Turbulent kinetic energy in interchange-dominated drift turbulence: \(k_{\perp}\) equation and relation to particle transport

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Abstract

This paper studies the turbulent kinetic energy \((k_{\perp})\) in isothermal electrostatic interchange-dominated ExB drift turbulence, and its relation to particle transport. An evolution equation for the former is analytically derived from the underlying turbulence equations. Evaluating this equation shows that the dominant source for the turbulent kinetic energy is interchange, while the current loss to the sheath constitutes the main sink. Transport of the turbulent kinetic energy seems to plays a minor role in the balance equation. The interchange source of the turbulence is analytically related to the average turbulent ExB energy flux, while a regression analysis of TOKAM2D data suggests a model that is linear in the turbulent kinetic energy for the sheath loss. A similar regression analysis yields a diffusive model for the average radial particle flux, in which the anomalous diffusion coefficient scales with the square root of the turbulent kinetic energy. Combining these three components, a closed set of equations for the particle transport is obtained, in which no nonlinear saturation terms are required to saturate the turbulence as the source of the turbulence depends on mean flow gradients and \(k_{\perp}\) through the particle flux. Implementation of this new model in a 1D mean-field code shows good agreement with the original TOKAM2D data over a range of model parameters.

1 Introduction

The anomalous transport observed in tokamaks is generally known to be caused by turbulent fluctuations. ExB drift turbulence, fluctuating drift flows caused by electric field fluctuations, is believed to be dominant in the plasma edge \[30, 35, 13\]. Usually, the interchange instability provides the main source of this turbulence in the scrape off layer (SOL), with the drift wave mechanism playing a less important role as perturbations without a parallel component can exist in this open field-line region \[27, 28, 18\].

Various approaches have been followed to simulate this ExB drift turbulence and the related particle and heat transport, ranging from gyrokinetic models (e.g. GENE \[31\]) to fluid turbulence codes (e.g. TOKAM2D \[29\] and TOKAM3X \[32\]). However, the high computational cost of these approaches inhibits their use for simulations of complete future fusion reactors with the existing computational resources. Hence, mean-field plasma edge transport codes
SOLPS-ITER [6]), which effectively calculate averaged quantities of the flow only, are expected to remain the main instruments for the design of divertors for future reactors. However, these transport codes do not resolve the turbulence, but instead use ad-hoc transport coefficients to model the resulting turbulent transport [1, 26, 10], limiting the predictive capacities of these codes. Also in hydrodynamic turbulence modelling, there is a wide gap between detailed turbulent simulations using Direct Numerical Simulation (DNS), and the application to flows in realistic configurations. A range of techniques has been developed to bridge this gap. In DNS, the Navier-Stokes equations are solved on very short length and time scales, such that all relevant scales of the turbulence are resolved. In Large Eddy Simulations (LES), only the larger scales of the flow are resolved, while the smaller scales are filtered out and modelled using a subgrid model instead. In the Reynolds-Averaged Navier-Stokes (RANS) approach, a decomposition in time-averaged and fluctuating components leads to transport equations for the mean-field quantities, complemented with models for nonlinear closure terms [25]. Recently, Bufferand et al. [7] proposed a mean-field model for the turbulent particle transport in the plasma edge that draws inspiration from these RANS models. More specifically, the model bears similarity to $k(-\epsilon)$ models, where equations for the turbulent kinetic energy $k$ (and dissipation $\epsilon$) are solved to provide time- and length scales to model the closure terms [25]. Bufferand et al. proposed a diffusive model for the radial particle transport where the anomalous transport coefficients scale linearly with the local turbulent kinetic energy. Bufferand’s equation for the turbulent kinetic energy is based on a predator-prey model for the turbulence intensity derived by Miki et al. [21] with some ad-hoc adaptations to obtain a transport model for the turbulent kinetic energy. This model has later been refined by using global confinement scaling laws in its closure of the dissipation [3, 4, 5].

Similar to Bufferand et al., the present paper relates the average turbulent particle transport to turbulent quantities and the turbulent kinetic energy in particular. However, in this study we perform a consistent analytical derivation of the equations governing the transport and the evolution of $k_{\perp}$. Fluid turbulence codes, which resolve all the fine length- and time scales of the flow (as DNS codes do for hydrodynamic turbulence), are then used to explore the physics that need to be included in the mean-field models and to propose models for the remaining closure terms. More specifically, the isothermal TOKAM2D turbulence code [20, 23] for the scrape-off layer (SOL) is used as reference in our study. As such, 2D, isothermal, quasi-neutral, electrostatic plasmas will be investigated. The turbulence is assumed to be dominated by the interchange instability and mean quantities will only vary in the radial direction, resulting in 1D averaged profiles and transport.

The rest of this paper is structured as follows. Section 2 introduces the model describing 2D isothermal interchange turbulence, as implemented in the TOKAM2D code, that is used as a reference in this work. Next, analytical equations for the total, turbulent and mean-flow kinetic energy are derived in section 3. Section 4 evaluates the turbulent kinetic energy equation using
TOKAM2D data and investigates the balance of the sources and sinks of turbulent kinetic energy. Models for the dominant closure terms will be proposed based on a regression analysis. The same regression analysis techniques will be used to identify possible models for the average turbulent particle flux in section 5. Section 6 then compares simulation results obtained with the newly developed model to the original TOKAM2D results and to the model proposed by Bufferand et al. Finally, section 7 summarises the main findings of this work and comments on suggestions for further research.

2 Model for 2D isothermal interchange turbulence

The 2D interchange turbulence model in TOKAM2D consists of the continuity equation, the vorticity equation and the corresponding definition of the vorticity:

\[ \frac{\partial n}{\partial t} + [\phi, n] = S_n - \sigma_n c_s n \exp(\Lambda - \phi \frac{T_e}{T_e}) + D_n \nabla^2 n, \]  
\[ \frac{\partial \omega}{\partial t} + [\phi, \omega] = \frac{1}{n} [nT, gx] + \sigma_W c_s (1 - \exp(\Lambda - \phi \frac{T_e}{T_e})) + \nu \nabla^2 \omega, \]  
\[ \omega = \nabla^2 \phi. \]

In these equations \( n \) is the density, \( \phi \) the electrostatic potential, \( S_n \) the particle source, \( \sigma_N \) and \( \sigma_W \) parameters quantifying the magnitude of the sheath losses (\( \sigma \sim 1/L_{||} \) with \( L_{||} \) the parallel connection length), \( c_s \) the sound speed, \( \Lambda \) the sheath potential, \( T_e, T_i \) and \( T = T_e + T_i \) the (constant) electron, ion and total temperatures respectively, \( D_n \) a diffusion constant, \( \omega \) the vorticity, \( g \) a parameter characterising the radial decay of the magnetic field (\( g \sim 1/R \) with \( R \) the major radius of the tokamak), \( x \) the radial position and \( \nu \) a viscosity. The Poisson bracket in these equations is defined as \([P, Q] = b \cdot (\nabla P \times \nabla Q)\) where \( b \) the magnetic field unit vector. Note that all quantities in these equations are normalised to the reference gyro-frequency \( \Omega_{\text{ref}} = qB_{\text{ref}}/m \) and gyro-radius \( \rho_{\text{ref}} = \Omega_{\text{ref}}^{-1} \sqrt{T_{\text{ref}}/m} \), where \( q \) is the ion charge, \( m \) the ion mass and \( B_{\text{ref}} \) the magnetic field strength. All equations in the remainder of this paper will follow this normalisation, unless specifically mentioned otherwise.

In deriving this equation set it is assumed that the ExB drift dominates the perpendicular velocity such that it is the only component that needs to be taken into account in the convective terms and in the polarisation current term. The convective operator takes the form \([\phi, x] = V_E \cdot \nabla x\), where \( V_E \) is the ExB drift velocity. However, the definition of the Poisson bracket implies that \( V_E = b \times \nabla \phi \), hence without taking variations of the magnetic field strength into account as is normally done, i.e. \( V_E = b \times \nabla \phi / B \). As a result, \( \nabla \cdot V_E = 0 \), such that the convective operator \([\phi, x] \) may equivalently be written as \( \nabla \cdot (xV_E) \). We will write the equations in this paper in the conservative form.
using the divergence operator to allow easier generalisation to more complex models. In equation 2 the Boussinesq approximation is also made, assuming that \( \nabla \cdot J_p = \nabla \cdot (qnV_p) \approx qn\nabla \cdot (V_p) \), where \( J_p \) and \( V_p \) are the polarisation current density and velocity respectively. The parallel direction is modelled by using an analytical relations for the sheath behaviour, assuming every 2D cell to be connected to the sheath in the unresolved third direction.

As mentioned before, we will try to find a mean-field model for the turbulent transport, drawing inspiration from RANS techniques for hydrodynamic turbulence. To this end, all turbulent quantities in the governing equations are split into a mean flow and a fluctuating component. Two types of decompositions are used for this: Reynolds decomposition and Favre decomposition. The Reynolds decomposition is defined as follows [25, 8]:

\[
x = \bar{x} + x',
\]

\[
\bar{x} = \lim_{T \to \infty} \int_0^T x dt,
\]

where \( x \) can be any statistically stationary quantity and \( t \) is time. Hence, \( \bar{x} \) is the time-averaged value of \( x \), while \( x' \) is the fluctuating component. The Favre or density-weighted average, is defined as

\[
x = \tilde{x} + x'',
\]

\[
\tilde{x} = \frac{nx}{\bar{n}}.
\]

This density-weighted average is introduced because it appears naturally in compressible flow cases. These definitions imply the following relationships, which will be frequently used in the derivations below:

\[
\frac{\bar{x}}{\bar{n}} = 0,
\]

\[
\frac{x''}{\bar{n}} = 0.
\]

Note also that the time-averaging operator \( \bar{x} \) commutes with time and space derivatives, but the Favre operator \( \tilde{x} \) does not.

Given these decompositions, we will start our analysis by time-averaging the continuity equation to obtain an equation describing the evolution of the time-averaged density \( \bar{n} \):

\[
\frac{\partial \bar{n}}{\partial t} + [\tilde{\phi}, \bar{n}] + [\phi', n'] = \bar{S}_n - \sigma_n c_n n \exp(\Lambda - \frac{\phi}{Te}) + D_n \nabla^2 \bar{n}.
\]

The terms in this equation can be compared to the corresponding terms in the turbulent equation. Linear terms, such as the time derivative and diffusive terms, retain the same form as in the original equation. Nonlinear terms, such as the convective term and the sheath loss term, lead to correlations between fluctuations, and give rise to terms that require closure. Finally, \( \bar{S}_n \) represents the time-averaged source term of particles, which is just a constant in our study.
Since the diamagnetic direction in TOKAM2D is periodic, averaged quantities only vary in the radial direction. Hence, the mean field models for the turbulence that will be developed in this work will be 1D, radial models. As a result, only the turbulent ExB particle flux \( \Gamma_{E,t} = \bar{n}'V_{E}' \) contributes to the averaged (radial) total ExB particle flux because the mean field ExB particle flux \( \Gamma_{E,m} = \bar{n}V_{E} \) is zero (since gradients in the diamagnetic direction of averaged quantities are zero). For this reason the term \([\phi, \bar{n}] = \nabla \cdot \Gamma_{E,m} \) drops from equation 9. Hence, the remainder of this paper will look for models to close the turbulent ExB particle flux \( \Gamma_{E,t} = \bar{n}'V_{E}' \) in mean-field transport models.

3 Derivation of \( k_{\perp} \) equation

As the average particle transport in the 2D interchange turbulence model has been shown to be governed by the correlations between density and potential fluctuations in section 2, we aim to find a measure for the intensity of these fluctuations, and relate it to the resulting particle transport. To this end, we define the total (\( E_{k,\perp} \)), mean flow (\( E_{k,\text{mean,} \perp} \)), and turbulent (\( k_{\perp} \)) perpendicular kinetic energies as

\[
E_{k,\perp} = \frac{V_{E}^2}{2},
\]

\[
\bar{n}E_{k,\text{mean,} \perp} = \frac{\bar{n}'V_{E}'}{2},
\]

\[
\bar{n}k_{\perp} = \frac{\bar{n}'V_{E}'^2}{2}.
\]

Note that \( E_{k,\perp} \) varies rapidly in time and space as it follows the instantaneous fluctuations, while \( E_{k,\text{mean,} \perp} \) and \( k_{\perp} \) are time averaged quantities that do not change at these small scales. The latter two are constant in time in a statistical steady state, while the former is not. Note also that the sum of mean flow and turbulent kinetic energy per volume equals the averaged total kinetic energy per volume:

\[
\bar{n}E_{k,\perp} = \bar{n}E_{k,\text{mean,} \perp} + \bar{n}k_{\perp}.
\]

The turbulent kinetic energy as defined in equation 12 provides a direct measure of the characteristic (density weighed) ExB drift velocity of ions in the fluctuating electrostatic field. This is exactly the motion that is believed to cause the anomalous transport observed in the SOL that is of interest in this paper[30, 35, 13, 2]. This close link between the average radial particle flux and the perpendicular turbulent kinetic energy \( k_{\perp} \) will be confirmed by TOKAM2D data in section 5.

In the present section, we analytically derive the equation governing the transport of \( k_{\perp} \) from the vorticity equation. This will provide some insight in the physics of the turbulence and the mechanisms for its transport, creation and destruction. First, an equation for the total kinetic energy is derived in
subsection 3.1 and then equations for the mean flow kinetic energy and the turbulent kinetic energy are derived in 3.2. We follow a procedure similar to Scott[30], Garcia et al.[15] and Tran et al.[34], but rigorously accounting for density fluctuations in the kinetic energy equation.

3.1 Total kinetic energy equation

To obtain an expression for the time change of the total kinetic energy, we multiply the divergence of the polarisation velocity \( V_p \) with \( n\phi \) and use the continuity equation 1 to rewrite:

\[
\frac{\partial}{\partial t} n E_{k,\perp} + \nabla \cdot (n E_{k,\perp} V_E) = n \phi \nabla \cdot V_p - n \nabla \cdot (\phi V_p) + E_{k,\perp} S_n.
\] (14)

Applying equation 14 to the vorticity equation 2, which is effectively a charge balance equation with the left hand side representing \(-e \nabla \cdot V_p\), we find the total kinetic energy equation for the model presented in section 2:

\[
\frac{\partial}{\partial t} n E_{k,\perp} + \nabla \cdot (\Gamma_{E_{k,\perp}}) = -\phi[nT, gx] - \sigma_{Wc_s} n \phi(1 - \exp(\Lambda - \frac{\phi}{T_e}))) - \nu n \phi \nabla^2 \omega + \phi V_p \cdot \nabla n + S_{E_{k,\perp}n},
\] (15)

\[
\Gamma_{E_{k,\perp}} = n E_{k,\perp} V_E + \phi J_p,
\] (16)

\[
S_{E_{k,\perp}n} = E_{k,\perp} S_n + D_n E_{k,\perp} \nabla^2 n - E_{k,\perp} \sigma_{Nc_s} n \exp(\Lambda - \frac{\phi}{T_e})
\] (17)

The terms on the LHS of this equation represent the time rate of change and transport of \( k_{\perp} \), with the transport terms written in conservative form. In equation 15 only the ExB velocity appears in the divergence terms on the LHS. The contributions of the divergence of the parallel and diffusive flow components appear on the RHS of the equation, as part of the source term 17 consistent with the notation in equations 1 and 2. In more complete models, these two flow components would naturally be moved to the transport term on the LHS of the equation to ensure particle and energy conservation. The RHS of the equation groups sources and sinks of \( k_{\perp} \). The first two are the interchange source and loss to the sheath through divergence of the parallel current, which will turn out to be the dominant ones. The following term is a dissipation term due to the viscosity. The second but last term on the RHS is a "Boussinesq correction term" introduced by bringing \( n \) in the divergence in \( n \nabla \cdot (\phi V_p) \). This term would not have been present if the Boussinesq approximation had not been made in the vorticity equation 2.

3.2 Mean flow and turbulent kinetic energy equations

In order to arrive at equations for \( E_{k,\text{mean},\perp} \) and \( k_{\perp} \) defined in equations 11 and 12 the \( E_{k,\perp} \) equation 15 should be split in a contribution due to mean flows and a contribution due to fluctuations.
We obtain an expression for the time change of \(E_{k, \text{mean}, \perp}\) by taking the scalar product of the average polarisation current \(\bar{J}_p\) and the Favre-averaged gradient of the electrostatic potential \(\nabla \phi\) and then using the averaged continuity equation \([9]\) to rewrite:

\[
\frac{\partial}{\partial t} \bar{n} E_{k, \text{mean}, \perp} + \nabla \cdot (\bar{n} \bar{V}_E E_{k, \text{mean}, \perp} + \bar{n} \bar{V}_E^2 \bar{V}_E \cdot \bar{V}_E) = -\nabla \phi \cdot \bar{J}_p \\
+ \bar{n} \bar{V}_E^2 \bar{V}_E : (\nabla \bar{V}_E)^T + \bar{V}_E \cdot \bar{V}_E S_n + E_{k, \text{mean}, \perp} \bar{S}_n. \tag{18}
\]

In the derivation of this equation, only the ExB velocity is considered to be important for the polarisation current.

In order to use this expression starting from an averaged charge balance equation \((\nabla \cdot \bar{J} = 0)\), \(\nabla \phi \cdot \bar{J}_p\) is rewritten to include \(\nabla \cdot \bar{J}_p\):

\[
-\nabla \phi \cdot \bar{J}_p = \bar{\phi} \nabla \cdot \bar{J}_p - \nabla \cdot (\bar{\phi} \bar{J}_p) - \frac{\bar{J}_p}{\bar{n}} \nabla \bar{\phi}. \tag{19}
\]

Note that this is more complicated than for the total kinetic energy case because Favre averages and gradients do not commute. As a result, an additional "Favre averaging term", which is the last term in \([19]\) originates. A relation between the time change of \(E_{k, \text{mean}, \perp}\) and the averaged charge balance equation is finally found by inserting equation \([19]\) in equation \([18]\):

\[
\frac{\partial}{\partial t} \bar{n} E_{k, \text{mean}, \perp} + \nabla \cdot (\bar{n} \bar{V}_E E_{k, \text{mean}, \perp} + \bar{n} \bar{V}_E^2 \bar{V}_E \cdot \bar{V}_E + \bar{\phi} \bar{J}_p) \\
= \bar{\phi} \nabla \cdot \bar{J}_p + \bar{n} \bar{V}_E^2 \bar{V}_E : (\nabla \bar{V}_E)^T \bar{V}_E \cdot \bar{V}_E S_n + E_{k, \text{mean}, \perp} \bar{S}_n - \frac{\bar{J}_p}{\bar{n}} \nabla \bar{\phi}. \tag{20}
\]

Relation \([20]\) can now be applied to the vorticity equation \([2]\) to obtain the \(E_{k, \text{mean}, \perp}\) equation for the 2D interchange turbulence model:

\[
\frac{\partial}{\partial t} \bar{n} E_{k, \text{mean}, \perp} + \nabla \cdot (\bar{\Gamma}_{\text{E}_{k, \text{mean}, \perp}}) \\
= -\bar{\phi} \nabla \phi - \sigma_W \bar{c}_n \bar{n} (1 - \exp(\Lambda - \phi / \bar{T}_e)) - \bar{n} \bar{v} \nabla \bar{\omega} \\
+ \bar{n} \bar{V}_E^2 \bar{V}_E : (\nabla \bar{V}_E)^T - \frac{\bar{J}_p}{\bar{n}} \nabla \bar{\phi} + \bar{\phi} \bar{V}_p \cdot \nabla \bar{n} + S_{\text{E}_{k, \text{mean}, \perp}, \perp}, \tag{21}
\]

\[
\bar{\Gamma}_{\text{E}_{k, \text{mean}, \perp}} = \bar{n} \bar{V}_E E_{k, \text{mean}, \perp} + \bar{n} \bar{V}_E^2 \bar{V}_E \cdot \bar{V}_E + \bar{\phi} \bar{J}_p, \tag{22}
\]

\[
S_{\text{E}_{k, \text{mean}, \perp}, \perp} = E_{k, \text{mean}, \perp} \bar{S}_n + \bar{V}_E \cdot \bar{V}_E S_n \\
+ D_{\bar{n}} E_{k, \text{mean}, \perp} \nabla^2 \bar{n} + D_n \bar{V}_E \cdot \bar{V}_E \nabla^2 \bar{n} \\
- \sigma_n c_s E_{k, \text{mean}, \perp} \bar{n} \exp(\Lambda - \phi / \bar{T}_e) - \sigma_N c_n \bar{n} \bar{V}_E^2 \exp(\Lambda - \phi / \bar{T}_e) \cdot \bar{V}_E. \tag{23}
\]

In this derivation, vorticity equation \([2]\) was multiplied by the density and averaged, and the relation \(-\epsilon \bar{c}_n \bar{n} \nabla \cdot \bar{V}_p = \bar{\phi} \nabla \cdot \bar{J}_p - \epsilon \bar{\phi} \bar{V}_p \cdot \nabla \bar{n}\) was used, leading to the appearance of a "Boussinesq correction term". Also, the parallel and diffusive particle fluxes are treated like volumetric particle sink as was done before,
in section 3.1. Note that the the last four terms in $S_{E_k, \text{mean}, \perp, n}$ are still a pure transport term. Due to symmetry, the parallel contributions to the Reynolds stresses vanish.

We find the $k_{\perp}$ equation by taking the difference of the average of the $E_k, \perp$ equation (average of equation 15) and the $E_{k, \text{mean}, \perp}$ equation 21:

$$\frac{\partial}{\partial t} \bar{n} k_{\perp} + \nabla \cdot (\bar{\Gamma}_{k_{\perp}}) = \frac{\phi'(nT, gx)}{\frac{\phi'}{T_e}} - \nu \phi'(n \nabla^2 \omega)',$$

$$-nV_{E} E_{k} : (\nabla \nabla_{E})^T + \frac{J_{p}}{n} n \nabla \phi' + \phi'(V_{p} \cdot \nabla)n' + S_{k_{\perp}, n}, \quad (24)$$

$$S_{k_{\perp}, n} = \frac{1}{2} V_{E}^{\prime \prime} S_{n} + \frac{D_{n}}{2} V_{E}^{\prime \prime} \nabla_{E}^{2} n - \frac{\sigma_{N} c_{s}}{2} n V_{E}^{\prime \prime} \exp(\Lambda - \phi) \quad (26)$$

The perpendicular transport terms (second term on LHS) and the Reynolds stress terms (fourth on RHS) in equations 21 and 24 have the same form as in hydrodynamic turbulence [25, 8]. The interchange, sheath loss and viscous terms (first, second and third terms on the RHS) correspond to the pressure, the sheath loss, and the viscous stress tensor terms in a typical plasma momentum equation respectively. Comparing the $E_{k, \text{mean}, \perp}$ and the $k_{\perp}$ equations, it can be seen that both the Reynolds stresses and the Favre averaging term (fifth term on RHS) exchange energy between the turbulence and the mean flow. The latter originates from the non-commutative properties of Favre averaging and the divergence operator (see equation 19). Close inspection reveals that the Favre term has a structure similar to the turbulent transport and Reynolds energy transfer terms, which is in accordance with it appearing as an energy transfer term.

### 3.3 Relation between interchange term and turbulent fluxes

The interchange term in the perpendicular energy equations will be shown to be the dominant source of kinetic energy in section 3.1. Hence, it is of crucial importance to model this term correctly. Interestingly, an analytical expression is found that relates this important term to the ExB energy flux. In order to more clearly demonstrate that this relation is generally applicable, this section will use equation in in dimensional units (not normalised).

The interchange term in the charge balance equation or vorticity equation is the divergence of the diamagnetic current $J_{\ast} = B \times \nabla p/B^2$. Using the low $\beta$ approximation $\nabla \times B \approx 0$, this is rewritten as

$$\nabla \cdot J_{\ast} = \nabla \cdot \left( \frac{B \times \nabla p}{B^2} \right) \approx \nabla p \cdot (\nabla \frac{1}{B^2} \times B). \quad (27)$$

In order to arrive at the interchange term in the $E_{k, \perp}$ equation inter$_{E_k}$, this
divergence needs to be multiplied by the electric potential $\phi$ which can be rewritten as

$$\text{inter}_{E_k} = -\phi \nabla \cdot J_s \approx -\phi \nabla p \cdot (\nabla \frac{1}{B^2} \times B)$$

$$= -\nabla (p \phi) \cdot (\nabla \frac{1}{B^2} \times B) - p V_E \cdot \nabla \ln(B^2). \quad (28)$$

An analogous derivation is carried out for the interchange source in the $k_\perp$ equation, yielding

$$\text{inter}_k = -\phi' \nabla \cdot J'_s = -\nabla (p' \phi') \cdot (\nabla \frac{1}{B^2} \times B) - p' V'_E \cdot \nabla \ln(B^2). \quad (29)$$

Formula (29) is derived under the assumption of electrostatic turbulence, such that there are no fluctuations in the magnetic field $\vec{B}$. The relations for the interchange term reported here are in accordance with similar relations reported by Garcia et al. [14, 15]. Scott [30] also applied a similar procedure to the divergence of the ExB drift velocity.

In a 1D geometry where the magnetic field only changes in the radial direction, the first term drops out of equations (28) and (29) as the diamagnetic gradient $\nabla \lambda (p \phi)$ vanishes on average. Thus, the relation between the interchange source of kinetic energy and the ExB energy flux $p V_E$ becomes even more clear. Also, the second term is purely driven by the fluctuations in that case, as there is no mean radial component of the ExB flow. In such a 1D case, the interchange drive for the turbulence can hence only be positive if the ExB energy flux is in the direction of a decreasing magnetic field. This is consistent with the ballooning turbulence observed in experiments [11, 7, 33, 17, 12]. This also implies that the interchange term on the high field side acts as a sink of the turbulence if there is an outward ExB turbulent energy flux. In real tokamaks, this effect may be reduced or compensated by the diamagnetic contributions that vanish in 1D or by other sources of the turbulence. If the plasma is additionally assumed to be isothermal, relation (29) simplifies to

$$\text{inter}_{k,1D,iso} = -T \overline{\Gamma}_E, t \cdot \nabla_r \ln(B^2). \quad (30)$$

For the TOKAM2D model presented in section 2, the magnetic field gradients appear in the form of the factor $g$, so

$$\text{inter}_{k,T2D} = -\phi'([p,gx])' = g p' V'_{E,r}, \quad (31)$$

$$\text{inter}_{k,T2D,iso} = g T \overline{\Gamma}_E, t, \quad (32)$$

which is written in the normalised TOKAM2D units again. Relation 32 will be retrieved exactly when processing TOKAM2D simulations in section 4.2.2. Hence, it suffices to model the turbulent ExB particle flux to model the interchange term in the $k_\perp$ equation in the considered case of an isothermal 1D transport model.
4 Characterisation of the different terms in the energy equation

In this section, we investigate the balance of turbulent kinetic energy described by equation 24. The different terms in this equation are evaluated for a set of TOKAM2D simulations to identify the dominant sources and sinks in section 4.1. Then, we propose closure models for the dominant terms in Section 4.2.

4.1 Turbulent kinetic energy balance in TOKAM2D

To assess the various terms in the $k_{\perp}$ equation, we performed a large set of TOKAM2D simulations with varying input parameters $\sigma$, $g$, $T_i$ and $\nu$. The reference simulation has parameters $\sigma = 1e-4$, $g = 6e-4$, $T_i = 1$ and $\nu = 5e-3$ as in Ref. 20. These parameters have then respectively been varied by factors $0.5 - 2$, $0.75 - 1.5$, $0.5 - 2$ and $0.4 - 3$ of the reference set. The complete set of input parameters for the simulations is provided in A.1.

Figure 1 shows the evaluation of the different terms in the $k_{\perp}$ equation 24 for the default case with the standard parameter settings. In this figure, the transport terms in the left hand side of equation 24 have been moved to the right hand side (i.e. a minus sign was added to those terms). This figure clearly shows that the interchange term is the dominant source of $k_{\perp}$ while the sheath loss term is the dominant sink. The viscous term provides a secondary sink for $k_{\perp}$. The other terms are much smaller than these first three. It is particularly interesting that the transport of $k_{\perp}$ is small (parallel and perpendicular transport of $k$ are summed in figure 1), which means that the turbulent kinetic energy balance almost reduces to a local balance. Note also that the Reynolds stresses exchanging energy between the mean flow and the turbulence are very small for the cases studied here. The Favre term (which entered the equations because Favre averaging and the divergence operator do not commute) also exchanges energy between turbulence and mean flow and appears to be larger than the Reynolds stresses. The Boussinesq term is very noisy, but its average value appears to be small. Hence, it seems to be more of a numerical artefact than a physical term, which indicates that the Boussinesq approximation made in the TOKAM2D equation set is self-consistent, as the corresponding correction term is not important. The $S_{k_{\perp,n}}$ term in equation 24 involving the source term and the diffusive term from the continuity equation, is observed to be very small in the considered part of the domain in figure 1. The "subgrid" term represents the unbalance on the evaluation of the $k_{\perp}$ equation. It will be shown below that it is a numerical discretisation error, that can be reduced through grid refinement.

In figure 1, all transport terms have been plotted together. Figure 2 shows the different fluxes that contribute to this transport term separately. It is important to note that this figure plots the fluxes $\Gamma_{k_{\perp}}$ of the turbulent kinetic energy, and not the transport. The divergence of the flux gives the transport term in the $k_{\perp}$ equation for all the perpendicular terms. Note again that the parallel term has to be interpreted as the divergence of the parallel flux of $k_{\perp}$. The
Figure 1: Evaluation of the different terms in the $k_{\perp}$ equation.

Figure 2: Evaluation of average fluxes of $k_{\perp}$ in the radial and parallel direction.
parallel flux itself is not available under the T2D model assumptions, and 3D turbulence studies are required to get more insight into the nature of this term. For this reason, the parallel flux of $k_\perp$ is much smaller than the other terms, whereas its contribution to transport is of the same order of magnitude as the mean flow convection term (but has the opposite sign). This figure shows that the transport of turbulent kinetic energy is dominated by mean flow convection.

It has to be remarked that the unbalance on the $k_\perp$ equation labelled subgrid model, is not negligible as it is actually the fourth largest term in this evaluation (see figure 1). Its magnitude is about 7% of the size of the interchange source in this case.

A grid refinement study has been conducted to verify that this error reduces with increasing grid refinement. Given the first order time integration and second order spatial discretization schemes used by the code, during grid refinement we systematically reduced the cell size with a factor 2 in both directions, and the time step with a factor 4, in order to keep the CFL number constant. The exact parameters used in the TOKAM2D grid refinement simulations can be found in appendix A.1.3.

Figure 3 shows the results for the radially averaged value of the relative error on the $k_\perp$ equation and $k_\perp$ itself as a function of the grid cell size. The figure shows that the relative error and thus the magnitude of the subgrid model decrease as the grid is refined. The figure also shows that the expected 2nd order convergence has not been reached yet. Hence, the grid would have to be refined even further to complete the grid convergence study. This has not been done yet for reasons of computational cost.

The second plot of figure 3 clearly shows that $k_\perp$ increases as the grid is refined. Indeed, as the grid is refined, the dissipative effect of the discretisation error is reduced, which leads to an increase of $k_\perp$. This numerical dissipation thus acts as an additional subgrid model that is not present in the governing equations. The commonly used cell sizes and time steps ($\Delta x = \Delta y = \rho, \Delta t = \Omega[20, 23]$) will be used in the remainder of this paper, despite the error that they seem to cause, because we found no significant impact on the underlying physics interpretation or saturation behavior of the turbulence at present. However, for a detailed analysis of the forward and inverse turbulence cascades, this implied subgrid model might play an important role, and requires further investigation.

### 4.2 Development of a model for the $k_\perp$ equation

In this section, we search a model for the $k_\perp$ equation. Figure 1 has shown that the interchange term, the sheath loss term and the viscous term are the dominant ones in the energy balance for $k_\perp$, which is also observed in other simulations. Hence, we focus on these terms here. First the interchange source of the turbulence will be analysed by means of a regression analysis. Then, the sheath loss and viscous sinks will be discussed, as well as the saturation mechanism of the turbulence.
4.2.1 Methodology of the regression analysis

In this paper, we use non-linear least squares regression to extract models for the different terms in the mean-field equations that require closure. The aim is to identify the parameters $p$ in a model $f(x,p)$ that allow to reproduce the observed output quantities $y$ as closely as possible given input quantities $x$. Samples $x_i$ and $y_i$ of these quantities are available through detailed turbulence simulations. This regression analysis will also help to identify irrelevant parameters as parameter that have no significant impact on the input-output relation.

In this work, power laws are suggested as the expected model form:

$$f(x,p) = p_0 \prod_{i=1}^{N_p} x_i^{p_i}. \quad (33)$$

In this expression, $N_p$ is the amount of parameters present in the model, which equals the amount of input quantities plus one. The exponents found in these power laws indicate whether or not a certain quantity $x_j$ in $x$ is important. This allows to trim the full set of available quantities down to those relevant for $y$.

The parameters $p$ are tuned by minimising an objective function over these parameters of the model, resulting in the optimisation problem

$$\minimize_{p} \ obj(p) \quad (34)$$

$$obj = \sum_{i=1}^{N_d} \left( \frac{f(x_i,p)}{y_i} - 1 \right)^2. \quad (35)$$
In these formulae, \( N_d \) is the number of available sample points. The objective function \( 35 \) should minimise the relative error.

The data for the regression analysis is provided by 19 TOKAM2D simulations with different combinations of the model parameters \( g, \sigma, T_i \) and \( \nu \) (see appendix A.1.2). The sample points \( x_i \) and \( y_i \) are the radial profiles of the relevant quantities of these simulations. To this end, the TOKAM2D data of each simulation are averaged both in time (which is allowed because only data after convergence to a statistical steady state is used) and in the diamagnetic direction (which is a symmetry direction).

### 4.2.2 Regression analysis of the interchange term

The interchange term in the \( k_\perp \) equation is crucial to the closure of this equation as it provides the main source of the turbulence. Subsection 3.3 has already established the analytic relation \( 32 \) between the interchange term and the turbulent ExB energy flux. Figures 4 and 5 show that this relation is indeed exactly observed in TOKAM2D. Figure 4 shows that the radial profile of the averaged interchange term for the exact TOKAM2D data and for the analytical model \( 32 \) evaluated using TOKAM2D data, coincide for the reference simulation with the standard parameter settings (see appendix A.1.1).

Figure 5 shows a scatter plot of the interchange term that is obtained by evaluating relation \( 32 \) using TOKAM2D data, versus an evaluation of the exact TOKAM2D interchange term. Each circle represents a single TOKAM2D simulation (i.e. fixed parameters \( g, T, \sigma, \ldots \)) that is not only averaged in time and in the diamagnetic direction, but also in the radial direction. These types of scatter plots tend to give a clear image of the trends in the data across simulations. Figure 5 shows that the analytical relation \( 32 \) also manages to perfectly capture the trends in parameter space.

As an alternative option to model the interchange source, we analyse a model inspired by Bufferand et al. They proposed to model the interchange term using a linear growth model \( \text{inter}_k = \gamma \bar{n} k_\perp \), where the growth rate of the interchange instability in dimensional form is

\[
\gamma = c_s \sqrt{\frac{\nabla p \cdot \nabla B}{p B}} - \frac{5(1 + T_i/T_e)}{R^2}.
\]  

Here, we adapt this model to the isothermal TOKAM2D case and remove threshold part of the growth rate is removed (which allowed to match the TOKAM2D data much better) yielding

\[
\text{inter}_k = C_{\text{inter,Buff}} c_s \sqrt{-g \frac{\nabla \bar{n}}{\bar{n}}} \bar{n} k_\perp.
\]  

To determine the constant \( C_{\text{inter,Buff}} \), we perform a nonlinear regression on the set of TOKAM2D simulations as described in section 4.2.1. In this case, the output quantity of interest is the interchange term \( y = \text{inter}_k \) and
Figure 4: Comparison of TOKAM2D interchange term with models 32 and 37

Figure 5: Scatter plot for the interchange term models 32 and 37
The results of this alternative model are also shown in figures 4 and 5. It can be seen from figure 4 that a somewhat different radial profile of $k_\perp$ is obtained with model 37. The magnitude of the relative error is around 10% in this case. The default TOKAM2D case used for figure 4 lies in the middle of the parameter range investigated in the regression analysis. As a result, the model parameters are very well matched to this case specifically. It is expected that simulations further away from the center of this TOKAM2D parameter range will differ more from the TOKAM2D results. This is indeed confirmed by figure 5 which shows that Bufferand’s model 37 captures the trends in parameter space rather well, but that some scatter, error, remains. This error is especially pronounced for simulations in which the viscosities differ from the default value.

4.2.3 Sinks of $k_\perp$ and turbulence saturation

A regression according to section 4.2.1 similar to the regression analysis for the interchange term from section 4.2.2 is conducted for the sum of the main sinks, the sheath loss and viscous terms ($y = \text{sheath}_k + \text{visc}_k$). The explanatory quantities $x$ could be any set of quantities that are expected to be related to these terms. These may include fluid parameters and gradients thereof (e.g. $k_\perp, n, \nabla n, ...$), and TOKAM2D parameters (such as $g, T_i, \sigma, ...$). The regression analysis has optimised the exponents on these explanatory variables. Quantities with lower exponents have been dropped and exponents have been rounded to make the models more interpretable and physically viable. This resulted in the following model:

$$\text{sheath}_k + \text{visc}_k = C_{\text{sink}}\sqrt{\sigma c_s n k_\perp} \quad \text{with} \quad C_{\text{sink}} \approx -0.538.$$  (38)

Quantities with subscript "ref" are normalisation parameters that should correspond to global reference values. It has to be noted that the sink is found to be proportional to $\sqrt{\sigma c_s}$, whereas it was expected to scale as $\sigma c_s$, as that is the factor determining the strength of the sheath loss in the original vorticity equation 2. This is subject to further investigation.

The performance of this regression model is assessed in figures 6 and 7. Figure 6 shows that the regression model manages to capture the radial profile of the sink terms very well, with very little error remaining. The maximum relative error is smaller than 4%. The scatter plot shown in figure 7 indicates that the regression model also captures trends in parameter space rather well. The largest errors here are found in simulations where the viscosity was significantly varied from its default value. The viscosity was not retained in regression model 38 because the regression analysis that was conducted showed the exponent on it to be relatively low. Another reason not to retain a scaling with the viscosity is that physically a second sink term due to viscosity would be expected, rather than a factor on the sheath loss term.

It is interesting to see that a purely linear sink follows from the regression analysis. This is different from the quadratic sink that was proposed in the
Figure 6: Comparison of TOKAM2D interchange term with model 38.

Figure 7: Scatter plot for the on-sink model 38.
model by Bufferand et al. In combination with the linear source growth rate model for the interchange source model, such sink then led to a $k_\perp$ model of the form

$$\frac{\partial n_{k_\perp}}{\partial t} + \nabla \cdot (\Gamma_{k_\perp}) = \gamma n_{k_\perp} - \Delta \omega \cdot n_{k_\perp}^2. \quad (39)$$

In such a model, the linear drive of the turbulence causes the turbulent kinetic energy to increase initially. As $k_\perp$ increases, the nonlinear sink increases faster than the drive term and finally saturates the turbulence. Hence, the absence of any nonlinear sinks that is observed in TOKAM2D implies that the saturation mechanism is also different.

Combining the analytical relation 32 for the interchange source and regression relation 38 for the sink, we construct following model for the $k_\perp$ equation:

$$\frac{\partial \bar{n}_{k_\perp}}{\partial t} + \nabla \cdot \left( \Gamma_{k_\perp} \right) = g_T \Gamma_{E,t} - C_{\text{sink}} \sqrt{\sigma_c} \bar{n}_{k_\perp}. \quad (40)$$

If steady state is assumed and the transport terms are neglected because of the quasi-local balance that is observed, the model reduces to an algebraic expression:

$$\bar{n}_{k_\perp} = \frac{g_T}{C_{\text{sink}} \sqrt{\sigma_c}} \Gamma_{E,t}. \quad (41)$$

The idea behind this model is the following: as soon as a turbulent ExB particle flux originates (in the direction of decreasing magnetic field, indicated by $g$), this leads to an increase in the turbulent kinetic energy (through the interchange source term), which in turn causes an increase of the particle flux (see section 5) and a further build-up of the turbulence. Finally, this is saturated by a sink that is proportional to the turbulent kinetic energy. Note that no nonlinear sinks are required to saturate the turbulence in this model. Hence, the physics of the model suggested here differ markedly from model 39. Note that the presented $k_\perp$ model now features a very simple model for the sink of turbulent kinetic energy, supposedly modelling mostly the sheath loss term. More complex models for the sink could easily be implemented, e.g. a second sink with an expression more specifically adapted to the viscous sink, or any nonlinear terms that would be found to be important could be added in the future. Nonetheless, the present model will be shown to explain the TOKAM2D results very well in section 6.

## 5 Particle transport model

In this section, models for the average radial turbulent ExB particle flux $\bar{\Gamma}_{E,t} = \bar{n}' V'_E$ are developed. In Section 2 we have already shown that this flux dominates the radial particle transport in the considered 1D case.

The regression methodology discussed in section 4.2.1 is applied to find a model for $\bar{\Gamma}_{E,t}$. The input quantities $x$ of the regression analysis are chosen as any set of quantities that are expected to be related to the particle transport.
It has to be noted that quantities with lower exponents have been dropped and exponents have been rounded to make the models more interpretable and physically viable.

Figures 8 and 9 compare regression model 42, evaluated using TOKAM2D data, to the particle flux obtained from TOKAM2D directly. Figure 8 shows that both models capture the radial profile of the particle flux rather well, however, a slight decreasing trend in the relative error seems to remain. The maximum relative error on the particle flux is 25.1%. Figure 9 shows that regression model 42 manages to capture the main trends in TOKAM2D parameter space, however, some trends seem not to be fully captured by this model. The clearest one is again the one with variations in viscosity. This time, the scaling with varying sheath loss parameter $\sigma$ does not seem to be fully captured either though. Correction factors for this have been dropped in the regression analysis as they seemed to be of secondary importance.

The diffusive model 42 for the average radial particle flux is very interesting in the sense that it proves to be rather robust, using a very limited number of parameters. This model indicates that the initial hypothesis that the turbulent kinetic energy $k_\perp$ plays an important role in the particle transport holds. In its dimensionless form $D = C_D \sqrt{\kappa_\perp}$, the diffusion coefficient in this model only depends on characteristics of the turbulence. It could be argued that these are the only parameters the diffusion coefficient should depend on as the
turbulence is the driver of the particle transport and no macroscopic, geometric parameters such as \( g \) or \( \sigma \) should be involved. Also, this square-root-scaling seems quite intuitive and is also found in hydrodynamic turbulence modelling. In RANS models for hydrodynamic turbulence, the turbulent transport of a passive scalar is often modelled using the gradient diffusion hypothesis. The diffusion coefficient therein is commonly related to the turbulent viscosity, which is assumed to scale as \( l_m \sqrt{k} \) in one-equation \( k \)-models, where \( l_m \) is a suitable length scale [25].

The diffusive model proposed by Bufferand et al. [7] provides an alternative model for this particle flux:

\[
\bar{\Gamma}_{E,t} \sim -\frac{a k_\perp}{c_s} c \nabla \bar{n}.
\] (43)

In this equation, \( a \) is the minor radius of the tokamak. This model is adapted to the 2D interchange turbulence model [13] by assuming a constant aspect ratio, such that the minor radius is proportional to the major radius, and thus inversely proportional to the magnetic field curvature \( a \sim 1/g \). Thus,

\[
\bar{\Gamma}_{E,t} = -C_{D,Buff} k_\perp \frac{k_\perp}{c_s g} \nabla \bar{n}.
\] (44)

The regression methodology presented in section 4.2.1 (with \( y = \bar{\Gamma} \) and \( x = k_\perp \nabla \bar{n} / (c_s g) \)) yields \( C_{D,Buff} \approx 0.507 \).

Figure 8 shows that the relative error on the radial profile of the particle flux is more pronounced for the adapted Bufferand’s model. The maximum
relative error is 35.7%. Figure 9 indicates that model 44 also performs less good in parameter space.

Despite the merits of the diffusive models presented here, literature seems to indicate that the nature of the particle transport in the plasma edge is not diffusive, but rather due to the convective/ballistic transport of radially propagating structures such as avalanches and blob-filaments [24, 15, 16, 11]. These blobs might be interpreted as a result from the gradient removal mechanism [28, 22, 18]. Possibly, the diffusive model proposed here could be interpreted as the averaged result of such intermittent blob transport. This may lead to diffusion-like behaviour on longer time scales, where particles seem to be transported down the gradient. Hence, the underlying particle transport physics may not be diffusive, but its statistical average may appear to be. It may nonetheless be interesting to research particle transport models that better incorporate these supposed underlying convective properties. Inspiration for such models might be drawn from characteristic blob propagation velocity models [14, 11].

6 Complete 1D transport model and implementation in DivOpt

The models developed above are combined to obtain a closed system of equations for the average density. This complete model is implemented in a 1D mean-field finite volumes code that can simulate the average turbulent transport, whereas all the previous sections have only post-processed TOKAM2D data. In this section, the results of simulations with this model are compared to the exact TOKAM2D results, and to our interpretation of the model proposed by Bufferand et al. [7].

6.1 Proposed mean-field transport models

Combining $k_\perp$ model [40,41] developed in section 4 with the particle flux model [42] that depends on $k_\perp$ found in section 5 the radial transport in the averaged continuity equation 9 can be closed. The resulting model equations proposed in this paper are repeated below in their dimensional form:

$$\frac{\partial \bar{n}}{\partial t} + \nabla \cdot (\bar{n} \bar{V}_E + \bar{\Gamma}_{E,t} - D_n \nabla \perp \bar{n}) = -\sigma c_s \bar{n}, \tag{45}$$

$$\bar{\Gamma}_{E,t} = -C_D \sqrt{k_\perp} \nabla \perp \bar{n} = -D \nabla \perp \bar{n}, \tag{46}$$

$$\frac{\partial \bar{n}k_\perp}{\partial t} + \nabla \cdot (\bar{\Gamma}_{k_\perp}) = gT \bar{\Gamma}_{E,t} - C_{sink} \sqrt{\sigma} c_s \bar{n}k_\perp \tag{47}$$

$$\bar{n}k_\perp = \frac{g c_s}{C_{sink} \sqrt{\sigma}} \bar{\Gamma}_{E,t}, \tag{48}$$

$$\bar{\Gamma}_{k_\perp} = k_\perp \bar{\Gamma} - C_{Dk} D \nabla (\bar{n}k_\perp), \tag{49}$$

$$C_D = 23.9, \quad C_{sink} = 0.561, \quad C_{Dk} = 0.24. \tag{50}$$
Note that either \( k_\perp \) equation 47 or its steady-state-local-balance-equivalent 48 should be used, not both. Also, some additional models have been filled out in these equations: in equation 45 the particle source has been neglected as none is present in the considered part of the TOKAM2D domain, the exponential in the sheath loss term in this equation has been dropped as it seemed to have very little influence and in equation 47 the turbulent kinetic energy flux has been modelled as the exact analytical mean flow convection term and a diffusive contribution for the turbulent convection. The constant \( C_{Dk} \) for the latter has been determined by means of a regression analysis. This last model is quite crude though and might need to be improved in the future. It also has to be noted that the value of the \( k_\perp \) sink parameter \( C_{\text{sink}} \) has been determined from a regression analysis for \( \text{inter}_k \approx C_{\text{sink}} \sqrt{\sigma_c \bar{n} k_\perp} \) and not as the value found in equation 38. In this way, all sinks are collected in this single sink and assumed to exactly balance the source of the turbulence locally (which is approximately observed, quasi-local balances). This allows to implicitly treat the effect of all the minor terms in the \( k_\perp \) balance without having to model all of them.

In the model presented here, the turbulence level and the transport are determined by the interaction between the source of the turbulence and the mean flow gradients. The source of the turbulence depends on the particle flux, which in turn depends both on \( k_\perp \) and the mean flow density gradient, where the density gradient depends on the magnitude of the turbulent diffusion coefficient that is determined by \( k_\perp \). Parallel sheath dynamics constitute main sink mechanism of the turbulence.

This behaviour seems to be compatible with the gradient removal mechanism for turbulence saturation. The idea behind this is that pressure or density gradients determine the growth rate of the turbulence (see for example equations 37 and 36). Due to the turbulence that develops, the mean flow pressure and density gradients are relaxed, leading to a reduced growth rate of the turbulence or even to its removal. This leads to intermittent behaviour, where gradients are first build up, until the instability threshold is reached and causes a sudden, large outburst due to turbulent transport [28, 22, 18]. Arguably, the model presented here contains the averaged result of these dynamics, which lead to a shift of the equilibrium due to the interaction between the mean-flow gradients, the resulting turbulence, and the transport caused by the turbulence. Note that the sheath losses also play a non-negligible role in the model presented here (constituting a linear sink of \( k_\perp \)). This seems to be in accordance with Ricci and Rogers [28] and Halpern et al. [18], who also seem to suggest that parallel transport to the wall is the main removal mechanism for the turbulence in the gradient removal regime. However, the sheath loss in our model is not directly due to the parallel convection, but rather due to the current to the sheath. More analysis of the gradient removal mechanism, and on its link with the model presented here is required though. It could be especially illuminating to investigate time series and transient behaviour in TOKAM2D.

The new model 45-50 introduced here forms an alternative to the model proposed by Bufferand et al., which has been adapted to the TOKAM2D case.
as summarised here:

\[ \Gamma_{E,t} = -C_{D,Buff} k_{\perp} \frac{mcg}{k_{\perp}} \nabla_{\perp} \bar{n} = -D_{Buff} \nabla_{\perp} \bar{n}, \quad (51) \]

\[ \frac{\partial \bar{n} k_{\perp}}{\partial t} + \nabla \cdot (\bar{\Gamma}_{k_{\perp}}) = C_{\text{inter,Buff}} cs \sqrt{-g \nabla \bar{n}} \bar{n} \bar{k}_{\perp} - C_{\text{sink,Buff}} \bar{n} k_{\perp}^2, \quad (52) \]

\[ k_{\perp} = \frac{C_{\text{inter,Buff}} cs}{C_{\text{sink,Buff}}} \sqrt{-g \nabla \bar{n}} \bar{n} , \quad (53) \]

\[ \bar{\Gamma}_{k_{\perp}} = k_{\perp} \bar{\Gamma} - C_{Dk} D_{Buff} \nabla (\bar{n} k_{\perp}), \quad (54) \]

\[ C_{D,Buff} = 0.507, \quad C_{\text{inter,Buff}} = 2.21, \quad C_{\text{sink,Buff}} = 5.84. \quad (55) \]

Either equation (52) or equation (53) should be used as \( k_{\parallel} \) model, again depending on whether or not the steady-state-quasi-local-balance-approximation is made. In these equations, the source term consists of the interchange term found in expression (37) and a sink term quadratic in \( k_{\perp} \) that saturates the linear source is assumed to exist. As a crude approximation, this sink is assumed not to scale with any TOKAM2D parameters, i.e. \( \text{sink}_{k_{\parallel}} \sim \bar{n} k_{\perp}^2 \) only. Note however that recent studies do include a dependence on machine parameters in this sink term in the Bufferand et al.’s model [3, 4, 5]. A regression analysis has been conducted to determine the corresponding constant \( C_{\text{sink,Buff}} \) such that equation (53) matches the TOKAM2D \( k_{\parallel} \) results across all simulations as good as possible. Note however that this sink term is ad-hoc as no large nonlinear sink terms have been identified in TOKAM2D in this analysis.

### 6.2 Implementation in DivOpt and results

DivOpt [9] is a 2D (poloidal plane) finite volume code that is used as a testing code in the KU Leuven TME-TFE research group. For the implementation of the above 1D models only the continuity equation is retained, in which models for the flux are filled out. The turbulent kinetic energy equation is also implemented. Note that the mean field transport terms in equation (45) have been neglected because \( D_{m} \) is very small and the radial ExB velocity is zero in the considered 1D case. DivOpt does not use normalised quantities, so the transport models and the \( k_{\perp} \) equation are implemented in their dimensional form. Neumann boundary conditions are applied in the diamagnetic direction to arrive at a 1D code. On the radial boundaries, either Dirichlet or flux boundary conditions that exactly match the TOKAM2D data are applied for the density.

No boundary conditions for \( k_{\perp} \) are required if a steady state local balance version of the \( k_{\perp} \) equation is used, i.e. equation (48) or (53) as these are just algebraic relations. This is a significant advantage of these models, next to the reduced complexity and computational cost. The PDE versions of the \( k_{\perp} \) equation (47) or (52) on the other hand do require boundary conditions on the radial boundaries for \( k_{\perp} \) as well. Dirichlet boundary conditions are again taken from the exact TOKAM2D data. Flux boundary conditions are obtained from the observed flux of \( k_{\perp} \) in simulations with Dirichlet conditions. However, if no
TOKAM2D results would be available (and no other additional information for that matter), it would be hard to determine suitable boundary conditions. In this work, no attempt is made to find generally valid boundary conditions for $k_{\perp}$. More research into this topic is certainly required.

If boundary conditions are chosen in this way, the type of boundary conditions (Dirichlet or flux) that are applied on radial edges does not seem to significantly alter the results for most of the models presented above. However, the Bufferand model using PDE 52 does become much less numerically stable for flux boundary conditions. Also, if a PDE model for $k_{\perp}$ (47 or 52) is used, the simulation becomes relatively sensitive to the exact value of the boundary conditions that are applied. The algebraic models 48 and 53 seem to perform very consistently for all types of boundary conditions and appear to behave robustly with respect to (relatively small) changes in the value of the boundary conditions.

Figures 10-13 show the resulting profiles for density, particle flux, diffusion coefficient and turbulent kinetic energy for four DivOpt simulations, compared to the exact TOKAM2D results (that have been dimensionalised). The four models that are compared are two simulations with the transport model 45-50 proposed in this paper, one with $k_{\perp}$ equation 47 and one with 48 and two simulations with the tuned Bufferand model 51-55 one with $k_{\perp}$ equation 52 and one with 53. Flux boundary conditions are applied on radial edges for the density and Dirichlet conditions are applied for $k_{\perp}$ for all four models. The results shown here are the ones for the default TOKAM2D case (see appendix A.1.1). Note that all forward simulations feature the exact dimensionalised TOKAM2D parameters $g$, $\sigma$, $T$, i.e. no attempt has yet been made to obtain these parameters from the DivOpt geometry. The 1D DivOpt geometry has only been matched to TOKAM2D by having the same radial domain length. In the future, the DivOpt code could of course be extended in that direction, however, the main goal of this section is to show that the models are capable of reproducing the TOKAM2D results with reasonable accuracy. The global reference values used for making the TOKAM2D variables dimension are $n_{ref} = 10^{19}\text{m}^{-3}$, $T_{ref} = 50\text{eV}$, $B_{ref} = 1.725T$ and $m = m_D$. The simulations are run on a 48x4 (radial cells x poloidal cells) grid, where the number of poloidal grid cells is unimportant because of the symmetry in that direction.

Figures 10 and 11 show that all four models are capable of predicting the density and the particle flux, which are ultimately the main macroscopic quantities of interest, up to a high accuracy. The "secondary quantities" being the diffusion coefficient and the turbulent kinetic energy are also approximated relatively well by the different models as can be seen in figures 12 and 13. However, the error on these quantities is significantly higher and the difference between the various models is much more pronounced.

A first thing that can be noted is that both PDE models show rather peculiar profiles for $k_{\perp}$. This is probably because the crude models for the transport of the turbulent kinetic energy that are used are slightly mismatched with the exact boundary conditions that are applied. The profiles of $k_{\perp}$ could indeed be brought closer to the desired profile by adjusting the boundary conditions.
Figure 10: Comparison of density profiles of forward DivOpt simulations with different models for $k_{\perp}$ and particle transport.

Figure 11: Comparison of particle flux profiles of forward DivOpt simulations with different models for $k_{\perp}$ and particle transport.
Figure 12: Comparison of diffusion coefficient profiles of forward DivOpt simulations with different models for $k_\perp$ and particle transport.

Figure 13: Comparison of turbulent kinetic energy profile of forward DivOpt simulations with different models for $k_\perp$ and particle transport.
and/or the constant \( C_{\text{sink}} \). However, this is not rigorously explored in this paper as the goal is to arrive at a physically viable model based on TOKAM2D data.

The steady state model proposed in this paper can be seen to match the TOKAM2D \( k_\perp \) profile the closest, while the steady state Bufferand profile seems to be too flat. However, the trend in the diffusion coefficient is more similar for both steady state models, because of the different scaling with \( k_\perp \) \( (D \sim \sqrt{k_\perp} \) and \( D_{\text{Buff}} \sim k_\perp \) respectively). Hence, surprisingly, the Bufferand model seems to perform about as good as the new model proposed here. Interestingly the inaccuracies on its particle transport and \( k_\perp \) models seem to compensate each other.

The model parameters are very well matched to the default TOKAM2D case used for the above simulations since it lies in the middle of the parameter range investigated in the regression analyses (see appendix A.1). Figure 14 on the other hand gives an idea of the kind of errors that can be expected with varying TOKAM2D parameters. It shows a scatter plot of the diffusion coefficient that is obtained by filling out \( k_\perp \) models 48 and 53 respectively in the corresponding particle diffusion coefficient relations 46 and 51 evaluated using TOKAM2D data, versus the exact TOKAM2D diffusion coefficient. Each circle in figure 14 represents a single TOKAM2D simulation (i.e. fixed TOKAM2D parameters \( g, T, \sigma, \ldots \)) that is not only averaged in time and in the diamagnetic direction, but also in the radial direction. Thus, this figure is constructed by post-processing TOKAM2D data, no forward DivOpt simulations have been run to make it. Figure 14 seems to indicate that the newly proposed model manages to capture the scalings of the particle transport in TOKAM2D parameter space relatively well, although some scatter, error, does remain. The Bufferand model on the other hand appears to miss the trends in parameter space. Including a scaling with TOKAM2D parameters in the sink for \( k_\perp \) in equations 52 and 53, as proposed in Refs. 3, 4, 5, might (partially) remedy this discrepancy.

7 Conclusion

This contribution has analysed the average turbulent kinetic energy in 2D isothermal electrostatic interchange-dominated ExB drift turbulence and its relation to particle transport. Models for both have been developed and tuned, based on data from the TOKAM2D turbulence code.

A time evolution equation for the turbulent kinetic energy has been derived analytically for this model and evaluated exactly using TOKAM2D data from numerous simulations across a range of parameters. The results indicate that the turbulent kinetic energy balance is dominated by the interchange source and a sink due to current losses to the sheath. The viscous dissipation term plays a secondary role, while transport of \( k_\perp \) is observed to be small.

An analytical relation between the interchange source term of turbulent kinetic energy and the average particle flux has been derived, which directly leads to ballooning effects, especially in 1D geometries. A regression analysis has identified a model for the sheath loss sink that is linear in the turbulent kinetic
energy. Based on a similar regression analysis of TOKAM2D data, a diffusive model that scales with the square root of the turbulent kinetic energy has been proposed for the average radial turbulent particle flux. Combining the latter three elements, a closed model for the radial particle flux is obtained. The transport in this model is determined by mean-flow gradients and the turbulence level, whose source is in turn controlled by the particle transport, while parallel dissipation due to the sheath provides a linear sink of the turbulence. This might be interpreted as a steady state effect of the gradient removal mechanism for turbulence saturation\[28, 22, 18\].

The developed transport model has been implemented in a 1D mean-field code and has been shown to be capable of reproducing the TOKAM2D results with high accuracy. The version of the model with the algebraic steady state quasi-local balance equation for the turbulent kinetic energy proved to be especially accurate and robust. This new model provides a significant improvement to the current best practises for modelling the radial particle transport in the SOL. The usual mean-field transport codes approximate the turbulent transport in the perpendicular directions by ad-hoc diffusion-type equations, which employ experimentally determined profiles for the diffusion coefficient, featuring a large amount of free parameters as the profiles are a function of the radial (and sometimes the poloidal) coordinate \[1, 26, 10\]. While the proposed particle transport model still features a diffusion relation, the diffusion constant now gets a clear physical background as it is shown to be determined by the energy in the ExB turbulence. The complete mean-field turbulent transport model only requires two or three (depending on whether or not the quasi-local
balance approximation is used) constants to be tuned instead of a 1D or 2D field.

The results of this relatively simple model are encouraging and entice the further development of it. Its accuracy could probably be further increased by the inclusion of more detailed models for the different sink and transport terms in the turbulent kinetic energy equation. The particle transport model might also still be improved; taking into account the underlying convective nature of transport might be especially interesting. Preliminary results indicate that the viscous dissipation term in the turbulent kinetic energy equation scales with the product of the viscosity with the enstrophy, while the scaling for the turbulent particle diffusion coefficient could also be improved by including the enstrophy.

Further research will also need to verify the main conclusions of this work in non-isothermal cases and for realistic tokamak geometries in which case other instabilities than the interchange term might also become important. The developed models should then be extended to model the turbulent thermal energy transport, new sources and/or sinks of the turbulence, as well as the additional terms present in 2D cases. Additionally, the analysis needs to be extended to include the part of edge region inside the last closed flux surface.

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A Appendices

A.1 Simulation parameters

In all simulations the parameters were chosen such that $D_n = \nu$, $\sigma_N = \sigma_W$, $\Lambda = 2.8388$ and $Te0 = 1$. All reported simulations were run for the isothermal version of the code with a non-periodic x-direction and using the strong Boussinesq assumption.

A.1.1 Default simulation

The default settings for the simulations are shown in table 1. The last four columns are not classical TOKAM2D parameters, but are parameters used in the post-processing. $x_{\text{start}}$ and $x_{\text{end}}$ denote the first and the last cell that are considered in the post-processing. Note that these are expressed in cell number, not in gyro-radii. They serve to remove the nonphysical fringe region and the zone where the particle source is large. $t_{\text{start}}$ and $t_{\text{end}}$ denote the first and the
last time steps used for the averaging, they serve to remove the non-converged first part of the simulation and to show the length of the simulation. Note that these are expressed in time steps, not in gyro-periods.

Table 1: Default parameters used in TOKAM2D simulations and their post-processing.

| Nr. | Lx  | Ly  | dx | dy | dt | Ti0 | σ  | ν   | x_{start} | x_{end} | t_{start} | t_{end} |
|-----|-----|-----|-----|-----|----|-----|-----|-----|-----------|---------|-----------|---------|
| 1   | 256 | 256 | 1   | 1   | 1  | 6e-4| 1   | 1e-4| 5e-3      | 51      | 199       | 2e5     | 8e5      |

A.1.2 Parameter scan simulations

Table 2 shows the parameters of the simulations used for the regression analysis. Only the parameters that differ from the default simulation (for which the parameters are listed in table 1) are shown, except for the first simulation which is the default simulation.

Table 2: TOKAM2D and post-processing parameters of the simulations used in the regression analysis.

| Nr. | g     | T{i0} | σ  | ν   | t_{start} | t_{end} |
|-----|-------|-------|-----|-----|-----------|---------|
| 1   | 6e-4  | 1     | 1e-4| 5e-3| 2e5       | 8e5     |
| 2   | 4.5e-4|       |     |     |           |         |
| 3   | 7.5e-4|       |     |     |           |         |
| 4   |       |       | 5e-5|     |           |         |
| 5   |       |       | 8e-5|     |           |         |
| 6   |       |       | 2e-4|     |           |         |
| 7   |       |       | 0.5 |     |           |         |
| 8   | 2     |       |     |     |           |         |
| 9   |       |       |     |     | 2e-3      |         |
| 10  |       |       |     |     | 4e-3      |         |
| 11  |       |       |     |     | 6e-3      |         |
| 12  |       |       |     |     | 1e-2      |         |
| 13  |       |       |     |     | 1.5e-2    |         |
| 14  | 4e-4  | 0.8   |     |     |           |         |
| 15  | 4e-4  | 1.4   |     |     |           |         |
| 16  | 9e-4  | 1.8   |     |     |           |         |
| 17  | 8e-4  | 0.75  |     |     |           |         |
| 18  | 0.9   | 0.75e-4|    |     |           |         |
| 19  | 4.5e-4| 1.5e-4|    |     |           |         |

A.1.3 Grid refinement simulations

Table 3 shows the parameters of the simulations used for the grid refinement analysis. Only the parameters that differ from the default simulation (for which
the parameters are listed in table 1 are shown.

Table 3: TOKAM2D and post-processing parameters of the simulations used in the regression analysis.

| Nr. | Lx   | Ly   | dx  | dy  | dt  | $x_{\text{start}}$ | $x_{\text{end}}$ | $t_{\text{start}}$ | $t_{\text{end}}$ |
|-----|------|------|-----|-----|-----|---------------------|-------------------|-------------------|-----------------|
| a   | 64   | 64   | 2   | 2   | 4   | 13                  | 49                | 8e5              | 1.04e7          |
| b   | 128  | 128  | 1   | 1   | 1   | 26                  | 99                | 2e5              | 2.6e6           |
| c   | 256  | 256  | 0.5 | 0.5 | 0.25| 51                  | 199               | 8e5              | 3.2e6           |
| d   | 512  | 512  | 0.25| 0.25| 1/16| 101                 | 399               | 1.6e6           | 8e6            |

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