Parallel transport modeling of linear divertor simulators with fundamental ion cyclotron heating

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Abstract
The Material Plasma Exposure eXperiment (MPEX) is a steady state linear device with the goal to perform plasma material interaction studies at future fusion reactor relevant conditions. A prototype of MPEX referred as ‘Proto-MPEX’ is designed to carry out research and development related to source, heating and transport concepts on the planned full MPEX device. The auxiliary heating schemes in MPEX are based on cyclotron resonance heating with radio frequency (RF) waves. Ion cyclotron heating (ICH) and electron cyclotron heating in MPEX are used to independently heat the ions and electrons and provide fusion divertor conditions ranging from sheath-limited to fully detached divertor regimes at a material target. A hybrid particle-in-cell code- PICOS++ is developed and applied to understand the plasma parallel transport during ICH in MPEX/Proto-MPEX to the target. With this tool, evolution of the distribution function of MPEX/Proto-MPEX ions is modeled in the presence of (a) Coulomb collisions, (b) volumetric particle sources and (c) quasi-linear RF-based ICH. The code is benchmarked against experimental data from Proto-MPEX and simulation data from B2.5 EIRENE. The experimental observation of ‘density-drop’ near the target in Proto-MPEX and MPEX during ICH is demonstrated and explained via physics-based arguments using PICOS++ modeling. In fact, the density drops at the target during ICH in Proto-MPEX/MPEX to conserve the flux and to compensate for the increased flow during ICH. Furthermore, sensitivity scans of various plasma parameters with respect to ICH power are performed for MPEX to investigate its role on plasma transport and particle and energy fluxes at the target.
1. Introduction

Understanding and controlling plasma-material-interactions (PMI) in future fusion reactors is considered a critical step towards the realization of commercially-viable power-producing fusion reactors. Present-day toroidal fusion confinement devices can explore important plasma physics questions towards this goal but are limited in their pulse duration and ion fluence on plasma facing components (PFCs). To address this limitation, steady state linear divertor simulators have been proposed [1]. In the USA, the response to this need has led to the development of a new linear divertor simulator: the Materials Plasma Exposure eXperiment (MPEX) [2, 3]. The MPEX device is currently under construction at Oak Ridge National Laboratory in the USA. A predecessor experiment, Proto-MPEX, has been used to develop the plasma source, transport, and heating concepts.

MPEX will have the capability to expose targets up to $10^6$ seconds and ion fluences ($\sim 10^{13} \text{ m}^{-2}$) not achievable in present-day and planned toroidal fusion devices. MPEX will allow exploration of questions relating to long pulse operation such as testing of novel PPC materials and power exhaust solutions, hydrodynamic retention in PFCs under steady-state conditions, etc. A key capability of MPEX will be the independent control of ion and electron temperature via the application of radio-frequency (RF) fields at suitably selected cyclotron resonant surfaces. The ion and electron heating R&D needed to develop the linear divertor simulator concept has been carried out in the Proto-MPEX device. References to previous numerical and experimental work on ion and electron heating in Proto-MPEX can be found in [4–12]. Noteable work on the subject of fundamental ion cyclotron heating (ICH) in open systems include the VASIMR electric thruster [13] and the HITOP device in Japan [14].

MPEX will expose material targets to steady-state plasma conditions that resemble those expected in the ITER divertor. The plasma conditions will be created using RF power to resonantly heat both electrons and ions via cyclotron interactions. However, these resonant heating schemes will create anisotropic and non-thermal features in the distribution function. Moreover, the open and non-uniform magnetic field used in MPEX will affect the parallel transport of particles and power to the target region due to kinetic and mirror effects during RF heating as demonstrated in [11, 12]. The final state of the plasma, subject to all these interactions (RF heating, collisions, kinetic transport, mirror effects, open and non-uniform magnetic field), cannot be fully described with fluid models [15–17] or bounced-averaged kinetic codes [18, 19]. Addressing this transport problem requires solving the Vlasov equation with appropriate particle and energy sources and coupled to electromagnetic field equations. A linearized solution to this problem has been carried out to model electron heating in Proto-MPEX subject to 2nd harmonic Electron Bernstein Wave (EBW) heating [11]; however, the electromagnetic fields and plasma moments were not coupled to the Vlasov equation. Linearization is suitable under certain scenarios but is not applicable in the general case where non-thermal and kinetic effects modify the bulk plasma.

The principal goal of the work herein presented is to investigate the parallel plasma transport in Proto-MPEX and MPEX during fundamental ion cyclotron RF heating (ICH) with up to 400 kW of power. More specifically, we aim to explore the effect of RF heating on the shape of the ion distribution function at the target, kinetic effects on parallel transport and modification of the background helicon plasma. The transport problem is addressed by solving the Vlasov equation coupled to electromagnetic fields [6] using the so-called ‘hybrid’ particle-in-cell (PIC) approach [20, 21] and adapted to the present scenario (volumetric particle sources, non-uniform magnetic field, open magnetic field lines, RF heating, Coulomb collisions). The term ‘hybrid’, in this context, refers to the process of describing ions kinetically and electrons as a fluid. In the present work, parallel transport is taken to be much greater than radial transport [11] and thus the transport problem is solved along magnetic flux surfaces; as a result, the Vlasov equation is solved by retaining one dimension in physical space (bounce-averaging is not used) and two dimensions in velocity space by describing ions using the guiding-center (GC) approximation. Moreover, Coulomb collisions are modeled with a Fokker–Planck (FP) operator [11, 22] and RF heating using a quasilinear operator [11].

The structure of this paper is as follows: in section 2, a brief description of Proto-MPEX and MPEX including the magnetic field profiles used is discussed; the hybrid PIC code: PICOS++, is introduced and its framework described in section 3; The various operators (RF heating, Coulomb collisions based on FP equation) used are described in section 4. In section 5, results from PICOS++ modeling to study the plasma parallel transport during ICH in Proto-MPEX and MPEX are presented. This includes various validation exercises of PICOS++ simulation results with existing experimental data on Proto-MPEX and predictions of plasma parallel transport for MPEX. The results are discussed in section 6 as well as the relationship to the future operation of MPEX.

2. The material plasma exposure eXperiment (MPEX)

MPEX can be divided into the following 5 regions as shown in figure 1: (a) plasma ‘Dump’, (b) ‘Helicon’ plasma source, (c) electron cyclotron heating (ECH), (d) ICH and (e) ‘PMI’
region. Each region has a different requirement for the magnetic field based on its function [3]. This leads to the non-uniform magnetic field presented in figure 1.

The ‘Dump’ region consists of a large diameter water-cooled target whose function is to terminate and recombine the incident plasma flux during steady-state operation. The magnetic field in this region needs to be diverging in order to spread out and minimize the plasma-induced heat flux. The neutral gas pressure in this region is in the order of 1 Pa.

The ‘Helicon’ plasma source [23, 24] is responsible for producing a low temperature plasma using 13.56 MHz RF fields with up to 200 kW. Based on experimental work in Proto-MPEX, the helicon plasma source operates best at a magnetic field below 0.2 Tesla and magnetic mirrors on either end. The MPEX helicon source is expected to provide around $5 \times 10^{21} \text{s}^{-1}$ deuterium ions per second to the target when operating at 200 kW and 0.2 T source magnetic field at an ionization fraction close to 0.9 [25].

The ECH region consists of a 70 GHz microwave system with up to 400 kW to drive 2nd harmonic (Electron Bernstein Wave) EBW heating via O-X-B [12]. At these conditions, the resonant magnetic field is about 1.25 T. The ICH system consists of a 4–9 MHz RF system with up to 400 kW to drive beach heating of ions at the fundamental ion cyclotron frequency [2]. In a deuterium plasma and an RF frequency of 8 MHz, the resonant magnetic field is 1.1 T.

The ‘PMI’ region consists of a water-cooled target exposed to the intense plasma flux and a magnetic field of 1 T. Given the high neutral gas pressure in both the ‘Helicon’ and PMI regions (>1 Pa), gas skimmers on either end of the heating regions are used to keep the neutral pressure in the ECH and ICH regions at about 0.01 Pa [24]. When considering all of the above, the MPEX magnetic field needs to be non-uniform (figure 1) to accommodate all the RF heating systems and PMI requirements. The magnetic field profile and the various heating scenarios for Proto-MPEX are discussed in [11, 26].

3. The PIC framework

In this section, we describe the general framework and equation set used in the ‘hybrid’ PIC code which is hereafter referred to as ‘PICOS++’ (PIC for Open Systems). PICOS++ is a multi-species, fully-parallel (MPI-openMP), electrostatic, 1D-2V hybrid PIC code used for simulating plasmas in open and non-uniform magnetic field geometries. The public repository for PICOS++ can be found in [27].

The PIC method evolves a collection of computational particles in phase space $(x,v,t)$ according to the equations of motion and subject to the self-consistent electromagnetic fields. The particle phase-space distribution is used to calculate charge and current density which become sources to the electromagnetic fields. This cycle is applied repeatedly to advance the phase-space distribution of particles forward in time. The basic PIC cycle is well illustrated in figure 1 of [28].

Fully-kinetic PIC codes have been used extensively in the plasma physics community to model processes such as laser-plasma interactions, electric thrusters, basic plasma physics, plasma instabilities, etc. Fully-kinetic PIC codes describe both electrons and ions kinetically. Due to the need to resolve both electron time and length scales, fully-kinetic codes can be computationally intensive especially if physics over ion time scales is required. A common way to reduce computational intensity while retaining ion kinetic physics is to use a ‘hybrid’ PIC approach. The term ‘hybrid’ in this paper refers to the process of describing ions kinetically while electrons as a fluid. More details of the hybrid approach can be found in [21, 29–47].
3.1. Ion distribution function

The basis of the PIC method is the Vlasov equation (equation (1)) which describes the time-evolution of the plasma consisting of charged particles which interact via long-range electromagnetic fields. In the form presented in equation (1), no collisional processes are present. The effect of Coulomb collisions, RF heating and particles sources are incorporated as source terms on the right-hand side of equation (1):

\[
\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \frac{q}{m} (E + v \times B) \cdot \frac{\partial f}{\partial v} = 0
\] (1)

The PIC method solves the Vlasov equation by using a so-called Klimontovich distribution function in equation (2), where \( N_R \) is the total number of particles in the system modeled. Each particle is described as a delta function in phase-space with a position given by \((x_i(t), v_i(t))\) and evolved in time according to the equations of motion:

\[
f_k(x, v, t) = \sum_{i=1}^{N_R} \delta(x - x_i(t)) \delta(v - v_i(t))
\] (2)

In all PIC codes, the delta functions are replaced by ‘shape’ functions to reduce shot noise [28]. Different shape functions can be used depending on the application; however, all have the effect of ‘spreading’ the particle’s dimension in phase space. All shape functions \( S \) must satisfy the property shown in equation (3) and effectively behave as a broadened delta function. More details on shape functions can be found in [25]. In PICOS++, a triangular-shaped cloud (TSC) function is used. Details are presented in appendix B: Shape and assignment function:

\[
S(x' - x_i) = \begin{cases} 
1 & \text{if } x_i \leq x' < x_i + A \left( x_i \right) \\
0 & \text{otherwise}
\end{cases}
\] (3)

An important assumption used in PICOS++ is that parallel transport dominates over radial transport; hence, particles are restricted to flow along magnetic flux surfaces only. The radial transport in Proto-MPEX and MPEX is found to be approximately two orders of magnitude slower than the paraxial transport in Proto-MPEX and MPEX is found to be. Hence, particles dominate over radial transport; hence, particles are described as a delta function over an annular cross section area \( A \) defined by the magnetic flux surface and letting the magnetic field vary along the ‘x’ coordinate leads to the Klimontovich distribution function shown in equation (4) where \( A(x_i) \) represents the plasma cross sectional area at location \( x_i \) and describes the ‘compression’ effect caused by the magnetic field:

\[
f_k(x, v, t) = \sum_{i=1}^{N_R} \frac{S(x - x_i(t))}{A(x_i)} S(v - v_i(t))
\] (4)

To proceed, the total number of real particles \( N_R \) in the plasma system is represented by a much smaller number of so-called computational particles \( N_C \). Moreover, each computational particle is given a variable weight \( a_i \) to represent an arbitrary number of super-particles. Moreover, using the paraxial approximation for the magnetic field (equation (6)), the term \( A(x_i) \) is calculated using conservation of magnetic flux \( \nabla \cdot B = 0 \) which leads to \( A(x_i) = A_0 \left( B_0 / B(x_i) \right) \), where \( A_0 \) represents a reference cross sectional area. Hence, the distribution function used in PICOS++ is shown in equation (5) where \( K = N_R / N_{SP} \) represents the number of real particles \( N_R \) for every super-particle, \( N_{SP} \) is the total number of super-particles (defined below), \( N_C \) the total number of computational particles, \( a_i \) is the number of super-particles represented by the \( i \)th computational particle and \( c_i \) is the compression factor of the \( i \)th particle. The \( S \) term represents the shape function used to represent the computational particles in both physical and velocity space. The distribution function in equation (5) is used in PICOS++ to calculate the various moments used throughout the calculation as presented in section 3.4 and appendix A:

\[
f(x, v, t) = \frac{K}{A_0} \sum_{i=1}^{N_C} a_i c_i S(x - x_i(t)) S(v - v_i(t))
\] (5)

Using the distribution function in equation (5), each computational particle has the following attributes: (a) weight \( a_i \), (b) compression factor \( c_i \), (c) position \( x_i \) and (d) velocity vector \( v_i \). These attributes are evolved in time in the PIC simulation according to the equations of motion, magnetic field profile and boundary conditions for the particles (see section 3.3). The normalization parameters used in the code is presented in appendix C.

3.2. GC equations of motion

In the PICOS++ framework, particles are described using the GC approximation. The GC description assumes the magnetic field can be described in the paraxial limit (equation (6)) and leads to the concept of magnetic moment. The use of the GC approximation removes the need to evolve the particle’s gyro-phase and as result can lead to important reduction in computational time when compared to the full-orbit description. The absence of the gyro-phase variable, however, requires the use of additional approximations to implement the RF operator and the associated heating as described in section 5. In the paraxial approximation for the magnetic field, the radial component is given by equation (6), where \( r \) is the radial coordinate. This means that the angle \( \gamma \) the magnetic field makes with the \( x \) axis satisfies \( \cos \gamma \approx 1 \). The paraxial approximation for the magnetic field is satisfied provided \( \frac{r}{B_x} \frac{\partial B_x}{\partial r} \ll 1 \):

\[
B_x(r, x) = -\frac{r}{2} \frac{d B_x}{d x}
\] (6)

The GC equations of motion employed in PICOS++ are presented in equations (7)–(9), where \( x_i \) is the position along
the ‘x’ coordinate of the ith particle, \( v_{||i} \) the parallel velocity of the ith particle, \( B_i \) and \( E_{||i} \) the magnetic and parallel electric field at the position of the ith particle respectively. The term \( \mu_i \) represents the magnetic moment of the ith particle. Note that equation (9) enforces conservation of magnetic moment.

In PICOS++, the equations of motion are advanced in time over a time step \( \Delta t \) using a 4th order Runge–Kutta method. The time interval \( \Delta t \) is chosen such that particles, on average, move less than a single grid cell \( \Delta x \) during each time step. After positions and velocities have been advanced using equations (7)–(9), other operations are applied such as projecting charge onto the grid, volumetric sources, Coulomb collisions and/or RF heating and electric field solution. These operations are described in the following sections 4 and 5:

\[
\frac{dx_i}{dt} = v_{||i} \tag{7}
\]

\[
m_i \frac{dv_{||i}}{dt} = -\mu_i \frac{dB_i}{dx} - q_i E_{||i} \tag{8}
\]

\[
d_{\mu i} = 0 \text{ where } \mu_i = \frac{m_i v_{||i}^2}{2B_i}. \tag{9}
\]

3.3. Computational domain and spatial grid

Particle positions and velocity vectors are defined continuously in phase-space (not constrained to a grid); however, all electromagnetic fields and ion moments are defined on a computational grid with finite resolution. The computational domain of length \( L \) is represented with a uniform grid with \( N_x \) number of grid cells. Each grid cell has a width \( \Delta x \) defined as a small fraction, typically 0.1–0.2, of the characteristic length \( d_i \) (see appendix C, table 1). From the MPEX example presented in appendix C, the characteristic length is defined as the ion skin depth and calculated to be about 45 mm; hence, the cell width would be defined between 4 and 9 mm.

The computational domain can be made periodic or finite in size as in the case of a linear divertor simulator. In the case of finite-sized computational domain, the left and right boundaries are labeled \( x_L \) and \( x_R \) respectively; for a given cell width \( \Delta x \) and number of grid cells \( N_x \), the spatial grid which defines the cell centers \( x_p \) is defined by equation (10). Fields and ion moments are defined at the cell centers \( x_p \). Gradients are calculated also at cell centers using central differencing. Moreover, ‘ghost’ cells are included in the computational grid to accommodate the finite size of computational particles upon introduction of ‘shape’ functions:

\[
x_p = p\Delta x + \frac{\Delta x}{2} + x_L \text{ where } p \in [0, 1 \ldots N_x - 1]. \tag{10}
\]

3.4. Moments of the distribution function

In PICOS++, moments of the distribution function are needed to: (a) calculate the electric field and (b) apply the collision operator. These moments are calculated at cell centers \( x_p \) and averaged over the cell width \( \Delta x \). These moments include the ion density \( n \), ion flux density \( \Gamma \), parallel and perpendicular ion temperature \( T_\parallel \) and \( T_\perp \), etc.

Using the distribution function in equation (5), the ion density at an arbitrary location \( x \) is defined by equation (11). Averaging over a cell width \( \Delta x \) using the operation in equation (12) leads to the ion density \( n(x_p) \) defined at the grid point \( x_p \) shown in equation (13) where \( W(x_p - x_i) \) is the so-called assignment function presented in appendix B (equation (48)) [15, 17]:

\[
n(x) = \int_{-\infty}^{+\infty} f(x') \, dx' = \frac{K}{d_x} \sum_{i=1}^{N_x} q_i c_i S(x - x_i) \tag{11}
\]

\[
n(x_p) = \frac{1}{\Delta x} \int_{x_p - \Delta x}^{x_p + \Delta x} n(x') \, dx' \tag{12}
\]

\[
n(x_p) = \frac{K}{d_x} \sum_{i=1}^{N_x} a_i c_i W(x_p - x_i). \tag{13}
\]

Having calculated all the ion moments at the cell centers \( x_p \), these values can be interpolated to the particle positions \( x_i \) using equation (14), where \( F \) represents any of the ion moment or field quantities and \( W \) is the assignment function:

\[
F(x_i) = \sum_{p=1}^{N_x} W(x_p - x_i) F_p. \tag{14}
\]

3.5. Solution to the electric field

PICOS++ solves the electric field at the cell centers \( x_p \) using the electrostatic approximation \( E = -\nabla \phi_E \) where \( \phi_E \) is the electric potential. From Faraday’s law, the electrostatic approximation leads to a time-independent magnetic field; hence, if no plasma currents are present at \( t = 0 \), no plasma currents will form at future times. This simplification is used at present for its simplicity and suitability for low-beta plasma such as those encountered in linear divertor simulators. As a result, only the electric field needs to be calculated and evolved in time.

In the ‘hybrid’ PIC approach, the electric field is solved using the generalized Ohm’s law (equation (1)) and not via the boundary value problem (BVP) defined by Poisson’s or Maxwell’s equation as in the case of fully-kinetic PIC codes. This distinction is important because the generalized Ohm’s law is an algebraic expression while Poisson/Maxwell’s equations are partial differential equations (PDEs). The critical difference lies in the fact that BVP defined by PDEs require boundary conditions to establish a unique solution; however, an algebraic equation such as the generalized Ohm’s law (equation (1)) does not need boundary conditions to establish
a unique solution. The electric field, as defined by the Generalized Ohm’s law, is a function of the moments of the distribution function as shown in equation (15) where \( n_e \) is the electron density and \( P_e \) is the electron pressure tensor, \( J_e \) the current density and \( U \) the bulk plasma flow:

\[
E = \frac{J_e \times B}{n_e} - U \times B - \frac{1}{n_e} \nabla \cdot P_e
\]  

(15)

In the absence of plasma currents and solving the transport along the magnetic flux (field-aligned) leads to a reduced version of the generalized Ohms law shown in equation (16), where \( P_{e\parallel} \) and \( P_{e\perp} \) are the electron pressure terms parallel and perpendicular to the magnetic field respectively:

\[
E_{\parallel} = -\frac{1}{en_e} \left( \frac{dP_{e\parallel}}{dx} - (P_{e\parallel} - P_{e\perp}) \right) \frac{1}{B} \frac{dB}{dx}.
\]  

(16)

3.6. Electron temperature

At present, PICOS++ uses as an isotropic description for the electron temperature profile which leads to an expression for the electric field shown in equation (17). In the event of uniform electron temperature, this expression reduces to the Boltzmann relations for electrons. In the general case, the specification of the electron temperature profile requires solution to the electron energy transport equation as presented in [20], where the effects of volumetric heating such as RF power, ion-electron energy exchange and electron-neutral elastic collisions can be incorporated. At present, PICOS++ does not have a self-consistent solution for the electron temperature profile; hence, it must be provided as an input profile to the code:

\[
E_{\parallel} = -\frac{1}{en_e} \frac{dP_e}{dx}.
\]  

(17)

4. Monte-Carlo based physics operators in PICOS++

Two Monte-Carlo based operators are used in PICOS++: (a) a Coulomb collision operator and (b) a quasi-linear RF heating operator. These are described next.

4.1. Coulomb collision operator based on Fokker-Planck (FP) equation

The Vlasov equation describes the evolution of a collection of charged particles which interact via smooth and long-range electromagnetic fields over length scales greater than the Debye length. This formulation does not include the effect of Coulomb collisions (sub-Debye length field fluctuations). Moreover, in fully ionized plasmas, small-angle cumulative Coulomb deflections is the dominant collisional process and is described via a Coulomb collision operator based on Fokker-Planck (FP) equation [48,49].

PICOS++ includes Coulomb collisions via a Monte-Carlo based FP collision operator based on [11, 22, 48]. Moreover, the FP operator is applied in the plasma reference frame. If we let \( v_i \) and \( U \) represent the \( i \)th particle velocity and plasma bulk velocity vector respectively in the laboratory frame, the \( i \)th particle velocity \( \mathbf{w}_i \) in the plasma frame is given by equation (18); hence, the particle’s pitch angle \( \theta_i \) is given by equation (19), where \( \mathbf{b} \) is the magnetic field’s unit vector:

\[
\mathbf{w}_i = v_i - U
\]  

(18)

\[
\cos \theta_i = \frac{\mathbf{w}_i \cdot \mathbf{b}}{|\mathbf{w}_i|}.
\]  

(19)

The FP operator scatters the kinetic energy \( E \) and cosine of the pitch angle \( \xi = \cos \theta \) (equation (1)) of the \( i \)th particle against all background species. This is performed in the plasma reference frame (equation (1)). The change in kinetic energy \( \Delta E_{ijk} \) and cosine of pitch angle \( \Delta \xi_{ijk} \) due to the \( i \)th particle colliding with the \( j \)th background species during the \( k \)th time step are presented in equations (20) and (21) respectively:

\[
\Delta E_{ijk} = -2\nu_{ij}^E \Delta t \left[ E_{ik} - \left( \frac{3}{2} + \frac{E_{ik} \nu_{ij}^E}{\nu_{ij}^E} \right) T_j \right]
\]  

\[
\pm 2\sqrt{T_j E_{ik} \nu_{ij}^E} \Delta t
\]  

(20)

\[
\Delta \xi_{ijk} = -\xi_{ijk} \nu_{ij}^D \Delta t \pm \sqrt{(1 - \xi_{ijk}^2) \nu_{ij}^D \Delta t}.
\]  

(21)

The terms \( \nu_{ij}^E \) and \( \nu_{ij}^D \) represent the energy loss (equation (22)) and deflection rates (equation (23)) the \( i \)th particle colliding with the \( j \)th background species. \( m_j \) and \( T_j \) represent the mass and effective temperature of the background species \( j \). The collision frequency term \( \nu_{ij}^D \) is given in equation (24). The so-called ‘Chandrasekhar’ function \( \psi(x) \) and the error function \( \phi \) are given in equation (25). The term \( w_{ij} \) represents the thermal velocity of the background species \( j \) and \( |w_i| \) the magnitude of the velocity vector of the \( i \)th particle in the plasma reference frame:

\[
\nu_{ij}^E = \nu_{ij}^0 \left( 2 \frac{m_i}{m_j} \frac{\psi(x)}{x} \right)
\]  

(22)

\[
\nu_{ij}^D = \nu_{ij}^0 \left( \frac{\phi(x) - \psi(x)}{x^3} \right)
\]  

(23)

\[
\nu_{ij}^D = \frac{n_i e^2 Z_i Z_j \ln \Lambda}{2 \pi m_i^2 c^2} \xi_{0,w_{ij}}^D
\]  

(24)

\[
x = \frac{|w_i|}{w_{ij}} \psi(x) = \frac{\phi - x (d\phi/dx)}{2x^2} \phi = \frac{2}{\pi} \int_0^\infty \exp(-y^2) \, dy.
\]  

(25)

The final kinetic energy \( E \) and cosine of pitch angle \( \xi \) of the \( i \)th particle is calculated by summing the scattering from all background species \( j \), including self-collisions and collisions with the electron fluid (equation (26)). Once the collision operator calculation is completed, the new velocity vector \( \mathbf{w}_i \) is
translated back to the laboratory frame to get \( v_i \) by inverting equation (18):

\[
E_{i,k+1} = E_{i,k} + \sum_j \Delta E_{ijk} \quad \xi_{i,k+1} = \xi_{i,k} + \sum_j \Delta \xi_{ijk}. \tag{26}
\]

It is important to note that the ‘background’ species terms \((n_i, T_i)\) referred to in equations (22)–(25) are calculated from the ion moments which have been evolved self-consistently by the code (equations (38)–(45)) and/or the electron temperature at the present time step \(k\). In this manner, the FP collision operator is non-linear since it depends on the present state of the moments of the distribution function; however, since it uses the moments rather than the distribution function itself, the operator does not capture the non-linear effects due to anisotropy in velocity space. To overcome this limitation, we plan to use the fully non-linear binary-collision FP operator described in [50].

In PICOS++, the FP operators in equations (20) and (21) are sub-cycled within the simulation time interval \( \Delta t \) in order to satisfy the Monte-Carlo condition. This is done by dividing \( \Delta t \) into \( N_s \) substeps to produce the subcycle time interval \( \delta t = N_s \Delta t \) to ensure the conditions \( \nu_i^\parallel \delta t \ll 1 \) and \( \nu_i^\perp \delta t \ll 1 \) are always satisfied. This is especially important for the low temperature plasmas to be encountered in MPEX. When these conditions are satisfied, the Monte Carlo operators are well behaved.

### 4.2. Quasilinear RF heating operator

In the GC approximation, the gyro-phase of particles is not evolved. In order to describe the resonant cyclotron interaction between charged particles and RF fields, a so-called quasilinear RF operator is implemented [11, 51, 52]. This RF operator effectively models the cyclotron resonant RF heating process as diffusion in velocity space when particles satisfy the cyclotron resonance condition shown in equation (27), where \( n \) is the harmonic number, \( \Omega_i \) the cyclotron frequency of the \( i \)th particle, \( \omega_{RF} \) the RF angular frequency, \( k_i \parallel \) the parallel wavenumber of the RF wave and \( v_{\parallel i} \) the parallel velocity of the particle in the laboratory frame:

\[
n\Omega_i = \omega_{RF} - k_i \parallel v_{\parallel i} \tag{27}
\]

For each computational particle, an attribute called ‘resonance number’ is calculated based on equation (27) in the form of \( g_i = n\Omega_i + k_i \parallel v_{\parallel i} - \omega_{RF} \), where \( i \) represents the particle index. Whenever the attribute \( g_i \) changes sign between two consecutive time steps, the particle is flagged and considered to have satisfied the cyclotron resonance condition. Particles in resonance receive a change in kinetic energy in both the perpendicular and parallel degree of freedom according to the Monte-Carlo rules given in equations (28)–(31) [11] The term \( \Delta E_{RF} \) represents the mean change in kinetic energy or ‘RF kick’ driven by the resonant interaction between the \( i \)th particle and the RF electric field and \( R_{n_i} \) is a random number between \( \pm 1 \):

\[
\Delta E_{\perp i} = \Delta E_{RF} + R_{n_i} \sqrt{2E_0 \Delta E_{RF}} \tag{28}
\]

\[
\Delta E_{\parallel i} = \left( k_i \parallel v_{\parallel i} / n\Omega_i \right) \Delta E_{\perp i}. \tag{29}
\]

The mean ‘RF-kick’ term \( \Delta E_{RF} \) in equation (28) is given in equation (30), where \( E_{RF} \) represents the amplitude of the RF electric field at the particle position, \( n \) is the harmonic number of the interaction, \( k_i \perp \) the perpendicular wave number of the wave field, \( \tau_{\parallel i} \) the gyro radius of the particle and \( \tau_{\perp i} \) the RF interaction time. This last term \( \tau_{\perp i} \) quantifies the time the particle spends in resonance with the RF wave fields based on the parallel velocity of the particle and the gradient of the magnetic field. Whenever \( \Omega_i \) is finite, such as away from turning points or in non-uniform magnetic fields, the RF interaction time is given by equation (31). Near turning points and/or near perfectly uniform magnetic fields, the interaction time is given by another expression as described in section 4.3 of [11]:

\[
\Delta E_{RF} = \left( \frac{e^2}{m} \right) \left( \frac{|E_{RF}|}{\sqrt{2\alpha_i}} \right)^2 \tag{30}
\]

\[
\tau_{\parallel i}^2 = \frac{2\pi}{n\Omega_i} \frac{d \Omega_i}{dx} \tag{31}
\]

Using equations (28) and (29) and summing over all computational particles, we can approximate the total absorbed RF power in the plasma by the expression in equation (32). This expression is a very good approximation whenever a large number of particles is used, and the following condition is satisfied: \( E_{\perp i} \ll \Delta E_{RF} \). In equation (32), \( f_{RF} \) is a flag which is equal to 1 when the particle has satisfied the resonance condition (equation (27)) in the current time step and is zero otherwise:

\[
P_{RF} \approx \frac{K}{\Delta t} \sum_{i} a_{\parallel i} f_{RF} \left( 1 + k_i \parallel v_{\parallel i} / n\Omega_i \right) \Delta E_{RF}. \tag{32}
\]

At the present stage of development, the RF electric field terms \( E_{\parallel \perp} \) in equation (30) are calculated based on the time-dependent absorbed RF power specified by the user. Using equation (32) and the value of the desired absorbed RF power, the RF wave electric field \( E_{\parallel \perp} \) is solved for at every time step. Given this power-constrained electric field, the Monte-Carlo RF operator (equations (28)–(31)) is applied to all resonant computational particles.

### 5. Results

In this section, we present the numerical results produced using PICOS++. To explore the various physics involved: (a) fluid plasma and (b) magnetic mirror effects, PICOS++ simulation results are benchmarked with the fluid code B2.5 EIRENE [15, 53] and Proto-MPEX experimental data. Next, we introduce the numerical setup used for modeling the parallel transport in MPEX with and without the use of ICH. This is followed by an exploration of the effects of ICH power on the parallel transport dynamics, plasma density profile, flow acceleration and ion flux at the target.
Details are provided in the caption. In general, the density profiles produced by PICOS++ and B2.5-EIRENE are in good agreement, except near the target region. Moreover, the parallel flow near the target region is over predicted. The mismatch between the models near the boundaries could be related to neutral gas dynamics, charge-exchange and recycling at the boundaries which is not presently included in PICOS++ where the fluid modelling with B2.5 EIRENE can capture these.

It is interesting to note that the parallel flow velocity predicted by PICOS++ near the target region agrees more with the experimental data than the B2.5 EIRENE simulations. This could be associated with the difference in flow boundary conditions in the two models. In B2.5 EIRENE, the flow at the boundary is forced to be sonic \( M = 1 \) (does not allow supersonic flows) \([15]\); whereas in PICOS++, the flow satisfies \( M \geq 1 \) at the boundary \([54, 55]\). The ion temperature \( T_i \) and electron pressure \( P_e \) from SOLPS and PICOS++ are very similar and are in reasonable agreement with the experimental data. However, there are small deviations in the PICOS+ profiles as compared to the EIRENE simulations mainly at locations where there are large gradients of magnetic field along the length of Proto-MPEX device. This is possibly due to the mirror force and magnetic compression effects captured in PICOS++. In addition, because of the strong electron-ion collisions and for long enough simulation time \( (t_{\text{sim}} = 1.3 \text{ ms}) \), the ion temperature \( T_i \) eventually slowly follows the electron temperature \( T_e \) (see figures 2 and 3(c)). Typically for \( n_e \simeq 5 \times 10^{19} \text{ m}^{-3} \), \( U \) and \( T_e \simeq 5 \text{ eV} \), the electron-ion collision time \( \tau_{ei} \simeq 0.2 \text{ ms} \) and thus, \( t_{\text{sim}} \gg \tau_{ei} \). Finally, the parallel energy flux shown in figure 3(c) predicted by PICOS++ are also in qualitative agreement with the B2.5 EIRENE data.

5.1.3. Comparison against Proto-MPEX experimental data for the helicon ± ICH case. In addition to helicon-only plasmas, research was carried out in Proto-MPEX to study fundamental
ICH in helicon plasmas. This was achieved by the installation of a left-handed ion cyclotron antenna to couple RF power at \( \sim 8 \) MHz to a preformed helicon plasma with the goal of increasing the ion temperature and thus heat flux to the target.

Recent ICH experiments in Proto-MPEX have observed ion heating with temperatures up to 15 eV at the target with up to approximately 25 kW ICH power. Both the target heat flux and ion temperature were observed to increase with ICH power. More details are in [56]. However, during ICH operations on Proto-MPEX experiments, the electron density at the target is found to decrease with ICH power. This ‘density-drop’ near the target is not desirable for Proto-MPEX and MPEX operations as the goal of the device is to operate with very high electron density (\( n_e > 10^{21} \) m\(^{-3}\)) and low electron temperature (\( T_e \sim 1 - 15 \) eV) similar to detached divertor condition in a fusion reactor [57, 58]. The ‘density-drop’ at the target as a function of ICH power obtained from PICOS++ simulations are compared against the experimental measurements in figure 5. It is evident from figure 5, that the electron density at the target \( n_e \) (normalized to electron density at the target for helicon-only case (\( n_e,\text{helicon} \)) obtained from PICOS++ simulations are in qualitative agreement with experimental observations. Both modelling and experiments on Proto-MPEX confirm that the ‘density-drop’ at the target increases with ICH power and shows signs of saturating beyond a certain threshold power as seen in figure 5. The physics-based explanation for this behavior is presented in detail in section 5.5.

5.2. MPEX simulation setup

In this section, PICOS++ is applied to the linear divertor simulator MPEX. The magnetic field profile is taken from the MPEX design requirements and the nominal plasma conditions are taken from experimental data and extrapolations from Proto-MPEX. The magnetic field profile is presented in figure 6. Because of the lack of neutral and atomic physics model and other assumptions, the primary goal is to apply PICOS++ to understand how the ICH physics and associated kinetic effects modify the parallel plasma transport on MPEX. The goal here is not to quantitatively predict the density and
temperature at the target. PICOS++ in its current formulation does not have the atomic and neutral physics to do so.

In figure 6, the axial magnetic field profile is represented by a thick black curve. The two red lines on each side are the location of left and right boundaries, the shaded green region is the location the ICH power is applied. The thin dashed horizontal line is the value of the magnetic field for ICH resonance. The dashed black curve centered around $x = 0$ m is the plasma source profile.

Table 1. Simulation parameters for Hybrid PIC modeling of MPEX.

| Simulation parameters | Physical value |
|-----------------------|----------------|
| Length of domain $L$  | 10 m           |
| Total simulation time  | 4.8 ms         |
| Peak magnetic field $B_m$ | 1.2 T        |
| Magnetic field at the source $B_0$ | 0.07 T |
| Plasma radius at the source $R_0$ | 0.05 m |
| Electron temperature $T_e$ | 15 eV |
| Initial ion temperature $T_{i||} = T_{i\perp}$ | 15 eV |
| Ion charge number $Z_A$ | 1              |
| Ion mass number $A_A$ | 2 AMU          |
| Ion density fraction   | 1              |
| Left boundary location $L_L$ | −2 m    |
| Right boundary location $L_R$ | +8 m     |
| Number of computational particles per cell | 2500 |
| Characteristic plasma density $\bar{n}_e$ | $5 \times 10^{19}$ m$^{-3}$ |
| Time step $0.5/\omega_{pi}$ |                |
| Spatial grid size      | 0.02 m         |
| Source temperature $T_{source}$ | 15 eV |
| Source spread length $\sigma_{source}$ | 0.3 m |
| Absorbed ICH power $P_{RF}$ | 0 − 400 kW |
| Harmonic number $n$    | 1              |
| RF frequency $\omega_{RF}/2\pi$ | 8.765 MHz |
| Location left of the resonance $RF_{1}$ | 4.5 m |
| Location right of the resonance $RF_{2}$ | 5.5 m |
| RF turn-on time        | 1.0 ms         |
| RF turn-off time        | 3.8 ms         |
| Parallel wave number $k_{||}$ | 20 m$^{-1}$ |
| Perpendicular wave number $k_{\perp}$ | 100 m$^{-1}$ |

Therefore, the ICH power in the simulation is applied between 4.0 m and 5.5 m as shown by the shaded green region. The initial conditions used in PICOS++ simulations for MPEX are shown in table 1.

5.3. MPEX: Helicon-only discharges

Before discussing discharges with RF heating, PICOS++ is first applied to helicon-only discharges on MPEX. The PIC simulation is evolved to steady state using a constant ion...
fueling at a rate of $G = 1 \times 10^{22}$ ions per second at a temperature of 15 eV that is expected on MPEX [2] and the spatial distribution shown in figure 6. Integrating over the entire device as a function of time produces the time-evolution of the total number of ions $N_R$ in the computational domain (equation (33)); this is shown in figure 3(a). In addition, the total ion flux [s$^{-1}$] and ion flux density [m$^{-2}$s$^{-1}$] arriving at the target as a function of time is shown in figure 3(b). The data indicate that the plasma reaches equilibrium within 2 ms. This is consistent with calculated transport timescales discussed later. Given the cross-sectional area of the plasma at the target, the mean ion flux density during steady-state reaching the target is $3 \times 10^{24}$ [m$^{-2}$s$^{-1}$]:

$$N_R(t) = \int n(x',t) A(x') \, dx'.$$

Let us now compare these numerical results with some analytical transport calculations for mirror-trapped collisional plasmas. The total number of particles in the device $N_R$ is governed by the simple differential equation shown in equation (34), where $G$ is the fueling rate and $\tau_c$ is the particle confinement time which represents the mean time to empty all the particles inside the volume of plasma. In the simple case of an isotropic plasma, usually a good approximation for a low temperature helicon plasma, the particle confinement time is given by equation (35) [59] where $R$ is the mirror ratio, $L$ is the mirror-to-mirror length and $C_s$ is the ion sound speed. This expression is only valid for plasmas which have a fully populated loss-cone distribution. Moreover, when the source $G$ is a constant in time, the solution to equation (34) with an initial condition of zero particles is given in equation (36). In steady-state, the solution becomes $N_R(t \to \infty) = \tau_c G$:

$$\frac{\partial N_R}{\partial t} + \frac{N_R}{\tau_c} = G$$

Choosing, a mirror-to-mirror length $L = 5$ and the mirror ratio of 6.7 based on figure 6, the confinement time using equation (35) is approximately 0.25 ms and is consistent with the rise time of the numerical data presented in figure 7(a). Moreover, using the fueling rate of $G = 1 \times 10^{22}$ s$^{-1}$ and the calculated confinement time of 0.25 ms, we get $N(t \to \infty) = 3.15 \times 10^{19}$. In fact, the red dashed line in figure 7(a) is obtained using equation (36) and is consistent with the numerical results. This comparison demonstrates that the simulated helicon plasma behaves as expected from simple analytical transport estimates for mirror-trapped collisional plasmas.

The steady-state plasma density $n_i$ and plasma parallel flow $U_\parallel$ (normalized to ion sound speed $C_s$) profiles calculated by PICOS++ are presented in figures 8(a) and (b) respectively. The most important observation is the accumulation of density in the source region between the magnetic mirrors. This is the mirror confinement effect produced in a collisional plasma. In addition, the parallel and perpendicular ion temperature profiles are shown in figure 9. At these temperatures and plasma densities, Coulomb collision relaxation is strong enough to fully equilibrate parallel and perpendicular temperatures. Small deviations are observed near large gradients in the magnetic field. However, from these simulations, the ion distribution is effectively isotropic.

5.4. MPEX: helicon discharges with ICH

Using the ‘helicon-only’ plasma profiles and conditions described in the previous section, ICH power is applied during the steady-state state of the helicon plasma. We now explore the effects of ion heating in MPEX.

5.4.1. Plasma confinement. ICH is applied to the helicon plasma once it reaches steady state (the time range of 1 ms and 3.8 ms) as shown by the shaded green region in figure 10. The RF power is on during a time interval of $\Delta t_{RF} = 2.8$ ms

$$N_R(t) = \tau_c G \left( 1 - e^{-\frac{t}{\tau_c}} \right).$$ (36)

**Figure 7.** (a) time-evolution of the total number of real particles $N_R$ in the simulation as a function of time; (b) total particle flux and (c) flux density with respect to time for a given constant fueling rate of $G = 1 \times 10^{22}$ ions per second.
Figure 8. (a) axial electron density $n_e$ profile for MPEX (thick black curve); (b) parallel flow $U_\parallel$ (normalized to $C_s$). The thin black line represents the magnetic field profile, provided for the reference.

Figure 9. Parallel $T_\parallel$ and perpendicular $T_\perp$ ion temperature profiles along the length of MPEX.

Figure 10. Time-evolution of (a) total number of particles in entire device, (b) ion flux arriving at the Target plate with and without 100 kW of applied ICH and (c) ion flux arriving at the dump plate with and without 100 kW of applied ICH.

and sufficiently long to enable a new steady state condition during RF heating. This can be understood from the fact that $\Delta T_{RF} \gg \tau_c$ or $\tau_\parallel$. Here $\tau_c = 1/\nu_{ij}^0$ and $\tau_\parallel = L/U_{\parallel,\text{antenna}}$ represents the collisional time and ion parallel transport time respectively, $L$ is the length between antenna and the target and $U_{\parallel,\text{antenna}}$ is the parallel bulk velocity measured at the ICH.
antenna. For electron-ion, electron-electron, and ion-ion Coulomb collisions, the 90°cumulative scattering rate $v_i^j$ of species $i$ colliding on a background species $j$ is approximately given by equation (24). For a typical ion temperature of $T_i \approx 480$ eV (maximum ion temperature observed in the simulation for 400 kW ICH power) and ion density $n_i = 4 \times 10^{19}$ m$^{-3}$, $\tau_e \sim 0.2$ ms and $\tau_i \sim 0.05$ ms which is very small compared to $\Delta t_{RF}$. The rise time in figure 10 when ICH is applied is also consistent with these calculated timescales. Because $\Delta t_{RF}$ is approximately 14 times larger than the slowest possible time scale $\tau_c$ in the simulation, we can expect plasma to reach steady state conditions during application of the RF power.

The plasma reaching steady state during ICH can also be seen from figure 10 which presents the time-evolution of (a) total number of particles in the entire device and (b) ion flux arriving at the target plate with and without 100 kW of applied ICH. It is visible from the figure 10(a) that the total number of ions increases during the heating process. In other words, application of ICH increases the confinement time of the plasma. This becomes more evident from figure 10(b) where the ion flux at the target is reduced during ICH; hence, less particles are arriving at the target. After the ICH power is turned off, the ion flux at the target further decreases and then rapidly increases as shown in the figure 10(b) at $t \approx 3.8$ ms. This is associated with the abrupt shut down of the RF power in the simulation. An increase in the ion flux is observed at the dump, albeit, later in the ICH pulse. This indicates that that in the present configuration, application of ICH reduces the ability of the plasma source to provide particles to the target and favors transport of particles to the dump. Figure 10 clearly shows that ICH increases the confinement time of the plasma (a) and that the ion flux at the target is reduced during ICH (b).

In figure 11, the (a) equilibrium electron density $n_e$ and (b) parallel flow $U_i$ (normalized to ion sound speed $C_s$) profiles along the length of MPEX during the application of the ICH are presented. The thick black curves are the ‘helicon-only’ profiles while the red curves the ‘helicon + ICH’ profiles. The shaded green region represents the location where the ICH power is applied near a resonance. The thin black curve is the axial magnetic field profile superimposed on these subplots for reference.

Figure 11. (a) electron density $n_e$ (b) parallel flow $U_i$ (normalized to ion sound speed $C_s$) profiles along the length of MPEX at 3.8 ms. The thick black curves represent the ‘helicon-only’ profiles, while the red curves the ‘helicon + ICH’ profiles. The shaded green region represents the location where the ICH power is applied near a resonance. The thin black curve is the axial magnetic field profile superimposed on these subplots for reference.

5.4.2. Ion distribution function. Figure 13 shows the distribution functions at the source, ICH and target regions during steady-state. This figure confirms that the ion distribution function at the source is essentially isotropic and Maxwellian. Moreover, the distribution function at the target has a significant drift velocity but is ‘stretched’ in the perpendicular degree of freedom indicating a two-temperature distribution as evidenced in figure 13. However, in the ICH region the distribution function is significantly anisotropic.
Figure 12. Parallel $T_{∥}$ and perpendicular $T_{⊥}$ temperature profiles along the length of MPEX at 3.8 ms. The thick black curve is the 'helicon-only' temperature profile. The thin black curve is the axial magnetic field profile superimposed on these subplots for reference.

Figure 13. Ion distribution functions at the plasma source (left), ICH region (center) and (right) target regions during the steady-state period (at 3.8 ms) with ICH power applied.

5.4.3. Force balance. The steady-state momentum transport equation along the magnetic flux [21] is given in equation (37). This expression includes the effect of magnetic compression arising due to a non-uniform magnetic field. In equation (37), first term on left hand side $f_{K} = B \frac{\partial}{\partial x} \left( \frac{M_{n} U_{∥}^{2}}{B} \right)$ is the plasma acceleration force, the first term $f_{∥} = -\frac{\partial P_{∥}}{\partial x}$ on right hand side (RHS) is the parallel pressure gradient force and the second term $f_{B} = -\frac{P_{⊥} - P_{∥}}{B} \frac{\partial B}{\partial x}$ on the RHS is the mirror force arising due to pressure anisotropy and modulated by the parallel magnetic field profile. The individual contribution from each term $f_{K}, f_{∥}$ and $f_{B}$ are analyzed using the PICOS++ simulation data as shown below in figure 14. The green shaded region is the location of ICH resonance.

A very important observation is the weak contribution of the magnetic force term ($f_{B}$) relative to the other two forces ($f_{K}$ and $f_{∥}$). This means that despite the strong ion temperature anisotropy (figure 13), the mirror force in the present situation is not important. This is mainly due to the uniformity of the magnetic field near the ICH region.

The numerical results demonstrate that the force balance is primarily between the parallel pressure and the plasma acceleration forces while the mirror force, even when significant temperature anisotropy exists, is only of secondary importance. The ICH directly accelerates the bulk plasma towards the target. This acceleration is balanced by the reaction force which pushes the bulk plasma away from the target via the pressure gradient force. These forces help to explain
5.5. Scaling with ICH power

The results presented in the previous section indicate that the plasma flux towards the target is reduced upon application of ICH power. Moreover, it indicates that the plasma flux was increased towards the dump. The main question now is how these two effects scale with increasing ICH power. In this section, we precisely investigate this question by systematically increasing the ICH power from 0 to 400 kW on MPEX while maintaining all other conditions fixed. The simulation setup is identical to that presented in the previous section.

5.5.1. Plasma density and parallel flow. Firstly, we represent the plasma density and flow velocity upstream and downstream of the ICH region as these are variables that are most strongly affected during ICH (see figure 11). Moreover, we also present the parallel and perpendicular ion temperatures at the target to quantify the level of anisotropy as a function of ICH power. The results are presented in figure 12.

During application of ICH power in MPEX, the plasma density (figure 15(a)) upstream of the ICH resonance increases but saturates to a maximum level at about 100 kW. The density drop at the target follows a similar trend. In other words, increasing the ICH power beyond 100 kW in these cases does not lead to further reduction in plasma density at the target. On the other hand, the plasma flow velocity is observed to continuously accelerate as we increase the ICH power (figure 15(b)); however, the plasma flow reduction upstream of the ICH region reaches saturation at about 100 kW.

The parallel and perpendicular ion temperatures at the target as a function of ICH power are presented in figure 15(c). The perpendicular component increases linearly with ICH power while the parallel component saturates for ICH powers greater than 200 kW. Since the parallel ion temperature is driven to a large extent by the collisional relaxation of the perpendicular degree of freedom, as the ICH power is increased, the higher temperatures mean that relaxation takes longer to occur and the increases plasma flow towards the target means that there is less time available for the ions to reach isotropy before they reach the target plate.

5.5.2. Ion flux towards the target. Given that the plasma density and flow velocity at the target scale inversely to each other as a function of ICH power, a critical question is what happens to the ion flux at the target as a function of ICH power?

In figure 16, the (a) total particle and (b) energy fluxes to the target and dump plates are presented. Figure 16(a) indicates that the total ion flux towards the target drops while at the
dump it increases when ICH power is applied; however, they both saturate at about 100 kW. This means that increasing the ICH power beyond 100 kW does not lead to further changes in parallel particle transport. This observation is very important as it suggests a potential pathway to circumvent density drops that may occur in MPEX. More details on this are presented in the discussion.

Finally, the power flux towards the target and dump as a function of ICH power are presented in figure 16(b). The results clearly demonstrate that most the ICH power absorbed is effectively coupled to the target. The other fraction of power is lost to electron-ion collisions. This collisional power should lead to an increase in electron temperature; however, this process is currently not available in PICOS++. We note that almost no ICH power is transported to the dump plate.

5.5.3. Analysis on plasma transport time scales. During ICH power scan from 0 to 400 kW, the electron density, particle flux, parallel flow $U_\parallel$, parallel ion temperature $T_{i\parallel}$ and parallel energy flux at the target (figures 15 and 16) are observed to saturate beyond 100 kW.

To gain insight into this process, it is important to note that ICH preferentially increases the ion’s perpendicular energy. It is through collisional relaxation between degrees of freedom that the parallel ion energy increases. This relaxation process takes time and increases as the ion temperature increases. However, as the plasma flow velocity increases, the time available for collisional relaxation decreases.

To quantify this process, we calculate the ratio between the ion collisional relaxation time $\tau_c$ and the parallel transport time $\tau_{i\parallel} = LU_{i\parallel}^{-1}$, where $L$ is the distance between the ICH region and target and $U_{i\parallel}$ is the ion parallel bulk velocity. As the ratio $\tau_c/\tau_{i\parallel}$ increases above 1, it indicates that collisional relaxation between degrees of freedom takes longer than the time for particles to leave the plasma. When $\tau_c/\tau_{i\parallel} \gg 1$, particles leave the plasma volume before enough time has elapsed to achieve complete collisional relaxation. Using the results from the PICOS++ numerical simulation, the ratio $\tau_c/\tau_{i\parallel}$ is shown in figure 17 as a function of ICH power.

Figure 17 indicates that at $\sim 100$ kW, the collisional and parallel transport times are similar. At lower ICH power (<100 kW), the parallel transport time is long enough to allow significant collisional relaxation. However, at higher ICH power (>100 kW), the increase in both ion temperature and parallel bulk velocity leads to incomplete collisional relaxation. Since collisional relaxation becomes less significant beyond 100 kW, the mechanism to convert perpendicular heating into parallel heating via collisions also becomes less significant. This leads to the saturation of plasma profiles beyond 100 kW measured at the target even when the ion perpendicular temperature continues to increase.

6. Discussion

In this work, a GC based 1D-2V Hybrid PIC code-PICOS++ is developed to model plasma parallel transport under the effect of (a) Coulomb collisions, (b) non-uniform magnetic field profiles (c) quasilinear RF heating operator, (d) Volumetric particle sources and (e) finite boundaries.

The main purpose for developing this Hybrid PIC code-PICOS++ is to study the plasma parallel transport with
ion cyclotron RF heating in the steady state linear divertor simulator-MPEX. The Hybrid PIC formalism [21, 47] is able to capture the evolution of distribution function determined by the interplay between RF-driven velocity space diffusion, collisional relaxation and magnetic mirror in MPEX. To test the various Monte-Carlo physics operators: Coulomb collision (FP equation) and quasilinear RF heating operators, the code is benchmarked with the existing Proto-MPEX experimental data for helicon only and helicon + ICH scenarios. PICOS++ is also benchmarked with results from the fluid code-B2.5-EIRENE. During this benchmarking exercise, the PICOS++ modeling is found consistent with the experiments and fluid simulations using B2.5-EIRENE.

6.1. ‘Density-drop’ at the target in MPEX

During the modelling with ICH in MPEX, density at the target drops significantly as compared to upstream density and consistent with past experiments observations on Proto-MPEX. This ‘density-drop’ near the target is not desirable for MPEX operations as the goal of the device is to operate with very high electron density (\(n_e > 10^{21} \text{m}^{-3}\)) and low electron temperature (\(T_e \sim 1 – 15 \text{eV}\)) similar to detached divertor condition in a fusion reactor [57, 58].

The most important observation from the modelling is that while both the density and flow velocity are strongly affected during ICH, the total particle flux towards the target is only weakly affected by the ICH power. In fact the total ion flux towards the target is observed to drop by 20% and saturates at about 100 kW (figure 16(a)). It is quite possible that the neutral gas recycling at the target along with the electron heating can be used to recover the ‘lost’ density at the target. PICOS++ currently does not have a model for neutral gas recycling and charge exchange. However, in future, a fluid neutral model can be added to PICOS++ to explore these effects on ‘density-drop’ near the target in MPEX under the effects of neutral gas recycling and charge exchange.

6.2. Particle splitting/merging algorithm

In general PICOS++ can be applied to any open magnetic field system, for instance the Wisconsin HTS Axisymmetric Mirror (WHAM) device [21, 60]. However, in the presence of very strong magnetic mirror ratios (~30) as those used in the WHAM device, the flux of particles into the loss-cone is significantly reduced relative to those observed in linear divertor simulators. This adversely impacts the computational particle statistics in the exhaust regions and the resulting numerical noise can lead to non-physical results. One possible way to deal with this is by either using adaptive mesh grids with finer spacing in the regions of interest and/or by increasing the number of computational particles in the region of poor statistics and merging the number of particles in regions of better statistics as described in [61, 62]. Noise associated with the electromagnetic fields can be smoothed out by choosing the finer grids whereas particle noise can be handled by particle splitting/merging algorithms. The particle splitting/merging algorithms are very helpful improving the statistics in specific velocity range. The implementation of adaptive mesh grid and particle splitting/merging techniques in PICOS++ to deal with simulations involving very high magnetic mirror ratios will be the subject of another paper.

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Appendix A. Ion moments

In PICOS++, the ion moments are calculated at all cell centers \(x_p\) and averaged over a cell width \(\Delta x\). The expressions used to perform these calculations are presented in equations (38)–(41). \(\Gamma_i\) represents the ion parallel flux density, \(P_{1i}\) and \(P_{2i}\) the (1,1) and (2,2) terms of the ion stress tensor (see 3.17 in [51]) respectively, and \(m\) is the ion mass:

\[
n(x_p) = \frac{K}{A_0} \frac{1}{\Delta x} \sum_{i=1}^{N_c} a_i c_i W(x_p - x_i) \tag{38}
\]

\[
\Gamma_i(x_p) = \frac{K}{A_0} \frac{1}{\Delta x} \sum_{i=1}^{N_c} a_i c_i W(x_p - x_i) v_{ii} \tag{39}
\]

\[
P_{1i}(x_p) = \frac{1}{\Delta x} \sum_{i=1}^{N_c} a_i c_i W(x_p - x_i) v^2_{ii} \tag{40}
\]

\[
P_{2i}(x_p) = \frac{1}{\Delta x} \sum_{i=1}^{N_c} a_i c_i W(x_p - x_i) v^2_{\perp i} \tag{41}
\]

Using the above ion moments, the ion parallel drift velocity, pressures (parallel and perpendicular) and temperatures are calculated using equations (42)–(44):

\[
u_{ii}(x_p) = \frac{\Gamma_{ii}}{n} \tag{42}
\]

\[
p_{ii}(x_p) = P_{1i} - m n u_{ii}^2 \quad \text{and} \quad p_{\perp}(x_p) = P_{2i} \tag{43}
\]

\[
T_{ii}(x_p) = \frac{P_{ii}}{n} \quad \text{and} \quad T_{\perp}(x_p) = \frac{P_{\perp}}{n} \tag{44}
\]
Summing over all ion species, the electron density and plasma bulk flow are given by equation (45):

\[ n_e = \sum_{\alpha} Z_{\alpha} n_{\alpha} \quad \text{and} \quad U_{||} = \frac{1}{n_e} \sum_{\alpha} Z_{\alpha} n_{\alpha} u_{\alpha||} \]  
(45)

**Appendix B. Shape and assignment function**

PICOS++ uses the TSC shape function given in equation (46) [15]. Given the position \( x_i \) of a computational particle, its charge is spread along the grid according to the shape function (equation (46)). Moreover, the fraction of the total charge assigned to an arbitrary cell center \( x_p \) with a width \( \Delta x \) is calculated using the integral in equation (47). The assignment function \( W(x_p - x_i) \) associated with equation (46) is given in equation (48):

\[
S(x_p - x_i) = \frac{1}{\Delta x} \left\{ \begin{array}{ll}
1 - \frac{|x_p - x_i|}{\Delta x} & \text{when } |x_p - x_i| \leq 1 \\
0 & \text{when } |x_p - x_i| > 1
\end{array} \right.
\]
(46)

\[
W(x_p - x_i) = \int_{x_p - \Delta x/2}^{x_p + \Delta x/2} S(x' - x_i) \, dx'
\]
(47)

\[
W(x_p - x_i) = \left\{ \begin{array}{ll}
\frac{3}{4} - \left( \frac{|x_p - x_i|}{\Delta x} \right)^2 & , 0 < |x_p - x_i| < \frac{\Delta x}{2} \\
\frac{1}{8} \left( 3 - 2 \frac{|x_p - x_i|}{\Delta x} \right)^2 & , \frac{\Delta x}{2} < |x_p - x_i| < \frac{3\Delta x}{2} \\
0 & \text{otherwise}
\end{array} \right.
\]
(48)

**Appendix C. Normalization of variables**

All input and output files used in PICOS++ are given in physical SI units. However, in the initialization stage of the computation, all physical quantities are normalized by a set of characteristic scales to reduce round-off errors. The characteristic scales selected for PICOS++ are the following: (a) the speed of light \( c \) (characteristic velocity), (b) the inverse ion plasma frequency \( (\omega_{pi})^{-1} \) (characteristic time), (c) average ion charge \( q_i \) (characteristic charge) and (d) average ion mass \( m_i \) (characteristic mass). The characteristic length \( d_i = c/\omega_{pi} \), which is the definition of the ion skin depth.

Since the plasma modelled by PICOS++ is in general time-dependent and multi-species, the inverse ion plasma frequency \( (\omega_{pi})^{-1} \) is calculated using: (a) the average ion mass \( m_i \), (b) average ion charge \( q_i \), and (c) a density value characteristic of the problem under investigation. For example, in a typical MPEX deuterium plasma, the characteristic density could be chosen to be \( 5 \times 10^{19} \text{ m}^{-3} \). This leads to a characteristic length of approximately 4.5 cm. Using the main characteristic scales: (a) time, (b) velocity, (c) mass and (d) charge, the expressions for the characteristic electric, magnetic fields and temperature are shown in table 1.

**Table A1. Characteristic plasma parameters used to normalize the simulation variables.**

| Scale       | Expression | Description |
|-------------|------------|-------------|
| Velocity    | \( c \)    | Light speed in vacuum |
| Time        | \( (\omega_{pi})^{-1} \) | Characteristic time (inverse ion plasma frequency) |
| Mass        | \( m_i \)  | Average ion mass |
| Charge      | \( q_i \)  | Average ion charge |
| Number density | \( n_i \) | Characteristic electron density |
| Length      | \( d_i = c/\omega_{pi} \) | Characteristic length (ion skin depth) |
| Electric field | \( c\omega_{pi} (m_i/q_i) \) | – |
| Magnetic field | \( \omega_{pi} (m_i/q_i) \) | – |
| Temperature | \( m_i c^2/k_B \) | \( k_B \) is the Boltzmann constant |

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