is that $k$ is positive.

We restrict ourselves to rapidly decaying functions of the speed because we are interested in behavior like the Maxwellian. Let us multiply through by $c^2 e^{mc^2/2T} F$ and integrate with respect to $c$. After an integration by parts we obtain the identity

$$k \int_0^\infty c^2 e^{mc^2/2T} F^2 \, dc = \lambda_1 \int_0^\infty \nu e^{mc^2/2T} F^2 \, dc + \int_0^\infty c^2 \nu e^{-mc^2/2T} \left( \frac{\partial}{\partial c} e^{mc^2/2T} F \right)^2 dc$$

from which we conclude that $k > 0$, since $\lambda_1$ is positive. The same argument shows that all moments of order greater than or equal to one converge to zero as $t \to \infty$. This proof fails for the moment of order zero because the spherical harmonic of order zero, which is constant, corresponds to the eigenvalue zero of the Laplacian on the unit sphere. In this case the eigenvalue problem admits $k = 0$ as a solution with the Maxwellian as the corresponding eigenfunction.

Next let us present numerical results demonstrating that conservation of momentum is not an essential issue for transport, so that we may set $\mathbf{u} = 0$ in the collision operator. Consider a flow parallel to $\mathbf{B}$. Monte Carlo calculations show that it produces no significant change in the confinement time. Although this flow is a typical one to consider in the guiding center approximation [10], its merit is limited. A comparison between the magnetostatic equations and Ohm's law suggests that a rotation of the plasma in the direction of $\mathbf{J}$ is to be expected because of the radial electric field. In choosing $\mathbf{u}$ parallel to $\mathbf{B}$ one could argue that we do not have a radial electric field. A simulation with $\mathbf{u}$ parallel to $\mathbf{J}$ would be more realistic. We therefore performed experiments with an arbitrary flow $\mathbf{u}_\perp$ perpen-

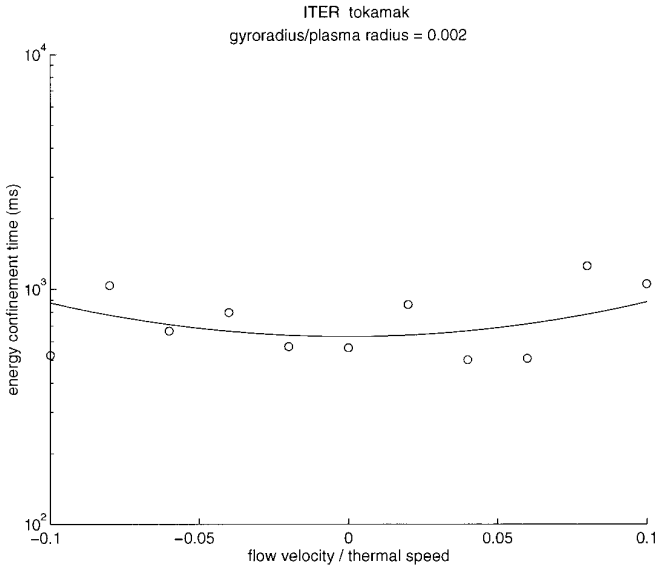


**FIG. 3.** Dependence of the energy confinement time on flow across the magnetic field. There is little change in the confinement time for values of the speed that are as much as 10% of the ion thermal speed, which suggests that conservation of momentum is a secondary issue.

dicular to **B**. We have raised $u_\perp$ to 10% of the ion thermal speed, a value bigger than is observed experimentally. Our calculations establish again that there is no significant change in the confinement time (see Fig. 3).

## 5. NUMERICAL EXAMPLES

We have shown in Section 2.2 that transport does not depend strongly on the choice of a three-dimensional mode of perturbation of the magnetic field. Now we consider the convergence of the spectral method that solves the quasineutrality equations. We shall study how the confinement time behaves when we increase the number of harmonics $P_{mn}$ of the electric potential and how the size of the perturbations of the spectrum of the magnetic field changes when we increase the number of harmonics $b_{mn}$.

In the TRAN code the guiding center ordinary differential equations are solved by a fourth-order Runge–Kutta method in which the step size is chosen so that well-defined drift surfaces can be observed in Poincaré sections. The approximation for the collision operator requires that $\nu\,\Delta t$ be small compared to one, where $\Delta t$ is the collision time step. Extensive runs have been made to assure that the Fourier coefficients $C_{mn}$ of the charge separation and the confinement times $\tau_e$ and $\tau_i$ are statistically significant.

For a convergence study we estimate the confinement time and the size of the magnetic field perturbations when we increase the number of Fourier modes $b_{mn}$ and $P_{mn}$ in the expansions of $1/B^2$ and $\Phi$. We have plotted the confinement time versus the dimensionless gyroradius for various modes, and the consistent agreement of the results at each gyroradius shows that the method does not depend strongly on the number of harmonics (see Fig. 4).

We have already discussed why quasineutrality takes precedence over Ohm's law in determining the electric field. An algorithm to solve the quasineutrality and ambipolarity equations was presented in which oscillations of the electromagnetic field and charge separation are modeled by asymmetric Fourier modes. Our contention is that three-dimensional perturbations are crucial for the existence of the quasineutral decaying solutions required for transport. The confinement times computed by this algorithm compare favorably with tokamak experimental data obtained from TFTR supershots and from the PLT, and also good agreement has been found with predictions for the ITER tokamak [5, 11].

We have compared numerical results from the TRAN code with one of the JET experiments reported in [12]. Satisfactory agreement with the experimental results once more shows that our model can explain the anomalous transport of electrons. We have also used extensive numerical calculations to derive semi-empirical scaling laws for the ITER tokamak, for the LHD stellarator now being constructed in Japan [6], and for the MHH advanced stellarator reactor [13].

Experimental parameters modeling JET are plasma major radius $R = 3$ m, horizontal plasma minor radius $a = 1$ m, and vertical plasma minor radius $b = 1.5$ m. The particle density and temperature are $n = 4 \times 10^{13}$

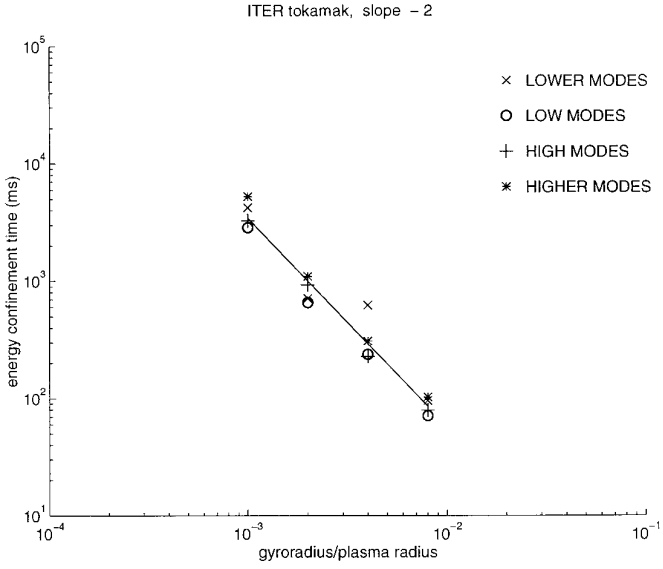


**FIG. 4.** Convergence study for the ITER tokamak. The collision frequency corresponds to the conditions $B = 5$ tesla, $T = 15$ keV, $n = 2 \times 10^{14}$ cm$^{-3}$, $\alpha = 2$, and $Z_{\text{eff}} = 1$. The scaling law $\tau_E \propto \rho_L^{-2}$ that is inferred turns out to depend only weakly on the number of Fourier modes $P_{mn}$ of the electric potential that are used.

$cm^{-3}$ and $T = 4$ keV, respectively, where we use average and not peak values. The average magnetic field strength is $B = 3$ tesla, the effective charge number is $Z = 2$, and the energy confinement time is $\tau_E = 260$ ms. These data give the values $\rho_L = 0.0025$ and $\nu = 2.5$ for the dimensionless gyroradius and the dimensionless normalized collision frequency needed in the TRAN code. We include both axisymmetric Fourier modes and three-dimensional modes with $m \leq 4$ and $n \leq 4$ that are resonant inside the plasma for our calculations. The radial electric potential is set to $-1.5$ times the temperature.

Two separate computations enabled us to study the iterative process. In a first run the three-dimensional modes of the electromagnetic field were put to zero and therefore the electron confinement time became much larger than the ion confinement time. A later run showed how three-dimensional perturbations of the fields affect transport by reducing the electron confinement time much more than the ion confinement time. The iteration continued until quasineutrality was achieved, and the resulting confinement times of the ions and electrons reached good agreement with the experimental value.

These simulations demonstrate that a two-dimensional model cannot explain experimental observations. The Monte Carlo method takes into account the complex geometry of the drift surfaces, so it models neoclassical transport that is dominated by toroidal curvature and banana orbits. If in the calculations the three-dimensional perturbations of $\Phi$ and $1/B^2$ are set equal to zero and no iteration in the electric potential is allowed, then the confinement times never come into line with measurements. However, when quasineutrality is imposed to determine the three-dimensional terms then the numerical answers agree well with observations (see Fig. 5).

Let us next discuss scaling laws. From a parameter study for the ITER tokamak we arrive at the rule

$$\tau_E \propto \rho_L^{-2}.$$

The exponent we have found for scaling with $\rho_L$ is slightly lower than would be obtained by semi-empirical rules, which suggest that the confinement time scales more like the volume. The dependence of the confinement time on $\rho_L$ deduced from runs of both the LHD and the MHH stellarators leads to a scaling law of the form

$$\tau_E \propto \rho_L^{-2.5}.$$

The results will enable us to compare the performance of these configurations at reactor conditions. All cases are run with typical values $2 \times 10^{14}$ $cm^{-3}$ for the particle number density, 10 keV for the average temperature, and 5 tesla for the average magnetic field strength, giving an approximate

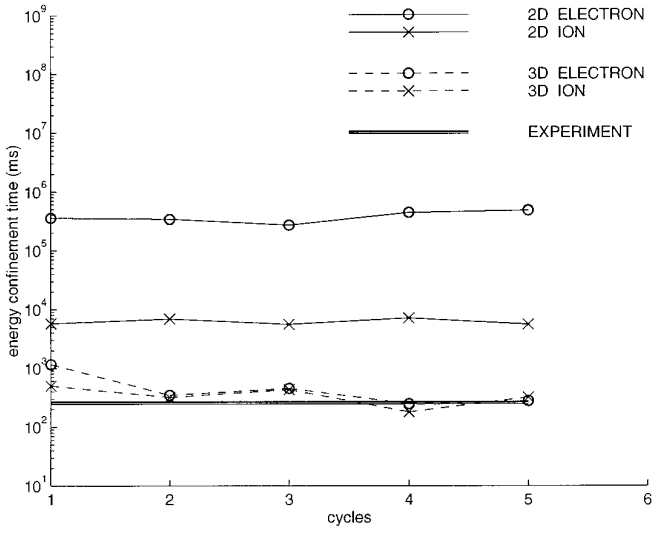


**FIG. 5.** Cycles of a Monte Carlo iteration toward quasineutrality for JET at the experimental conditions $B = 3$ tesla, $T = 4$ keV, $n_i = n_e = 4 \times 10^{13}$ $cm^{-3}$, $\alpha = 2$, $Z_{\text{eff}} = 2$, $a = 100$ cm, $b = 150$ cm, and $R = 300$ cm. Two-dimensional calculations of the electron and ion confinement times are an order of magnitude apart. When a three-dimensional perturbation brings them together then both agree with experimental data.

value of 0.002 for $\rho_L$. The LHD calculations predict an energy confinement time of 20 ms at reactor conditions, which is poor compared with the values 1 s for the ITER tokamak and 1.5 s for the MHH stellarator (see Fig. 6).

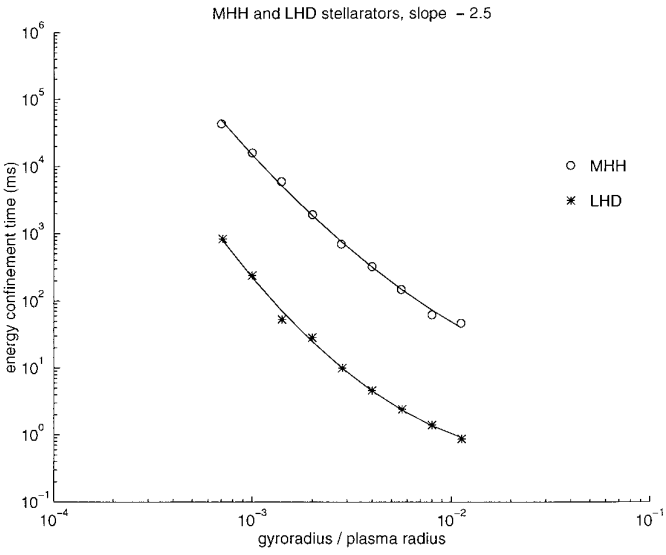


**FIG. 6.** Scaling law for the MHH and LHD stellarators. These runs are compatible with the average reactor specifications $B = 5$ tesla, $T = 10$ keV, $n = 2 \times 10^{14}$ $cm^{-3}$, $\alpha = 2$, and $Z_{\text{eff}} = 1$. The rule $\tau_E \propto \rho_L^{-2.5}$ applies to both devices, but the constants of proportionality are different. Each point required 30 min machine time on the CRAY Y-MP C90 computer.

This suggests that the latter might be as good a candidate as any for the ITER project.

## 6. CONCLUSIONS

Our study demonstrates that transport is essentially a random walk among drift surfaces. The mean free path is very much larger than the plasma radius, so the complicated geometry of the drift surfaces plays a major role. Details of the geometry are handled computationally by an appropriate ordinary differential equation solver. Conservation of momentum is a secondary issue for transport and cannot account for quasineutrality, which is a requirement for the existence of the magnetic field. Three-dimensional perturbations in the electric potential and in the spectrum of the magnetic field simulate the turbulence triggered by the displacement current.

Most models of turbulence include a factor that needs to be determined from additional information, like the eddy viscosity in the time-averaged Navier–Stokes equation. In our model we do not need any extra hypothesis because the capability of the TRAN code to compute not only the ion confinement time, but also the electron confinement time, allows us to determine auxiliary factors from quasineutrality equations. This computer code seems to be a reliable tool to investigate transport and assess experiments. By performing numerical simulations we learn that two-dimensional models are inadequate, and it is when both the ion and the electron confinement times are computed that an algorithm can be developed that compares favorably with experimental results.

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