Turbulent impurity transport in tokamak fusion plasmas

Andreas Skyman

Transport Theory, Department of Earth and Space Sciences
Chalmers University of Technology

Thesis for the degree of Licentiate of Engineering
a Swedish degree between M.Sc. and Ph.D.

Abstract

With the enormous growth of high performance computing (HPC) over the last few decades, plasma physicists have gained access to a valuable instrument for investigating turbulent plasma behaviour. In this thesis, these tools are utilised for the study of particle transport in fusion devices of the tokamak variety, focusing in particular on the transport of impurities.

The transport properties of impurities is of high relevance for the performance and optimisation of magnetic fusion devices. For instance, the possible accumulation of He ash in the core of the reactor plasma will serve to dilute the fuel, thus lowering fusion power. Heavier impurity species, originating from the plasma-facing surfaces, may also accumulate in the core, and wall-impurities of relatively low density may lead to unacceptable energy losses in the form of radiation. In an operational power plant, such as the ITER device, both impurities of low and high charge numbers will be present.

This thesis studies turbulent impurity transport driven by two different modes of drift wave turbulence: the trapped electron (TE) and ion temperature gradient (ITG) modes. Principal focus is on the balance of convective and diffusive impurity transport, as quantified by the impurity density gradient of zero flux ("peaking factor", $PF$). The results are scalings of $PF$ with impurity charge number, as well as with the driving background gradients of temperature and density, as well as other plasma parameters.

Quasi- and nonlinear results are obtained using the gyrokinetic code GENE, and compared with results from a computationally efficient multi-fluid model. In general, the three models show a good qualitative agreement. Results for ITG mode driven impurity transport are also compared with experimental results from the Joint European Torus, and also in this case a good qualitative agreement is obtained.

Keywords: fusion plasma physics, tokamaks, gyrokinetic theory, fluid theory, turbulence, impurity transport, ion temperature gradient mode, trapped electron mode, Joint European Torus, e-science
List of Appended Papers

This thesis is a summary of the following three papers. References to the papers will be made using roman numerals.


Other contributions (not included)

This is a list of conference contributions and non-peer reviewed articles.

A – A. Skyman, H. Nordman, P. Strand, et al,
Impurity transport in ITG and TE mode dominated turbulence,
Proceedings of EPS 2010, Europhysics Conference Abstracts, vol. 34A,

B – H. Nordman, A. Skyman, P. Strand, et al,
Modelling of impurity transport experiments at the Joint European Torus,
Proceedings of EPS 2010, Europhysics Conference Abstracts, vol. 34A,

C – A. Skyman, H. Nordman, P. Strand, et al,
Impurity transport in ITG and TE mode dominated turbulence,
EPS Conference 2010, (poster), Dublin, Ireland
http://publications.lib.chalmers.se/records/fulltext/local_126484.pdf

D – P. Strand, A. Skyman, H. Nordman,
Core transport studies in fusion devices,
SNIC progress report 08/09,
http://publications.lib.chalmers.se/records/fulltext/local_126485.pdf

E – P. Strand, A. Skyman, H. Nordman,
Core transport studies in fusion devices,
PDC 20th Anniversary & SNIC Interaction Conference 2010, (poster),
Stockholm, Sweden
http://publications.lib.chalmers.se/records/fulltext/local_126486.pdf

F – A. Skyman, H. Nordman, P. Strand,
Turbulent impurity transport in fusion plasmas,
RUSA meeting 2010, (poster), Stockholm, Sweden
http://publications.lib.chalmers.se/records/fulltext/local_131418.pdf

G – A. Skyman, P. Strand, H. Nordman,
Turbulence and transport in multi ion species fusion plasmas,
PDC Newsletter, vol. 11, no. 1, p. 12,

H – A. Skyman, P. Strand, H. Nordman,
Turbulent impurity transport driven by temperature and density gradients,
13th International Workshop on H-mode Physics and Transport Barriers, (poster),
Oxford, UK
http://publications.lib.chalmers.se/records/fulltext/local_147191.pdf
Acknowledgements

I would like to express my sincere gratitude to my friends in Hederligheten & Assoc., without whose continuous (and firm, sometimes almost to a fault) support the writing of this thesis would not have been possible (or at least not enjoyable).

I would also like to thank my co-workers, and in particular my supervisor Prof H. Nordman, for rewarding discussions on the finer points of plasma turbulence.¹

Further, I wish to thank my family, the Lunch Squad and Dr J. M. Grebo, whose support has been unwavering over the years.

Finally, some credit is long overdue for Lady Ada Lovlace and Dr Grace Hopper, without whose groundbreaking work none of this would be possible.

Credits & About

This thesis was written in \LaTeX{}, using latex templates made by Markus Billeter and Ludde Edgren.

Markus Billeter’s template was originally created by Fredrik Warg, and updated by Martin Thuresson. The new, modified version of the template will be made available at

http://www.cse.chalmers.se/~billeter

This document uses images from the “Silk Icons Set 1.3” by Mark James. The icons are licensed under a Creative Commons Attribution 2.5 License, and available at

http://www.famfamfam.com/lab/icons/silk/.

The document also uses “ccBeamer 0.1” by Sebastian Pipping, which is licensed under Creative Commons Attribution–ShareAlike 3.0, available at

http://blog.hartwork.org/?p=52

In compliance with the Swedish Research Council’s policy on Open Access, the whole thesis is licensed under the Creative Commons Attribution-ShareAlike 3.0 License. For details on the licenses, see page ii. To learn more about Open Access, go to

http://www.openaccess.se

An up to date version of this thesis will be available on the author’s homepage. To get the \LaTeX{} source, please go to

https://gitorious.org/skyman-s-licensiate-thesis

Long live \(\odot\)!

¹and on other topics, ranging from pens to electrodynamics, on the topic of which the Royal Blenheim pub in Oxford deserves a special mention...
Table of contents

I Summary

1 Introduction 1
   1.1 Nuclear fusion ........................................... 1
   1.2 Fusion plasmas ........................................... 3
       1.2.1 The fourth state of matter ......................... 3
       1.2.2 Confinement – the “Tokamak” ....................... 5
       1.2.3 Stability and quality of the confined plasma ....... 7
   1.3 Plasma impurities ........................................ 8
   1.4 Transport processes ..................................... 9

2 Turbulent impurity transport 11
   2.1 TE and ITG mode turbulence ............................. 11
   2.2 Impurity transport ....................................... 13

3 Gyrokinetic simulations 15
   3.1 GENE ..................................................... 15
   3.2 Experiments in silico .................................... 16

4 Summary of papers 19
   4.1 Fluid and gyrokinetic simulations of impurity transport at JET . 19
   4.2 Impurity transport in temperature gradient driven turbulence . . 20
   4.3 Particle transport in density gradient driven TE mode turbulence 22

Bibliography 23

II Appended Papers 27

Paper I – Fluid and gyrokinetic simulations of impurity transport at JET 29

Paper II – Impurity transport in temperature gradient driven turbulence 55

Paper III – Particle transport in density gradient driven TE mode turbulence 69
Part I

Summary
1

Introduction

1.1 Nuclear fusion

In a conventional nuclear power plant, the fuel consists of heavy elements whose nuclei split naturally, forming lighter atoms, in what is known as fission. Fusion, on the other hand, is the nuclear process where two lighter nuclei combine to form a heavier element. This does not happen naturally on Earth, but elsewhere in the universe it is commonplace: it is fusion that powers the stars. This was realised around the 1920s by Sir Arthur Eddington, and the dream of utilising this process for energy production was kindled at the same time [1].

Though fusion and fission power require very different operating scenarios, the fundamental principle that allows both fusion and fission to occur and release energy is the same. As can be seen in the curve in figure 1.1, the mass of an atom is not simply the sum of its nucleons – its neutrons and protons. This phenomenon is called the mass defect. [2] As neutrons and protons are added to or subtracted from an element, the combined mass is decreased if the product is closer to the minimum in the curve. The most common isotope of iron, $^{56}$Fe, has been highlighted (□) in the figure. As can be seen, iron is at the minimum of the mass curve, meaning that it is the element with the least mass per nucleon.

By Einstein’s relation $E = mc^2$ [3] mass is a form of energy, wherefore the decrease in mass is also a decrease in energy, and generally, decreased energy means increased stability. The tendency of elements combining or falling apart to form more “iron like” elements is spontaneous, in the sense that it is statistically more likely to occur than the opposite. This can be understood from figure 1.1, by observing that in order to bring an element away from the minimum, mass in the form of energy has to be supplied from somewhere, whereas going toward $^{56}$Fe the excess mass/energy need not fulfil any particular requirements – it has
a whole universe into which it can disperse. The conservation of energy – one of the most fundamental principles in all of Physics – demands that the missing mass be turned into other forms of energy, and it is this energy that is captured in nuclear power plants of both varieties. The typical fuel for fusion and fission are represented in figure 1.1 by the two highlighted isotopes $^2\text{H}$ and $^{238}\text{U}$ (Uranium) respectively. The $^2\text{H}$ is the isotope of Hydrogen called “heavy Hydrogen”, which is more commonly known as Deuterium and denoted D in fusion science. As can be seen, the energy that can potentially be gained by fusing light elements is many times greater per nucleon, and hence per kilogramme of fuel, than that which fission yields.\footnote{The scale in figure 1.1 is in eV, or electron Volts. 1 eV \approx 1.6 \cdot 10^{-19} \text{ J}, meaning that you would need roughly 2.5 \cdot 10^{19} \text{ eV} to heat 1 g of water 1 \text{°C}, but considering that Deuterium atoms are \sim 1.5 \cdot 10^{26} to a kilo, there is still a lot of energy in one nuclear reaction [4].} This is one of the reasons why fusion as a power source is so attractive.

That the fusion process is essentially spontaneous does not mean, however, that it is easy to accomplish. Whereas fission happens spontaneously on Earth, fusion requires much more exotic circumstances. In fission power plants, the nuclear process is mediated by neutrons, whereas for fusion to occur, the electrostatic repulsion between both the atoms’ negatively charged electron clouds, and then between the positively charged nuclei themselves, need to be overcome. Methods of accomplishing this normally require either extreme temperatures, extreme pressure, or a combination of the two. At sufficiently high temperature, collisions between atoms will be energetic enough to separate the electrons from the nuclei. If the frequency of recombining collisions is sufficiently low, a plasma is the result [5], meaning that it is easier to ionise a thin gas than a dense one. For fusion to occur, however, the resulting ions need to collide with enough force, that they break through the repulsive potential of the nuclear charges, which is many orders of magnitude higher than the repulsion from the electron clouds. The probability of a nuclear reaction to occur is quantified by the cross section for the reaction. The most favourable cross section for fusion is obtained for the fusion between Deuterium and Tritium ($^3\text{H}$) in the reaction [2, 5]:

$$D + T \equiv ^2\text{H} + ^3\text{H} \longrightarrow ^4\text{He} + n + 17.6 \text{ MeV} \tag{1.1}$$

where $^4\text{He}$ is an ordinary Helium ion, more often referred to as an $\alpha$-particle, and $n$ is a neutron. The total excess energy from the reaction in equation (1.1) is 17.6 MeV, distributed on the fusion products according to their mass, so that the total momentum is conserved, meaning that $\sim 4/5$ of the energy is deposited on the neutron. Because the neutron is uncharged, it is not confined by the magnetic fields used to contain the plasma, and will therefore leave the core region, depositing it energy in the wall of the plasma chamber, which is how energy will be extracted in a working power plant. The $\alpha$-particles, on the other hand, will be caught in the magnetic field and, through collisions, deposit their excess energy to the fuel ions, heating the plasma. Efficient $\alpha$-particle heating.
therefore is the key to achieving self-sustained nuclear fusion. Unfortunately, Tritium is not a stable isotope of Hydrogen. It is radioactive with a half-life of 12.33 years, and so must be bred, for instance from from Lithium [2, 4].

A striking example of fusion in Nature is the sun, which relies on the force of gravity to create the immense pressure needed for the fusion of protons and other elements to occur, which is the process that makes it and all other stars shine. The circumstances under which fusion can take place are very exotic from an Earthly stand-point, and very difficult to produce in a laboratory. Creating the conditions of allow for a high enough fusion cross section requires highly specialised devices and knowledge, which is why the engineering and science aspects of fusion research are both very important.

1.2 Fusion plasmas

1.2.1 The fourth state of matter

Super-heating or sufficiently depressurising a gas will eventually, through the processes outlined in section 1.1, lead to the separation of the electrons from the atoms in the material, resulting in an ionised gas – a plasma. In analogy with the solid, liquid and gaseous states of matter, plasmas are often referred to as
Figure 1.2: Illustration of the origin of the helical magnetic field lines in a tokamak. The toroidal ($B_\phi$; ↕) and poloidal ($B_\theta$; ↘) contributions to the total ($B_{\text{tot}}$; ←) magnetic field are indicated. Neither $B_\phi$ nor $B_\theta$ exhibit the necessary twist, but their sum $B_{\text{tot}}$ is a magnetic field whose field lines spiral around the torus. The safety factor in the figure is $q \approx r \frac{B_\phi}{B_\theta} = 0.35$. The surfaces spanned by the field lines of $B_{\text{tot}}$ for different (minor) radii are referred to as flux surfaces. In most tokamaks their cross section is not fully circular. The poloidal magnetic field is induced by the plasma current ($J$; !) running along the toroidal axis of the plasma. Also indicated are the major ($R$; →) and minor ($r$; ↗) radii.

the fourth state of matter.

A more rigorous definition of a plasma is that

“[a] plasma is a quasineutral gas of charged and neutral particles which exhibits collective behaviour” [5],

where quasineutral means that the plasma is electrically neutral when viewed from a distance, but may exhibit charge fluctuations on small scales. In many ways a fluid,\textsuperscript{2} plasmas are subject to the already complicated laws of fluid mechanics, but their behaviour becomes even more embroiled by the electromagnetic properties of the plasma, which introduce long range effects not present in

\textsuperscript{2}in physics, the term fluid is used for both liquids and gasses, as opposed to solids
other media. These effects are what lead to collective behaviour in the plasma, and this property is the most important difference between a partly ionised gas and a proper plasma. The intermingling of these two areas of physics further implies, that acoustic and electromagnetic waves of all kinds coexist in the plasma, but often on very different time and length scales. This makes both analytical and numerical studies of the governing equations very challenging, if one wishes to capture the entirety of this intricate interplay.

Though exotic in many ways, plasmas exist in our everyday surroundings: in fluorescent tubes, neon signs and modern television sets. The kind of plasmas that occur naturally on Earth are rarer, but not uncommon. The Northern lights and lightning are perhaps the most well known examples. Fusion plasmas, however, need to be much hotter in order to have a high enough fusion cross section for fusion power to be feasible. In order to sustain a fusion grade plasma in a laboratory or a reactor, it needs to be separated from the surroundings; it needs to be confined.

In the sun and the stars, the confinement is accomplished by gravity, where the mass of the stellar body is enough to create the pressure needed for the fusion process to be self sustained. This is not, however, an option for earthbound plasmas. Instead, research into confining plasmas is divided into two main areas: magnetic and inertial confinement.

1.2.2 Confinement – the “Tokamak”

In the presence of a magnetic field, charged particles will experience a force perpendicular to their velocity and to the magnetic field. Because the force is always at a right angle to the velocity, it can not lead to an increase in the velocity of the particle, but only change its direction. This means that the particles will be confined to move in orbits around the magnetic field lines, but they remain free to move parallel to the field. In order to fully confine the particles, the parallel motion has to be restricted as well. This can be accomplished by increasing the magnetic field at the edges of the device, creating what is called a “magnetic mirror”. Though this will cause many particles to bounce back into the core of the plasma, it can be shown that particle losses at the ends of the device are unavoidable [5]. Therefore, most research into potential power plant designs have been devoted to the study of toroidal magnetic geometries – instead of tying off the ends of the magnetic field, the field lines are bent into a ring, closing on themselves. The toroidal configuration is illustrated in figure 1.2.

Since the ends are eliminated this way, so are the end losses, however, this setup comes with its own difficulties, stemming from the inhomogeneity of the magnetic field. For a simple toroidal magnetic field, it can be shown that, due to a combination of effects due to the gradient and curvature of the magnetic field, it can be shown that...
field, the plasma will tend to be expelled from the core, toward the outside of the torus [5, 7]. This problem can be solved by introducing a twist (or “helicity”) in the magnetic field, so that the field lines – and the particles following them – spend time on both the in- and the outside of the device. In that way, the particles pushed toward the edge of the plasma when on one side of the torus, will be pushed back into the core when on the other side.

The twist is created by adding a field in the poloidal direction to the toroidal field; their sum will be a field with field lines spiralling around the torus. Figure 1.2 presents an illustration of how the helical field lines are generated. The first method of inducing this twist utilised external coils for both the poloidal and the toroidal magnetic fields. The devices were called “stellarators”, referring to the ambition of reproducing the workings of the sun and her stellar sisters here on Earth. Though stellarator research is a very active field (see e.g. [8, 9]), due to the difficulties of creating a favourable magnetic geometry by external means, most research since the sixties has shifted toward what is known as the “tokamak”, a configuration where the twist is accomplished by running a current through the core of the plasma. The rate of the helicity is measured by a parameter called the safety factor \(q\), which can be seen as the number of toroidal turns a magnetic field line make in one poloidal turn. It is directly proportional to the ratio of the toroidal magnetic field strength \(B_\phi\) to the poloidal magnetic field strength \(B_\theta\) [11], see figure 1.2.

In the tokamak design, instead of relying on external coils to crate this twist, an axial current is induced in the plasma, creating the poloidal field through Ampere’s law [4]. This is done by treating the plasma – a very good conductor due to the free mobility of the electrons – as a the secondary winding of a transformer, thus inducing a current in the plasma. The relationship between the plasma current and the helicity of the magnetic field lines is illustrated in figure 1.2.

A drawback of this method of introducing a helical twist in the magnetic field is that the electromagnetic field driving the plasma current is proportional to the change in the magnetic flux, as described by Faraday’s law of induction [4]. Therefore, the current can only be induced as long as the magnetic flux increases.

---

5There seems to be some confusion as to where the name “tokamak” came from, originally. Today, it is most often said to be an acronym for “toroidalnaya kamera s magnitnym polem”, which is Russian for “toroidal chamber with axial magnetic field” [1]. In older works, however, one can instead read that it originates from “toroidalnaya kamera s akshialnym magnitnym polem”, or “toroidal chamber with axial magnetic field” [10]. While how and why the name came to shift its meaning remains a mystery, both acronyms are suitably descriptive of the device: the tokamak was developed in the Soviet Union in the middle of last century, and is indeed a toroidal chamber, with magnetic coils generating a magnetic field along the toroidal axis of the chamber. But this is common to all toroidal magnetic confinement devices, and so the name does not cut to the core of what sets the tokamak design apart from the others.

6this also helps to heat the plasma through resistive (or “ohmic”) heating, though at high temperatures the plasma is too good a conductor for this to be the only source of heating power.
which it cannot do indefinitely. Eventually the transformer core will saturate, meaning that the plasma current can no longer be sustained. Though there are advanced operating scenarios under investigation that may circumvent this, tokamak operations are currently limited to pulsed mode. This is not a problem for the study of plasma dynamics, which usually involve time scales much shorter than the pulse time, but certainly a drawback when it comes to efficient power production.

1.2.3 Stability and quality of the confined plasma

Plasma confinement is a precarious process, only possible for precisely tuned parameters. One such parameter is the so called plasma $\beta$, which expresses the ratio of the particle pressure to the confining magnetic pressure. This parameter cannot supersede a few percent in tokamaks, or the plasma will be subject to large scale instabilities and disrupt, losing confinement almost at once [7, 11]. Pressure is related to the particle density and the temperature through the Boltzmann constant: $p = n_e k_B T$ [4]. Therefore, an increase in either the number of particles or temperature would proportionally increase the pressure, eventually bringing it above the $\beta$-limit.

Though the $\beta$-limit constrains puts a severe constraint on the operating regimes available to achieve fusion power, it also makes the process inherently safe from anything like a nuclear melt-down. “Disruption” and “loss of confinement” may sound dire enough, considering that the temperature of the plasma can reach in excess of a hundred million degrees Celsius. The actual energy content of the plasma, however, is very modest, which can also be seen from the definition of pressure. Dimensionally, pressure is a measure of the energy density in a fluid. For a typical fusion plasma in ITER [12], the particle density will be $n_e \approx 10^{20} \text{m}^{-3}$ for a volume of $V \approx 10^3 \text{m}^3$, and the temperature will be roughly $T \approx 10^8 \text{K}$. With $k_B \approx 10^{-23} \text{J/K}$, combining these gives an energy density of approximately $10^5 \text{J/m}^3$. This is equivalent to $10^3 \text{kPa}$, which is of the same order as the normal atmospheric pressure at sea level.\footnote{The energy associated with the free electrons has been neglected here: the ionisation energy for Hydrogen is $\sim 10 \text{eV}$, which translates to roughly $10^2 \text{J/m}^3$, so this contribution is negligible compared to the thermal energy of the ions}

Based on the energy content of the plasma, a measure of the quality of the confinement can be defined as the quotient of the energy content $E$ and the power input $P_{in}$ needed to sustain the plasma at that level of energy: $\tau_E \equiv E/P_{in}$, which has the dimension time. This is a measure of how quickly the energy would be lost, if power were not supplied, and is therefore called the energy confinement time. By dimensional arguments it can be shown that the power balance leads to a requirement for net energy production of $\tau_E n_e > (\tau_E n_e)_c$, for some critical value $(\tau_E n_e)_c$ [11]. This is called the Lawson criterion, and

\footnote{The subset $e$ is for electrons, which is conventionally used, since the electron density in a fully ionised gas is a measure of the ion density, regardless of the number of different ion species}
expresses the condition for power break-even. A more concrete performance parameter is that of the “fusion triple product”: \( n_e T \tau_E > (n_e T \tau_E)_c \), valid in the temperature range considered for fusion. The triple product is a condition for a self sustained plasma, meaning that the necessary power to heat the plasma comes from the \( \alpha \) particles generated by fusion events.\(^9\) In fusion experiments, the achieved triple product has been increasing exponentially over time since the dawn of fusion research, and the ITER device currently under construction is expected to continue this trend, with an estimated output power of five to ten times the input power [2, 7, 12]. Because of stability requirements, such as the \( \beta \)-limit mentioned above, the particle density and temperature are both restricted. Therefore, significantly increasing the Lawson parameter or the fusion triple product requires increasing the energy confinement time, which requires an understanding of the transport mechanisms at work.

1.3 Plasma impurities

Impurities – any ions that are not part of the fuel – tend to dilute the fuel, making collisions that produce fusion rarer, and thus reducing the fusion power. Heavier elements also tend to cool the plasma through radiative processes. Their high nuclear charge make them hard to ionise fully, even at the temperatures of a fusion plasma, and the electrons remaining bound to the impurity can then, rather than separate from the nucleus, respond to a collision by jumping to a higher electron orbit [13]. As the electrons relax, returning to the lower energy levels, they lose the energy gained in the collision, which is released in the form of photons. This is called line radiation, because the frequencies of the released photons correspond to lines in the light spectrum characteristic to the element that produced them. Since some heavy elements may never be fully ionised, line radiation can continue indefinitely. Therefore, even a small dilution of heavy impurities, can lead to significant energy losses in the plasma.

There are mainly three potential sources of impurities: the first being the walls of the reactor chamber. Due to the different roles played by different parts of the walls, they contribute both light and heavy impurities. The divertors, for instance, need to withstand the heavy power loads from energetic particles, and are therefore made of heavy metals such as Tungsten (W; nuclear charge \( Z = 72 \)). Because of the danger of line radiation, using an element as heavy as Tungsten is not practical for all of the chamber, and hence lighter candidates with high heat resilience are used elsewhere. For example, at the Joint European Torus (JET, [14]) the new ITER-like wall project was recently initiated, testing the feasibility of using a coating of the light metal Beryllium (Be, nuclear charge \( Z = 4 \)) on the plasma facing first wall of the reactor chamber [15].

---

\(^9\)both the Lawson criterion and the fusion triple product are valid measures of the quality of fusion plasmas for magnetically as well as initially confined fusion plasmas, but in magnetic confinement fusion \( n_e \) is typically small and \( \tau_e \) large, while the opposite holds for inertial confinement fusion
Not all impurities, however, are contaminants. The second main source of plasma impurities is injections of particles for control purposes. Here the cooling mechanisms are beneficial to the operation of the fusion reactor. By injecting elements such as Argon (Ar, $Z = 18$) that radiate energy in the right locations, the heat load on components such as the divertors can be spread out, protecting them from wearing out [16]. Impurities are also injected for experimental purposes, in order to study their transport properties.

Finally, the fuel ions will, in a working power plant, be diluted by the steady production of $\alpha$-particles (sometimes referred to as “Helium ash”) through fusion reactions.

Of major concern is whether different kinds (or “species”) of impurities will experience an inward or an outward pinch. Simulations of this is the main topic in this thesis.

### 1.4 Transport processes

Understanding the transport of particles, heat, momentum etc. in fusion plasmas is a very important topic of research. As mentioned above, controlling the transport properties of the plasma may be the only way forward when it comes to increasing the fusion efficiency, as measured by the Lawson parameter and the fusion triple product (section 1.2.3).

In fluids, it is common to describe the transport as consisting of diffusion and convection.\(^{10}\) Diffusion is the (seemingly) random spreading of a quantity in a fluid. It can often be understood as being mediated by collisions in the flow leading to a dispersive random walk [17]. Diffusive transport is driven by gradients, and so diffusion is directed from areas of abundance, to areas of scarcity. Thereby diffusion tends to even out profiles of temperature, density etc.

The convective part of the transport relates to bulk motion of particles in a fluid. It can either be up or down gradient, depending on the situation. In fusion plasmas, an net convective velocity is often referred to as a “pinch”.

Transport is often separated into classical and anomalous transport, where classical refers to transport dominated by collisions, whereas all other observed transport is termed anomalous [18]. Experiments have shown that, for most regions of the fusion plasma, anomalous transport clearly dominates over classical transport [18]. The most common example of anomalous transport in plasmas is turbulent transport. Turbulence is often associated with strong gradients, which represent free energy within a system that can drive drive instabilities. It is difficult to envision any classical situation, where the gradients are more pronounced than in a modern magnetic confinement fusion device, however, turbulence is a very common phenomenon in all of Nature. Hence it has been a topic of study for

\(^{10}\)advection is often used in place of convection, using convection to mean the sum of advective and diffusive transport
scientists and engineers for the better part of three hundred years, but its nonlinear character means that studying the effects of turbulence is very challenging. One main feature of turbulence is the interaction and interchange between different time and length scales, meaning that turbulent transport cannot be properly described by simple convection and diffusion. Locally, however, this approximation can be valid, when looking at space and time averaged fluxes [19–22]. The turbulent transport then manifests itself as effective diffusivities and pinches, at different minor radii.

All turbulent dynamics exhibit nonlinearities, making exact analytical solutions to equations of motion hard to come by, necessitating the application of numerical methods. To aid researchers when predicting and interpreting experimental outcomes, numerical tools have been developed to study the transport. Both dedicated transport solvers and more general plasma codes are used to this end, and one main topic in this thesis is comparing results from two such models: a multi-fluid and a gyrokinetic model.
2

Turbulent impurity transport

2.1 TE and ITG mode turbulence

The turbulence in magnetically confined fusion plasmas, such as those in Tokamaks like the proposed ITER device [12], has important and non-trivial effects on e.g. the quality of the energy confinement – effects that are hard to tackle both analytically and numerically. The problem of transport of energy and particles in a Tokamak plasma is an area of research where turbulence plays a major role, and that is intimately associated with the performance of future fusion reactors.

Many types of instabilities that exhibit this behaviour can be explained as analogous to the Rayleigh–Taylor instability, where a dense fluid is supported by a less dense fluid against the influence of gravity [5, 7, 11]. This is the case on the outboard side of the tokamak, which for its propensity for driving instabilities is called the bad curvature region. The profiles of the density and temperature perturbations will therefore have maxima on the outside, and minima on the inside, which is called ballooning [7, 23].

The origin of turbulent transport in tokamak plasmas is the fluctuations in the electric and magnetic fields. Crucially, the magnitude of the transport does not only depend on the magnitude of the fluctuation, but also on the extent of the phase correlation between the fluctuating quantities. For instance, for a net particle flux, the fluctuation in the velocity field needs to be accompanied by a fluctuation in the particle density that is correlated with the velocity fluctuation.

For the linear modes driving the turbulence considered in this thesis – ion temperature gradient (ITG) and trapped electron (TE) modes in low β plasmas – the perturbation can be considered to be mainly electrostatic. Both the ITG and the TE mode are examples of so called reactive drift wave modes. They are both
associated with length scales known to cause transport \(k_\theta \rho_s \approx 0.3\), and their mode frequencies are of the same order as the magnetic and diamagnetic drift frequencies \(\omega_r \sim \omega_D, \omega_\ast\).

The ITG mode can be understood as arising from a fluctuation in the temperature distribution, which under the influence of the poloidal magnetic drift causes a response in the ion density. If the electrons are considered adiabatic, they will respond by quickly redistributing according to the new landscape, creating an electric potential difference between the compressible ions, and the thermal electrons. The resulting electric field \(E\) will, in turn, lead to a drift velocity perpendicular to \(E\) and to the magnetic field \(B\) – the \(E \times B\) drift – acting on the temperature perturbation, and thus closing the feedback loop. In the bad curvature region, this feedback will be positive leading to an instability. The origin of the TE mode instability is similar in nature to the origin of the ITG mode [7].

In the case of a purely electrostatic perturbation, the particle flux of ion species \(j\) can formally be written [18]:

\[
\Gamma_j = \langle \delta n_j v_E \rangle, \quad (2.1)
\]

where \(\delta n_j\) is the perturbation in the density of species \(j\) and \(v_E\) is the \(E \times B\) drift velocity [7]. The angled brackets imply a time and space average over all unstable modes.

Deriving expressions for the drift velocities and the density response etc. can be done using different theoretical frameworks. In kinetic theory the plasma is described through distribution functions of velocity and position for each of the included plasma species. Hence, kinetic equations are inherently six-dimensional, however, in magnetically confined fusion plasmas the confined particles are generally constrained to tight orbits along field lines. This motivates performing an average over the gyration, reducing the problem to five-dimensional gyrokinetic equations [24–27]. Since the equations governing the evolution of the distributions are all coupled, the resulting decrease in numerical complexity is considerable. Fluid theory, on the other hand, is derived by taking the moments of the kinetic equations to some order, making them tractable by finding an appropriate closure [7]. In addition to making the workings of the plasma more accessible, by reintroducing familiar physical concepts such as pressure and density, fluid models are also several orders of magnitude more computationally efficient.

Whether \(\delta n_j\) and \(v_E\) are derived from fluid or gyrokinetic theory, performing the average in equation (2.1) for a fixed length scale \(k_\theta \rho_s\) of the turbulence, leads to an expression of the following form:

\[
\frac{R \Gamma_j}{n_j} = D_j \frac{R}{L_{n_j}} + D_{T_j} \frac{R}{L_{T_j}} + R V_{p,j}. \quad (2.2)
\]
The first term in equation (2.2) corresponds to diffusion, the second to the thermodiffusion and the third to the convective velocity (pinch), where \( R/LX_j = -R/\nabla X_j/X_j \), with \( X = n, T \), are the normalised logarithmic gradients of density and temperature for species \( j \), and \( R \) is the major radius of the tokamak. The pinch here contains contributions from curvature and parallel compression effects, however, the thermodiffusive term in equation (2.2) is sometimes referred to as the thermopinch and included in the convective velocity, so as not to confuse it with the proper (i.e. density gradient driven) diffusion. These terms have been described in detail in previous work, see e.g. [19–21] and Paper I and Paper II in this thesis.

### 2.2 Impurity transport

For trace impurities, equation (2.2) can be uniquely written as a linear function of \( \nabla n_Z \), offset by a convective velocity or “pinch” \( V_Z \):

\[
\Gamma_Z = -D_Z \nabla n_Z + n_Z V_Z \Leftrightarrow R\Gamma_Z = n_Z \frac{R}{L_n} + R V_Z,
\]

where \( D_Z \) is the impurity diffusion coefficient, and \( V_Z \) is the impurity convective velocity with the thermopinch included. Both the \( D_Z \) and \( V_Z \) are independent of \( \nabla n_Z \) in the trace impurity limit [19]. \( Z \) refers to the charge number of the impurity.

In the core of a steady-state plasma with fuelling from the edge (i.e. no internal particle sinks or sources), the impurity flux \( \Gamma_Z \) will go to zero. The zero-flux impurity density gradient (peaking factor) is defined as

\[
PF_Z = -\frac{R V_Z}{D_Z},
\]

for the value of the impurity density gradient that gives zero impurity flux.¹ Solving the linearised equation (2.3) for \( R/L_n \) with \( \Gamma_Z = 0 \) yields the interpretation of \( PF_Z \) as the gradient of zero impurity flux, and it quantifies the balance between convective and diffusive impurity transport. Specifically, the sign of the peaking factor is determined by the sign of the pinch, meaning that \( PF > 0 \) is indicative of a net inward impurity pinch, giving a peaked impurity profile. Conversely, if \( PF < 0 \) the net impurity pinch is outward, leading to a hollow impurity profile. The latter condition is called a flux reversal, and conditions leading to this are of particular interest, since an accumulation of impurities in the core of the plasma is preferably to be avoided (see section 1.3). The relationship of \( PF \) to \( D_Z \) and \( V_Z \) is illustrated in figure 3.3.

Much of the observed difference between the TE and ITG mode dominated cases – a major topic in the appended articles – can be understood from the convective

¹This number is also sometimes referred to the Péclet number [28, 29]
velocity $V_Z$ in equation (2.3). Particularly, the pinch contains two terms that depend on the impurity charge number $Z$ [19]:

- thermodiffusion (thermopinch):
  - $V_{\nabla T_Z} \sim \frac{1}{Z} \frac{R}{L_T Z}$,
  - inward for TE mode ($V_{\nabla T_Z} < 0$), outward for ITG mode ($V_{\nabla T_Z} > 0$),
- parallel impurity compression:
  - $V_{\parallel Z} \sim \frac{Z}{A_Z} k_{\parallel}^2 \sim \frac{Z}{A_Z q^2} \approx \frac{1}{2q^2}$,
  - outward for TE mode ($V_{\parallel Z} > 0$), inward for ITG mode ($V_{\parallel Z} < 0$).

Here $1/k_{\parallel}$ decides the wavelength of the parallel structure of the turbulence. Due to the ballooning character of the modes considered, this is proportional to the safety factor ($q$). The $Z$ dependence in the parallel impurity compression is expected to be weak, since the mass number is approximately $A_Z \approx 2Z$ for an impurity species with charge $Z$. The thermodiffusive contribution, however, can dominate the transport for low $Z$ impurities (such as the Helium ash). The direction of these contributions to the pinch are governed mainly by the considered mode’s drift direction, which is different for TE and ITG modes [7].
3

Gyrokinetic simulations

3.1 GENE

The GENE code [30–33] is a massively parallel gyrokinetic Vlasov code, solving the nonlinear time evolution of the gyrokinetic distribution functions on a fixed grid in phase space. The gyrokinetic equations are derived from the kinetic equations by performing an average of the particles’ gyrations around the field lines, so that the equations follow the centre of gyration, rather than the explicit orbits. This reduces the velocity space coordinates from three to two directions: parallel velocity and magnetic moment. Following the conventions of GENE, these are represented by $v$ and $\mu$ respectively. In real space, the radial ($x$) and bi-normal ($y$) dependencies are treated spectrally, i.e. those directions are discretised explicitly in $k$-space, whereas the toroidal ($z$) direction is discretised in real space. Because all phase space coordinates are coupled nonlinearly, the decrease from six to five phase space coordinates means a significant increase in computational efficiency.

There are some requirements that need to be fulfilled, for this simplification of the equations to be appropriate. First of all, the Larmor gyro-radii ($\rho$) of the plasma species have to be small, and the associated cyclotron frequencies ($\Omega$) large, compared to the system size ($\sim R$) and frequency ($\omega$) of the turbulent fluctuations respectively; secondly, the fast motion of the particles along the field lines lead to the requirement that the typical wave length of the parallel structure of the turbulence ($1/k_\parallel$) is much longer than the perpendicular ditto ($1/k_\perp$); and third, the energy associated with turbulent fluctuations need to be small compared to the thermal background energy. This is called the gyrokinetic ordering, which generally holds for tokamak plasmas [25, 31]. Formally, this can be written:

$$\frac{\rho}{R} \sim \frac{\omega}{\Omega} \sim \frac{k_\parallel}{k_\perp} \sim \frac{q\phi}{T} \ll 1.$$  \hspace{1cm} (3.1)
3.2 Experiments in silico

In this work, GENE simulations were performed in a flux tube geometry with periodic boundary conditions in the perpendicular directions. The flux tube is in essence a box that is elongated and twisted along with the \( B \) field as the field lines traverse the tokamak. Its application relies on the assumption that the scales of the phenomena of interest are all small compared to the size of the flux tube. The periodic boundary conditions also imply the assumption, that local effects dominate over global. This is generally true in the core of the plasma.

The instantaneous memory usage of a nonlinear GENE simulation is often of the order of several gigabyte. This means that even conservatively saving runtime data is unfeasible. Instead, GENE reduces the raw field data to physically comprehensible fields, which are saved to disk at intervals specified by the user. An example of this is shown in figure 3.1, where a cross section of the simulation domain is shown. The highlighted area corresponds to a cross section of the flux tube, whereas the rest of the annulus is approximated from the whole three dimensional data set. The quantity shown is the fluctuations in the electrostatic potential \( \phi \) near the end of a TE mode simulation. The saved data can be loaded into e.g. GENE’s native diagnostics tool, and after further refinement, data for specific physical quantities can be extracted.

Images such as the one presented in figure 3.1 are useful for providing a quick “sanity checks” for the simulations:

- Are the turbulent features sufficiently small, compared to the domain size?
- Are they large enough, compared to the resolution?
- Are there features that look artificial?

Beyond that, however, the derived data is still difficult to compare directly with experiments – numerical and physical alike – before it has been further distilled. By performing different averages over the simulation domain, scalar quantities are derived, such as mean fluctuation levels of particle densities and of the electrostatic potential, and integrated particle and heat fluxes across the flux tube boundaries. Since such scalar quantities are often what is needed for further analysis, GENE by default calculates and saves a number of such averages at regular intervals. Because they are scalars rather than fields, the resulting time series can afford a very good temporal resolution, without hampering simulation performance or running out of disk space. Two such time series are presented in figure 3.2. They show the space averaged fluctuations in background ion density \( (n_i^2) \) and impurity flux \( (\Gamma_Z) \) for the same simulation as in figure 3.1.

In order to reach the quantities of principal interest in this study, however, the data needs to be even further condensed. First, a time average is performed on time series of the impurity flux in order to obtain a mean flux \( \langle (\Gamma_Z) \rangle \), as illustrated in 3.2. This average is performed for simulations with at least three
Figure 3.1: A cut from the toroidal annulus made up of the flux tube as it twists around the torus following the $B$ field; see figure 1.2. Shown are the fluctuations in the electrostatic potential ($\phi$). A cross-section of the flux tube with the side $\sim 125 \rho$ is indicated. Data from NL GENE simulation of TE mode turbulence at $t \approx 300 R/c_s$; parameters as in figure 4.1a.

different values for the impurity density gradient ($-R\nabla n_Z / n_Z = R/L_{n_Z}$). As is illustrated in figure 3.3, the linearised impurity flux equation (2.3) is then fitted to the obtained average fluxes. The quotient of the obtained diffusion coefficient ($D_Z$) and convective velocity ($V_Z$) then yields the peaking factor ($PF$), which quantifies the balance of diffusive and convective transport for the impurity species (see section 2.2 for details).

Finally, $PF$ is calculated for several different values of e.g. the impurity charge ($Z$) in order to obtain a scaling, which can be compared to experiments and other models. Such a scaling is presented in figure 4.1a, where the sample followed in the figures mentioned previously has been highlighted (○).

In the process of generating a scaling such as the nonlinear scaling in figure 4.1a, the equivalent of several terabyte of instantaneous data is distilled into just a couple of floating point numbers – a remarkable compression rate, to say the least. GENE can also be run in quasilinear mode, a method that is considerably less demanding when it comes computer resources since the non-linear coupling between length scales is ignored [32–34]. The method is only used to study one mode at a time, and only for the particular length scale $k_\theta \rho_s$ of choice. If the length scale is chosen appropriately, however, the quasilinear simulation will capture the essential features of the dynamics, and it is useful for getting a qualitative understanding of the physical processes. As used in this work, it captures the contribution from the most unstable mode, not from any subdominant modes. The methodology is the same as for the nonlinear simulations.
Figure 3.2: Time series showing fluctuations in the main ion density ($n_{H^2}^2$) and impurity flux ($\Gamma_Z$) after averaging over the whole flux tube; see figure 3.1. The average impurity flux ($\langle \Gamma_Z \rangle$) is calculated from $\Gamma_Z$, discarding the first portion so as not to include the linear phase of the simulation. $\langle \Gamma_Z \rangle$ is used for finding the peaking factor for the impurity species; see figure 3.3. NL GENE simulation with He impurities; parameters as in figure 4.1a, with $R/L_{n_{H^2}} = 1.5$. An estimated uncertainty of one standard error is indicated.

Figure 3.3: Impurity flux ($\Gamma_Z$) dependence on the impurity density gradient ($R/L_{n_{H^2}}$), illustrating the peaking factor ($PF$), the diffusivity ($D_Z$) and pinch ($V_Z$), and the validity of the linearity assumption of equation (2.3) for trace impurities. $\Gamma_Z$ is acquired as a time average of the impurity flux; see figure 3.2. $D_Z$ and $V_Z$ are calculated from the data, taking the estimated uncertainty into account. NL GENE simulations with He impurities; parameters as in figure 4.1a. An estimated uncertainty of one standard error is indicated.
Summary of papers

4.1 Fluid and gyrokinetic simulations of impurity transport at JET

*Paper I* deals with impurity transport due to ion temperature gradient (ITG) mode dominated turbulence in the core plasma region of dedicated impurity injection experiments #67730 and #67732 at JET. The main results are comparisons between experimental results and results from nonlinear and quasilinear gyrokinetic and nonlinear fluid simulations for the impurity peaking factor (see section 2.2) in the form of scalings of the peaking factor ($PF$) with the impurity charge number $Z$. The simulations were performed both with one impurity species alone, and with impurities along with 2% C background, which is the common scenario at JET.

A good qualitative agreement between the experimental impurity peaking and both models was obtained, except for Carbon impurities, where the flat or hollow profiles observed in experiments were not reproduced by the numerical simulations. It was observed that the peaking factor increased rapidly for low impurity charge, reaching a saturation for higher values of $Z$ with $2 \leq PF \leq 3$, which is much lower than neoclassical predictions. Further, the effects of increasing the charge fraction of impurities, of collisions, and of $E \times B$ shearing on the impurity peaking were investigated. All three resulted in lowered peaking factors for the low $Z$ impurities. Scalings with the ion temperature gradient for different species of impurities were also obtained, and also here a good qualitative agreement between the models was observed, though the nonlinear gyrokinetic simulations predicted substantially higher fluctuation levels than the fluid model.

The article was published in Plasma Physics and Controlled Fusion in October 2011 (vol. 53, no. 10, p. 105005–18).
4.2 Impurity transport in temperature gradient driven turbulence

Rather than comparing with experiments, as in Paper I, the main focus in Paper II is the comparison of numerical models: nonlinear and quasilinear gyrokinetics, and a computationally efficient nonlinear multi-fluid model. The secondary focus is the comparison of temperature gradient driven TE mode scalings of the impurity peaking factor, with results for the ITG mode similar to those studied in Paper I.

Scalings of the impurity peaking factor with the impurity charge number, and with the background temperature and density gradients ($R/L_{T_i,e}$ and $R/L_{n_e}$) were obtained for both modes of turbulence. Nonlinear gyrokinetic scalings with $Z$ and $R/L_{T_e}$ were obtained for the TE mode dominated case.

A falling trend of $PF$ observed for increasing $Z$ in the TE mode case was observed, whereas for the ITG mode the same trend as in Paper I was seen, with the peaking factor saturating at higher values of $Z$ for both modes. This is illustrated in in figure 4.1. A theoretical explanation for this difference was found from the signs and $Z$ dependence of the thermodiffusive contribution to the impurity convective velocity.

For all the scalings, the results show a good qualitative agreement between the models. The quasilinear gyrokinetic simulations were observed to overestimate the peaking factor, compared to the nonlinear results. The fluid results were, however, shown to be sensitive to the choice of the parallel mode structure assumed in the simulations, which may hint at an avenue of improvement for the fluid model.

The impurity peaking factor was also compared to the main ion peaking factor as calculated from fluid simulations. The main ion peaking was found to be slightly larger than the corresponding impurity peaking factors.

The work included in this paper builds in part on results presented at the EPS, PDC, and RUSA conferences in 2010; see page vi. The article has been submitted to Physics of Plasmas.
(a) dependence of the peaking factor ($PF$) on $Z$ for the TE case

(b) dependence of the peaking factor ($PF$) on $Z$ for the ITG case

Figure 4.1: Scalings of the peaking factor ($PF$) with impurity charge ($Z$). Parameters are $q = 1.4$, $s = 0.8$, $\epsilon = \tau / R = 0.143$ in both subfigures, with $R/L_T_i = R/L_T_x = 3.0$, $R/L_{T_e} = 7.0$, $R/L_{n_e} = 2.0$ for the TE case (figure 4.1a), and $R/L_T_i = R/L_T_x = 7.0$, $R/L_{T_e} = 3.0$, $R/L_{n_e} = 3.0$ for the ITG case (figure 4.1b). The error bars for the NL GENE results in figure 4.1a indicate an estimated error of one standard deviation. The sample for the He impurity acquired from the data illustrated in figure 3.3 and figure 3.2 is highlighted (○).
4.3 Particle transport in density gradient driven TE mode turbulence

The work in Paper III complements the work in Paper II by investigating impurity transport in TE mode turbulence driven by steep background density gradients, as relevant to H-mode physics.

Main ion and impurity transport were both examined, and scalings with $Z$ and $R/L_{ne}$ obtained from a quasi- and nonlinear gyrokinetic model were compared with results from the fluid model. The scaling with impurity charge was observed to be weak for the parameters considered, and the peaking factor was shown to saturate at values significantly smaller than the driving electron gradient in the steep electron gradient regime. Good qualitative agreements between the models were obtained, and it was observed that, for the TE mode, the quasilinear gyrokinetic simulations usually overestimated $PF$, whereas the fluid results underestimated it, compared to the nonlinear gyrokinetic results.

The work included in this paper was presented at the 13th International Workshop on H-mode Physics and Transport Barriers in 2011; see page vi. The article has been submitted to the Nuclear Fusion special issue for the above mentioned workshop.
Bibliography


---

1formerly “International Thermonuclear Experimental Reactor”


Part II

Appended Papers
Fluid and gyrokinetic simulations of impurity transport at JET

H. Nordman, A. Skyman, P. Strand, C. Giroud, F. Jenko, F. Merz, V. Naulin, T. Tala and the JET–EFDA Contributors

Postprint, see DOI link for the published version

Plasma Physics and Controlled Fusion
vol. 53, no. 10, p. 105005–18

doi:10.1088/0741-3335/53/10/105005

https://publications.lib.chalmers.se/cpl/record/index.xsql?pubid=147198
Fluid and gyrokinetic simulations of impurity transport at JET

H. Nordman\textsuperscript{1}, A. Skyman\textsuperscript{1}, P. Strand\textsuperscript{1}, C. Giroud\textsuperscript{2}, F. Jenko\textsuperscript{3}, F. Merz\textsuperscript{3}, V. Naulin\textsuperscript{4}, T. Tala\textsuperscript{5} and the JET-EFDA Contributors.*

JET-EFDA, Culham Science Centre, OX14 3DB, Abingdon, UK.

\textsuperscript{1}Department of Earth and Space Sciences, Chalmers University of Technology, Euratom-VR Association, SE-412 96 Göteborg, Sweden.
\textsuperscript{2}EURATOM/CCFE Association, Culham Science Centre, Abingdon, OX14 3DB UK.
\textsuperscript{3}Max-Planck-Institut für Plasmaphysik EURATOM-IPP, D-85748 Garching Germany.
\textsuperscript{4}Association EURATOM/RISO-Technical University of Denmark, Roskilde, Denmark.
\textsuperscript{5}Association EURATOM/Tekes, VTT, P.O. Box 1000, FIN-02044 VTT, Finland.

* See annex of F. Romanelli et al., “Overview of JET Results”, (Proc. 23\textsuperscript{rd} IAEA Fusion Energy Conference, Daejeon, Korea (2010)).

Abstract

Impurity transport coefficients due to Ion-Temperature-Gradient (ITG) mode and Trapped-Electron (TE) mode turbulence are calculated using profile data from dedicated impurity injection experiments at JET. Results obtained with a multi-fluid model are compared with quasi-linear and nonlinear gyrokinetic simulation results obtained with the code GENE. The sign of the impurity convective velocity (pinch) and its various contributions are discussed. The dependence of the impurity transport coefficients and impurity peaking factor $-\nabla n_Z/n$ on plasma parameters like impurity charge number $Z$, ion logarithmic temperature gradient, collisionality, ExB shearing, and charge fraction are investigated. It is found that for the studied ITG dominated JET discharges, both the fluid and gyrokinetic results show an increase of the impurity peaking factor for low $Z$-values followed by a saturation at moderate values of impurity peaking, much below the neoclassical predictions, for large values of $Z$. The results are in qualitative agreement with the experimental trends observed for the injected impurities (Ne, Ar, Ni) whereas for the background carbon species the observed flat or weakly hollow C profiles are not well reproduced by the simulations.
I. INTRODUCTION

It is well known that the presence of impurities in tokamak fusion plasmas may have a limiting effect on the performance by their contribution to radiation losses and plasma dilution resulting in lower fusion power. Impurities arise in the fusion plasma from the sputtering of the wall and divertor materials (e.g. Be, C and W), from impurity seeding in the edge in order to reduce power loads (Ne, Ar), and from the D-T reaction in the form of He-ash. In ITER, the material configuration for the main chamber/divertor is beryllium/tungsten which will also be tested in JET as part of the ITER like wall project [1]. Accordingly, the scaling of impurity transport with impurity charge Z, from He to high Z impurities like W, is crucial for the performance and optimisation of a fusion reactor.

Impurity transport, both neoclassical and anomalous caused by turbulence, has been investigated in a number of theoretical [2-26] and experimental [27-34] studies. Theoretically, detrimental high-Z impurity accumulation is predicted in the core region by collisional transport theory [2-4]. This is usually not seen in experiments where neoclassical impurity transport coefficients are typically one or two orders of magnitude too small to explain the experimental results in the confinement zone. In this region, anomalous transport due to ITG/TE mode turbulence is expected to dominate for all channels of transport. Early studies of ITG mode driven impurity transport [12] reported an outward impurity flux for sufficiently peaked impurity density profiles, thereby avoiding severe impurity peaking in the core. In experiments it has also been observed that with the addition of ion cyclotron resonance heating to neutral beam heated discharges, accumulation of high-Z impurities can be avoided if most of the heating power is deposited on the electrons, while if the heating is deposited on the ions, the impurities accumulate in the core [31-33].

To study the Z-dependency of impurity transport in more detail, a set of dedicated impurity injection experiments has been performed at JET [33]. Extrinsic impurities were injected by laser ablation (Ni) and gas injection (Ne, Ar) and the diffusivity $D_Z$ and convective velocity $V_Z$ were determined by matching spectroscopic data with predictive
results obtained with the transport code UTC-SANCO [34]. In addition, the Carbon peaking factor was determined from the background C profile.

In the present paper, background data taken from the impurity injection experiments in JET are used in interpretative transport calculations based on anomalous transport due ITG/TE mode mode turbulence. The transport coefficients are calculated using the Weiland multi-fluid model [35] which is compared and contrasted with results from quasi-linear (QL) and nonlinear (NL) gyrokinetic simulations using the code GENE [36]. In particular, the dependence of the impurity transport coefficients and impurity density peaking factor $-\nabla n_i/n_e$ on plasma parameters, in particular the impurity charge number which is varied from $Z=2$ to $Z=74$, is discussed and compared with experimental trends. The main purpose of the work is to obtain an increased understanding of impurity transport in the confinement zone of tokamaks and to quantify to what extent a computationally fast and efficient fluid model can reproduce the gyro-kinetic results. Understanding the ITG/TE mode driven transport properties of main fuel (deuterium and tritium), ash (helium) and impurities are vital for the prediction of ITER performance. The paper aims to further establish the physics background for this and to provide input to support the validation of reduced physics models aimed at integrated predictive codes.

The remainder of the paper is organised as follows. In Sec. II the fluid and kinetic models used to describe the ITG/TE driven impurity transport are presented. Section III discusses the interpretative analysis of the discharges and the parameter scalings, in particular the scaling with impurity charge number $Z$, and comparison with experiments. Finally, the conclusions are given in Sec. IV.

**II. IMPURITY TRANSPORT MODELS**

a) Fluid model

The Weiland multi-fluid model [35] is used to describe the ITG/TE mode turbulence and the impurity species. The model equations consist of a set of fluid equations for each species, i.e. ions, trapped electrons and impurities [7-8, 12]. The equations for the perturbations in impurity density, parallel velocity and temperature, neglecting effects of finite impurity Larmor radius, take the form:
\[
(\tilde{\omega} + \tau_z^*) \tilde{n}_z - \left( \frac{R}{2L_{nz}} - \lambda \right) \tilde{\phi} + \tau_z^* \tilde{T}_z - \frac{k \delta \mathbf{v} \| \mathbf{l}^z}{\omega_{De}} = 0 \]  
\[
(\tilde{\omega} - 2\tau_z^*) \frac{k_1 \delta \mathbf{v} \| \mathbf{l}^z}{\omega_{De}} = \frac{Z}{A_z q_z^*} \tilde{\phi} + \frac{\tau_z^*}{A_z q_z^*} (\tilde{n}_z + \tilde{T}_z) \]  
\[
\left( \tilde{\omega} + \frac{5}{3} \tau_z^* \right) \tilde{T}_z - \left( \frac{R}{2L_{\tau z}} - \frac{1}{3} \frac{R}{L_{nz}} \right) \tilde{\phi} - \frac{2}{3} \tilde{\omega} \tilde{n}_z = 0 \]  

Here \( \tilde{\phi} = e\phi / T_e \) is the electrostatic potential, \( \tilde{n}_z = \delta n_z / n_z \) is the density, \( \delta_i \) is the parallel velocity, \( \tilde{T}_z = \delta T_z / T_z \) is temperature, and \( \tilde{\omega} = \omega_\tau + i \tilde{\tau} \) and \( k \) are the normalized eigenvalue and wavevector of the unstable ITG/TE modes and tilde denotes normalization with respect to the electron magnetic drift frequency \( \omega_{De} \). The normalized gradient scale lengths are defined as \( R/L_{nj} = -(R/n_j)(dn_j/dr) \) and \( R/L_{Tj} = -(R/T_j)(dT_j/dr) \) where \( R \) is the major radius of the tokamak. The other parameters are \( \tau_z^* = \lambda T_z / ZT_e \), \( \lambda = \cos \theta + \sigma \theta \sin \theta \), \( \theta \) is the poloidal angle, \( \tau_z = T_z / T_e \), \( A_z = m_z / m_i \) where \( m_i \) (\( m_e \)) is the ion (impurity) mass, \( \sigma \) is the magnetic shear, \( Z \) is the impurity charge, \( q_* = 2qk_\theta \rho_s \), where \( q \) is the safety factor, \( \rho_s = c_s / \Omega_{ci} \) is the ion sound scale with \( \Omega_{ci} = eB / m_i \) and the ion sound speed \( c_s = \sqrt{T_z / m_i} \). The curvature terms in Eqs. (1)-(3) enter through the magnetic drift \( \omega_{DZ} = \omega_{DZ}(\theta = 0) \lambda \) and originate from the compression of the ExB drift velocity, the diamagnetic drift velocity, and the diamagnetic heat flow. The term proportional to \( 2\tau_z^* \) in the left hand side of Eq. (2) corresponds to curvature effects from \( \tilde{\nabla} \cdot \tilde{\xi}_z \) (the stress tensor). Combining Eqs. (1)-(3), neglecting the ion pressure perturbations in the parallel ion dynamics for simplicity (Eq. 2), the relation between \( \tilde{n}_z \) and \( \tilde{\phi} \) can be written as [7]

\[
\tilde{n}_z = \left[ \tilde{\omega} \left( \frac{R}{2L_{nz}} - \lambda \right) - \tau_z^* \left( \frac{R}{2L_{\tau z}} - \frac{7R}{3L_{nz}} + \frac{5\lambda}{3} \right) + \frac{Z}{A_z q_z^*} \left( \tilde{\omega} + \frac{5\tau_z^*}{3} / \tilde{\omega} \right) \right] \tilde{\phi} / N 
\]  

where \( N = \tilde{\omega}^2 + \frac{10\tau_z^*}{3} \tilde{\omega} + \frac{5\tau_z^*}{3} \).

The perturbations in impurity, main ion and electron densities are coupled through the quasineutrality condition \( \delta n_i / n_e = (1-Zf_Z) \delta n_i / n_i + Zf_Z \delta n_Z / n_Z \) where \( f_Z = n_Z / n_e \) is the impurity
fraction. Here, the electron response is $\delta n_e/n_e = f_t \delta n_{et}/n_{et} + (1-f_t) \delta n_{ef}/n_{ef}$, where $f_t$ is the fraction of trapped electrons. The trapped electron response is calculated using the Weiland fluid model [35] and the free electrons are assumed adiabatic with $\delta n_{ef}/n_{ef} = e \phi/Te$. The linear eigenvalue equation obtained from the quasineutrality condition is solved for an electrostatic potential of general mode width where the magnetic drift $\omega_{Dj}$ and parallel wave number $k_{||}$ are calculated as averages over the poloidal mode structure [8].

From the impurity density response, the quasilinear impurity particle flux can be calculated as $\Gamma_m = -n_z \rho_s c_s \left\{ \bar{n}_z \frac{\partial \phi}{r \partial \theta} \right\} = -D_z V n_z + n_z V_z$ where $D_z$ and $V_z$ are the impurity diffusivity and convective velocity respectively:

$$\Gamma_m = \frac{k_z \rho_s \gamma N_z}{n_z c_s |N|^2} \left[ \frac{R}{2L_{nz}} \left( |\bar{\omega}|^2 + \frac{14}{3} \tau_z^* \bar{\omega}_r + \frac{55}{9} \tau_z^* \right) - \frac{R}{2L_{Tz}} \left( 2 \tau_z^* \bar{\omega}_r + \frac{10}{3} \tau_z^* \right) - \left\langle \lambda \right\rangle \left( |\bar{\omega}|^2 + \frac{10}{3} \tau_z^* \bar{\omega}_r + \frac{35}{9} \tau_z^* \right) + \frac{Z}{A_z q_s^2 N_{||}} \left( \tau_z^* \left( \frac{19}{3} \bar{\omega}_r^2 - \frac{1}{3} \bar{\gamma}^2 + \frac{100}{9} \tau_z^* \bar{\omega}_r - 5 \tau_z^* \right) + 2 \bar{\omega}_r |\bar{\omega}|^2 \right) \right]$$

where $N_{||} = \bar{\omega} - 2 \tau_z^*$ and $\left\langle \ldots \right\rangle$ represents an average over the poloidal mode structure. The impurity flux is calculated from Eq. (5) by summing over all unstable modes for a fixed length scale of the turbulence. Isotropic turbulence is assumed with $k_r \rho_s = k_\theta \rho_s$, where $r$ and $\theta$ are the radial and poloidal coordinates, and the saturated fluctuation level is estimated as $|\phi_k| = \frac{1}{\alpha_n} \frac{1}{k_n L_{nz}}$ [35]. In Eq. (5), the first term is the diffusive flux and the other terms represent the impurity convective velocity $V_z$ which includes contributions from three different sources. The first term is called thermodiffusion and is usually outwards ($V_z > 0$) for ITG-modes ($\bar{\omega}_r < 0$) and inwards for TE-modes ($\bar{\omega}_r > 0$). Its leading term scales as $V_z \sim 1/Z \cdot R/L_{Tz}$ and hence it is negligible for large $Z$ impurities. The second term is the curvature pinch which is proportional to $\left\langle \lambda \right\rangle$ and usually inwards. It is often
the dominant term and leads to a positive peaking factor. The third term represents parallel impurity compression \([6]\) and scales as \(V_Z \sim Z/A_Z \approx Z/\langle A q^2 \rangle\). It is usually inward for ITG-modes and outward for TE-modes. Effects of toroidal rotation would modify the above expression (Eq. 5) and add a new term proportional to the background rotation gradient (roto-diffusion) \([19]\). These effects may be potentially important in NBI heated tokamak discharges but are not included in the present work. In the trace impurity approximation, the trace species is neglected in the quasi-neutrality condition and in this limit \(D_Z\) and \(V_Z\) are independent of \(\nabla n_Z\). For the trace results presented below, an impurity fraction of \(f_Z=10^{-6}\) was typically used.

In steady state plasmas with impurity fuelling through the edge, the zero impurity flux condition \(\Gamma_Z = 0\) holds in the core. The balance between outward diffusion and convection \(V_Z\) then determines the normalised impurity peaking factor as \(\text{PF} = -RV_Z/n_Z = -RV_Z/D_Z\). For inward convection, a peaked impurity profile is obtained with \(\text{PF}>0\). For large \(Z\) impurities, neglecting parallel impurity compression and assuming a strongly ballooning eigenfunction with \(\langle \lambda \rangle = 1\) \((\omega_{\text{DZ}}(\theta) \approx \omega_{\text{DZ}}(\theta=0))\), the simple analytical result \(\text{PF}=2\) is obtained from Eq. 5 by balancing the outward diffusion with the dominant curvature pinch.

b) Gyrokinetic model

The gyrokinetic results have been obtained with the code GENE \([36]\). The main part of the simulations have been performed by treating the impurities as a trace species using an impurity fraction of \(f_Z=10^{-6}\). The impurity flux is calculated for a few different values of the impurity gradient \(\nabla n_Z\) and then the diffusivity \(D_Z\) and convective velocity \(V_Z\) are obtained assuming a linear dependence between impurity flux and impurity density gradient. In addition, simulations with larger fractions of impurities and with two impurity species present in the plasma have been performed in order to test the validity of the trace impurity approximation for the cases considered. In these simulations, the peaking factor is found by varying impurity gradient until the condition of zero impurity flux is approximately satisfied. Both quasi-linear (QL) and nonlinear (NL) simulations have been performed. The QL simulations calculate the flux from the dominant mode, which is the ITG mode for the JET discharges considered, whereas the fluid and NL
GENE simulations also include the contribution from the subdominant TE mode. The QL simulations assume isotropic turbulence with a fixed length-scale of the turbulence with \( k_\rho = k_s \rho_s \) as used in the fluid model. A more refined QL kinetic model, not used here, was constructed in [21-22] based on comparisons with NL GENE simulations. The GENE simulations also include impurity FLR effects which are neglected in the fluid case. Impurity FLR effects are expected to be weak and scale as \( A_Z/Z \) and should therefore not influence the main results presented in this paper. The NL fluxtube simulations using GENE were performed with a box size of \( L_x = L_y = 125 \rho_s \) with \( n_x \times n_y \times n_z = 96 \times 96 \times 32 \) grid points in real space and \( n_v \times n_\mu = 48 \times 12 \) in velocity space. Convergence tests were performed linearly and non-linearly to determine an appropriate numerical resolution in all coordinates [36]. Fig. 1 illustrates the results of a nonlinear GENE fluxtube simulation of JET discharge \#67730 with parameters taken at \( r/a = 0.5 \) (see below for parameter values). Figure 1a shows the time evolution of the impurity particle flux and the background density fluctuations. From the time evolution, the time average of the impurity flux is calculated for a few different values of \( R/L_nz \). The simulations were typically run over the interval \( 0 \leq t(c_s/R) \leq 300 \) and the time average was calculated in steady-state for \( t(c_s/R) \geq 100 \) as indicated in the figure. The result of such a scan is displayed in Fig. 1b where the error bars represent the rms deviations from the average. The scan shows a linear relationship between impurity flux and impurity density gradient and confirms the validity of the trace impurity approximation used here. The space scale of the nonlinear structures relative to the box size is illustrated in Fig. 1c which shows the contour plot of the background density fluctuations in the nonlinear saturated state of Fig. 1a.

### III. SIMULATION RESULTS

The anomalous impurity diffusivity \( D_Z \), convective velocity \( V_Z \), and normalised impurity peaking factor \( PF = -RV_Z/D_Z \) are calculated using the background profiles of JET L-mode discharges \#67730 and \#67732 [33]. The main parameters are taken from \#67730 at \( r/a = 0.5 \) with \( R/L_{Te} = 5.6 \), \( R/L_{Ti} = R/L_{Tz} = 5.6 \), \( f_1 = 0.55 \), \( q = 2.4 \), \( s = 0.6 \), \( T_e/T_{i,z} = 0.98 \), and \( R/L_{ne} = 2.7 \). The other parameters are \( B = 3 \) T, \( R = 3 \) m, \( T_e = 1.55 \) keV, and \( n_e = 1.84 \times 10^{19} \) m\(^{-3} \). The radial profiles of the impurity transport coefficients are calculated and compared.
with experiments. In addition, the sensitivity of the impurity transport and peaking factors to variations in the plasma parameters around the experimental values are studied. All simulations are performed in a simple s-α equilibrium in the low beta (β≤10⁻³) electrostatic limit. Effects of non-circular geometry are not included in the present study but have been shown to be rather weak for ITG dominated plasmas using the present fluid model [37-38].

a) Z-scaling of impurity transport and comparison with experiment
First, the scaling of the normalised impurity density peaking factor $PF = -RV_Z/D_Z$ with impurity charge $Z$ is studied, assuming an impurity mass $A_Z=2Z$. The results obtained with fluid, QL GENE and NL GENE simulations are illustrated in Fig. 2a. The parameters are taken from discharge #67730 at r/a=0.52. For these parameters, the ITG mode is the dominant instability. The kinetic eigenvalues are $\omega_{ITG}=-1.23+i0.43$ and $\omega_{TE}=0.62+i0.28$ (for $k\rho_s=0.3$, $\omega$ is normalized to $\omega_{De}$). The results are shown for 2 different values of the wave-number, $k\rho_s=0.2$ and $k\rho_s=0.3$. For low $Z$-values, the QL results are quite sensitive to the choice of $k\rho_s$, indicating the difficulty of predicting QL transport based on a single mode. The scaling with $Z$, with an increase in the peaking factor for small $Z$, is mainly a result of the thermodiffusive pinch (included here since $VT_Z=VT_i$ is assumed), which is outward for ITG modes and scales as 1/Z. The fluid and GENE results are in good agreement and show a saturation of the peaking factor for large values of $Z$ ($Z>10$) at a value slightly above the simple analytical fluid result $PF=2$, which is obtained when neglecting parallel impurity compression. For tungsten ($Z=74$), the peaking factors are $PF=2.18$ (fluid) and $PF=2.23$ (QL GENE) for $k\rho_s=0.3$. For the experimentally more relevant case with partially ionized tungsten, assuming an ionization stage with $Z=46+$ and $A_Z=184$, we obtain the peaking factor $PF=2.06$ (fluid) and $PF=2.11$ (QL GENE), i.e. a downward shift of the peaking factor with about 5%. The ratio $D_Z/\chi_i$ has been calculated using fluid ($k\rho_s=0.3$) and NL GENE simulations. The ratio shows a very weak scaling with $Z$ with $D_Z/\chi_i=1.1$ (fluid) $D_Z/\chi_i=1.0$ (NL GENE) for He.

In Fig. 2b the various contributions to the convective velocity $V_Z$ (in m/s) as a function of $Z$ are illustrated for the same parameters as in Fig. 2a. The results are obtained with the
fluid model for wave-number \( kp_s = 0.2 \). The results show that the curvature pinch (inward) dominates for all values of \( Z \). The compression term (inward) and the thermopinch (outward) are substantially smaller and have opposite sign as expected from the previous discussion. As observed, the main \( Z \) scaling originates from the thermopinch which becomes significant for \( Z < 10 \). The diffusivity \( D_Z \) (not shown) is weakly dependent on \( Z \) varying from \( D_Z = 2.6 \text{ m}^2/\text{s} \) to \( D_Z = 2.2 \text{ m}^2/\text{s} \) in going from \( Z = 2 \) to \( Z = 74 \).

The NL GENE simulations predict substantially larger turbulent fluctuation levels and hence larger values of \( D_Z \) and \( V_Z \) than obtained with the fluid model. For He, the NL GENE result is \( D_Z = 9.1 \text{ m}^2/\text{s} \). This is a consequence of the sensitivity of the fluctuation levels to the driving ion temperature gradient and is often observed in fixed gradient simulations of ITG turbulence. However, the peaking factors are much less sensitive to variations in the driving gradient. This is illustrated in Fig. 3a, b which shows the peaking factors for \( Z = 6 \) and \( Z = 28 \) and the ion heat diffusivity, versus \( R/L_{Ti,z} \), with the other parameters as in Fig. 2a. The stiff behaviour of the ion heat diffusivity \( \chi_i \) is apparent in Fig. 3b which shows the \( R/L_{Ti,z} \) scaling of \( \chi_i \) (in \( \text{m}^2/\text{s} \)) obtained with the fluid model. For comparison, the NL GENE result for \( \chi_i \) is also shown at the experimental value of the temperature gradient with \( R/L_{Ti,z} = 5.6 \). The impurity peaking factors, however, are only weakly sensitive to variations in the gradients around the experimental values as shown in Fig. 3a. For very weak ion temperature gradients (\( R/L_{Ti,z} < 4.5 \)), the TE mode dominates. This results in lower levels of the peaking factors for large \( Z \) impurities due to the reversal of the parallel compression pinch [6,13].

Figure 4 a, b, c shows the comparison between the Weiland fluid predictions and experimental results for \( D_Z \) (in \( \text{m}^2/\text{s} \)) and \( V_Z \) (in \( \text{m/s} \)) and peaking factor \( PF = RV_Z/D_Z \) [30]. The radial profiles of the coefficients are shown for L-mode discharge #67730 (Ne, Ar) and #67732 (Ni). The results are shown for \( r/a > 0.3 \). In the inner core region, the ITG/TE modes are stable according to both fluid and kinetic calculations. Crosses indicate Weiland model predictions whereas dashed lines are neoclassical values. The interpretative comparison used here is very sensitive to the background gradients and a small change of the profiles results in a large change in the diffusivities. This is
particularly true close to marginal stability (i.e. for r/a<0.3) which makes comparisons in this region questionable. The region r/a>0.8 is also outside the region of validity, at least for the fluid model used. Hence the comparison with experiments is made around mid-radius. The qualitative trends observed in experiments for Ne, Ar and Ni are reproduced by the theoretical predictions [30]. The calculated diffusivity at mid radius does not scale with Z (from Ne (Z=10) to Ni (Z=28)) and is of the right order of magnitude, two orders of magnitude larger than the neo-classical predictions (Fig. 4a). The calculated convective velocity is inward (i.e. an impurity pinch) for Z=10-28 and is also of the correct order of magnitude, one order of magnitude larger than neoclassical predictions (Fig. 4b). For Carbon, the predicted peaking with PF\textsubscript{C}=1.9 (fluid) and PF\textsubscript{C}=1.7 (NL GENE) is larger than the measured peaking of the C profile which is flat or hollow at mid-radius. This may indicate that the thermodiffusion is larger than predicted by the present models. Alternatively, some of the approximations used in the simulations (trace approximation, collisionless plasma, circular geometry etc) may not be valid for the experimental parameters used. Some of these approximations are examined next.

b) Trace versus self-consistent treatment
The validity of the trace impurity approximation is investigated in Fig. 5a,b. Fig. 5a displays the normalised impurity density peaking factor PF=-RV\textsubscript{Z}/D\textsubscript{Z} versus the charge fraction Z\textcdot f\textsubscript{Z} for Z=6 and Z=18 obtained with the Weiland fluid model and QL GENE simulations. The parameters are the same as in Fig. 2a. As observed, the peaking factors remain close to the trace results (Z\textcdot f\textsubscript{Z}=0) for low levels of impurities. The slight increase in the peaking factor for Ar in the fluid case, not seen in the QL GENE simulations, is due to the presence of a subdominant impurity mode which is neglected in the QL GENE simulations which is based on the most dominant mode. The peaking factor obtained using the experimental fraction of Carbon (2% C) is only slightly reduced compared to the trace result of Fig. 2a. This is in line with several previous investigations [5,13,23] which show that the trace approximation is valid for up to 2% C. In Fig. 5b the results for the experimentally relevant case including 2 impurity species is studied. The peaking factor of the trace species with/without a background of 2% Carbon obtained by QL GENE simulations are displayed. The result confirms that the presence of 2% C in the
plasma does not significantly modify the trace impurity results of Fig. 2a. We have also performed NL GENE simulations including 2% Carbon to check for possible non-linear effects of the Carbon species on the peaking factor. However, the NL GENE simulations give a peaking factor for Carbon of $PF_C \approx 1.5$ which is close to the NL GENE trace results of Fig. 2a.

c) Collisions and sheared rotation

The influence of collisions on the results presented is investigated in Fig. 6. The peaking factors for He and C are shown as a function of the normalized effective collision frequency $\nu_{\text{eff}} = \nu_{ei} / (\epsilon \omega_{De})$. The parameters are taken from L-mode discharge #67730 at mid radius which has a relatively high collision frequency with $\nu_{\text{eff}} \approx 0.7$. As observed, collisions tend to reduce the peaking factor for low Z impurities. This is expected since the Z=1 background ions are strongly affected by collisions [39]. For Carbon however, the effect is marginal. Larger values of Z (not shown) are less affected [17].

Next, the stabilizing effects of sheared plasma rotation on the ITG/TE mode growth rate is implemented in the impurity transport expressions and the implication for the impurity peaking factor is investigated. This is done by treating the ExB shearing rate $\gamma_E = dV_{\text{ExB}}/dr$ as a parameter and applying the Waltz rule [40] to the linear growth rates where $\gamma_{\text{lin}}$ is replaced by $\gamma_{\text{net}} = \gamma_{\text{lin}} - \alpha \gamma_E$ in the fluid transport coefficients (Eq. 5, $\alpha=1$ is used here). The impurity peaking factor versus the shearing parameter $\gamma_E/\gamma_l$ is displayed in Fig. 7 for the same parameters as in Fig. 2a and with $k\rho_s=0.3$. The effective reduction of the ITG growth rate with ExB shearing is found to significantly reduce the peaking factors for low values of impurity charge Z. For Z=2, a flux reversal, from an inward to an outward convective impurity velocity, is obtained for $\gamma_E/\gamma_l \approx 0.25$. The effective reduction of the ITG growth rate leads to a reduction of all contributions to the impurity particle flux in Eq. 5. However, the main effect is that the thermodiffusion is less affected than the other pinch terms resulting in a relative increase of its contribution compared to the other contributions to the impurity transport. Since the thermodiffusion is outward for ITG dominated cases, the result is a reduction (or reversal) of the impurity peaking factor for
small values of Z. However, it is found that the experimental value of the shearing parameter at mid radius of JET discharge #67730 is too small \( \gamma_E/\gamma_l \approx 0.1 \) to significantly affect the peaking factor for Carbon and hence the flat or hollow C profile obtained in the discharge remains unexplained. We emphasize that the explicit effects of rotation and rotation shear studied in [19] are not included here.

V. CONCLUSIONS
Impurity transport coefficients driven by ITG/TE mode turbulence were calculated using the Weiland multi-fluid model as well as quasi-linear and nonlinear gyrokinetic simulations using the code GENE. The analysis was performed using profile data from dedicated impurity injection experiments at JET. The sign of the impurity convective velocity (pinch) and the dependence of the impurity transport coefficients and impurity density peaking factor \( PF=-R\nabla n_z/n_z \) on plasma parameters, in particular the impurity charge number Z, were studied. It was shown that the fluid, quasilinear and nonlinear gyrokinetic simulations predict similar impurity behaviour for the considered ITG mode dominated L-mode discharges. The impurity peaking factors were found to increase with Z for low Z-values \( (Z \leq 10) \) and saturate at moderate values of the impurity peaking factor for large values of Z. The saturated peaking factors for \( Z \gg 1 \) were found to be substantially smaller than the neo-classical predictions with typically \( 2 < PF \leq 3 \). The results are in qualitative agreement with the experimental findings at mid-radius for the injected impurities Ne, Ar, and Ni. For Carbon however, the predicted peaking is substantially larger than the peaking obtained from the measured profile which is flat or even hollow.

Various effects that could potentially explain this discrepancy between theory and experiment were investigated. The effect of sheared plasma rotation was included by implementing the Waltz rule \( \gamma_{\text{net}} = \gamma_{\text{lin}} - \gamma_E \) in the Weiland transport model (Eq. 5), where \( \gamma_E = \partial V_{\text{ExB}}/\partial r \) is the shearing rate. Sheared plasma flows were found to have a significant effect of the impurity peaking factor for low Z impurities \( (Z < 10) \) where a reduction or even a reversal (for He) of the impurity peaking was obtained. The reduction of the peaking factor is a result of the increased relative contribution from thermodiffusion in cases where the ITG growth rate is reduced by ExB shearing. Also effects of collisions...
and 2% background Carbon (vs trace) were found to reduce the low Z peaking factors. However, these effects were not sufficient to significantly reduce the Carbon peaking factor for the studied L-mode experimental parameters values. The results may indicate that some important ingredient is missing in the models used. Work is in progress in order to investigate if the effects of roto-diffusion [19] are as significant for the interpretation of low Z impurity transport at JET as indicated by recent analysis of AUG experiments [41]. Effects of realistic tokamak geometry will also be included. In addition, the computationally efficient fluid model will be used in predictive transport code simulations of JET discharges, allowing for the self-consistent evolution of temperature, density, momentum and impurity profiles.

ACKNOWLEDGEMENT

This work was supported by EURATOM and carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission.
REFERENCES

4. P. Helander and D. J. Sigmar, Collisional Transport in Magnetized Plasmas
   (2007).
9. N. Dubuit, X. Garbet, T. Parisot, R. Guiirlet, and C. Bourdelle, Phys. Plasmas 14,
   042301 (2007).
10. R. Guiirlet, C. Giroud, T. Parisot, M. E. Puiatti, C. Bourdelle, L. Carraro, N. Dubuit,
    (2010).
33. C. Giroud et al., 12th International Workshop on “H-mode Physics and Transport Barriers”, September 30-October 2 2009, Princeton, USA.
41. C. Angioni et al., submitted to *Nucl. Fusion* (2010).
Figure Captions

Fig. 1a Time traces of the impurity particle flux (in units of $10^6 c_s \rho_{ref}^2 n_e / R^2$) and ion density fluctuations $n_D^2$ (in units of $n_e^2 \rho_{ref}^2 / R^2$) obtained from NL GENE fluxtube simulations in the trace impurity limit (collisionless, electrostatic). The parameters are taken from JET Pulse No: 67730 (I=1.8MA, $B_T=3T$, $P_{NBI} = 4.2MW$) at $r/a=0.5$ with $Z=42$, $R/L_{nz}=2.6$, $R/L_{ne}=2.7$, $R/L_{Tj}=5.6$, $T_e/T_i=1$, $q=2.4$, and $s=0.6$.

Fig. 1b Time averaged impurity particle flux (in units of $c_s \rho_{ref}^2 n_e / R^2$) versus $R/L_{nz}$ for $Z=42$. Results obtained from NL GENE simulations with parameters from Fig. 1a.

Fig. 1c Contour plot of background ion density fluctuations obtained in the non-linear saturated state of Fig. 1a, at $t \sim 300 R/c_s$.

Fig. 2a Scaling of normalised impurity density peaking factor $PF=-RV_Z/D_Z$ with impurity charge $Z$ for $Z \geq 2$ for wave-numbers $k\rho_s=0.2$ and $k\rho_s=0.3$. Results from Weiland fluid model and QL and NL GENE simulations are compared in the trace impurity limit (collisionless, electrostatic). The parameters are taken from JET Pulse No: 67730 at $r/a=0.5$.

Fig. 2b Scaling of impurity convective velocity $V_Z$ with $Z$. Results from Weiland fluid model with $k\rho_s=0.2$. The parameters are the same as in Fig. 2a.

Fig. 3a Peaking factors for C and Ni versus the driving gradient $R/L_{T_{i,Z}}$. Results from QL GENE and Weiland fluid model with $k\rho_s=0.2$. The other parameters are the same as in Fig. 2a.

Fig. 3b Ion heat diffusivity $\chi_i$ (in $m^2/s$) versus the driving gradient $R/L_{T_{i,Z}}$ for the same case as in Fig. 3a. Results from Weiland fluid model with $k\rho_s=0.2$ and NL GENE simulations.
Fig. 4 a,b,c Comparison between the Weiland fluid predictions and experimental results for $D_Z$ ($m^2/s$, a), $V_Z$ ($m/s$, b) and $PF=-RV_Z/D_Z$ (c). The radial profiles of the coefficients are shown for L-mode Pulse No’s: 67730 (Ne, Ar) and #67732 (Ni). Crosses indicate Weiland model predictions whereas dashed lines are neoclassical values.

Fig. 5a Normalised impurity density peaking factor $PF=-RV_Z/D_Z$ versus charge fraction $Z\cdot f_Z = Z\cdot n_Z/n_e$ for $Z=6$ and $Z=18$. Comparison between Weiland fluid model and QL GENE simulations. Parameters taken from Pulse No: 67730 at $r/a\approx0.5$. The experimental value for the Carbon charge fraction is $Z\cdot f_Z \approx 0.12$.

Fig. 5b Normalised impurity density peaking factor $PF=-RV_Z/D_Z$ versus $Z$ in the trace impurity limit compared to a case with two impurity species; one trace species in the presence of 2% C which is included self-consistently. Results obtained by QL GENE simulations. The parameters are the same as in Fig. 2a.

Fig. 6 Normalised impurity density peaking factor $PF=-RV_Z/D_Z$ versus normalised effective collision frequency $\nu_{\text{eff}}=\nu_{ei}/(\epsilon\omega_{De})$ for $Z=2$ and $Z=6$. The parameters are the same as in Fig. 2a.

Fig. 7 Normalised impurity density peaking factor $PF=-RV_Z/D_Z$ versus shearing parameter $\gamma_E/\gamma$ for the same parameters as in Fig. 2a. The results are obtained using the Weiland fluid model for $k\rho_s=0.3$. 

47 (Paper I:17)
Fig. 1a

Fig. 1b
Fig. 1c

Fig. 2a
Fig. 2b

Fig. 3a
Fig. 3b

Fig. 4a
Fig. 5a

Fig. 5b
Fig. 6

Fig. 7
Impurity transport in temperature gradient driven turbulence

A. Skyman, H. Nordman, P. Strand

Postprint, see DOI link for the published version

Physics of Plasmas
vol. 19, no. 3, p. 032313

doi:10.1063/1.3695014

http://publications.lib.chalmers.se/records/fulltext/local_156282.pdf
Impurity transport in temperature gradient driven turbulence

A. Skyman,a) H. Nordman,b) and P. Strandc)
Euratom–VR Association, Department of Earth and Space Sciences,
Chalmers University of Technology, SE-412 96 Göteborg, Sweden
(Dated: 21 December 2012)

In the present paper the transport of impurities driven by trapped electron (TE) mode turbulence is studied. Non-linear (NL) gyrokinetic simulations using the code GENE are compared with results from quasilinear (QL) gyrokinetic simulations and a computationally efficient fluid model. The main focus is on model comparisons for electron temperature gradient driven turbulence regarding the sign of the convective impurity velocity (pinch) and the impurity density gradient \( R/L_{nz} \) (peaking factor) for zero impurity flux. In particular, the scaling of the impurity peaking factors with impurity charge \( Z \) and with driving temperature gradient is investigated and compared with results for the more studied Ion Temperature Gradient (ITG) driven turbulence. The question of helium ash removal in TE mode turbulence is also investigated. In addition, the impurity peaking is compared to the main ion peaking obtained by a self-consistent fluid calculation of the density gradients corresponding to zero particle fluxes.

For the scaling of the peaking factor with impurity charge \( Z \), a weak dependence is obtained from NL GENE and fluid simulations. The QL GENE results show a stronger dependence for low \( Z \) impurities and overestimates the peaking factor by up to a factor of two in this region. As in the case of ITG dominated turbulence, the peaking factors saturate as \( Z \) increases, at a level much below neoclassical predictions. The scaling with \( Z \) is, however, weak or reversed as compared to the ITG case. The results indicate that TE mode turbulence is as efficient as ITG turbulence at removing He ash, with \( D_{He}/\chi_{eff} > 1.0 \).

The scaling of impurity peaking with the background temperature gradients is found to be weak in the NL GENE and fluid simulations. The QL results are also here found to significantly overestimate the peaking factor for low \( Z \) values.

For the parameters considered, the background density gradient for zero particle flux is found to be slightly larger than the corresponding impurity zero flux gradient.

PACS numbers: 28.52.Av, 52.25.Vy, 52.30.Ex, 52.30.Gz, 52.35.Ra, 52.55.Fa, 52.65.Tt

I. INTRODUCTION

The transport properties of impurities is of high relevance for the performance and optimisation of magnetic fusion devices. For instance, the possible accumulation of He ash in the core of the reactor plasma will serve to dilute the fuel, thus lowering fusion power. Heavier impurity species, originating from the plasma-facing surfaces, may also accumulate in the core, and wall-impurities of relatively low density may lead to unacceptable energy losses in the form of radiation. In an operational power plant, both impurities of low and high charge numbers will be present.

In the confinement zone of tokamaks, the transport of the background species is usually dominated by turbulence. The Trapped Electron (TE) mode and the Ion Temperature Gradient (ITG) mode are expected to be the main contributors. Turbulent impurity transport has been investigated in a number of theoretical and experimental papers. In tokamak experiments, also the impurity transport is usually dominated by turbulence, resulting in impurity peaking factors well below the neoclassical predictions. The main theoretical effort has, with a few exceptions, been devoted to quasilinear studies, primarily focused on ITG mode driven impurity transport. For the directly relevant regimes, however, where \( \alpha \)-particle heating dominates, as will be the case in the ITER device, or in electron cyclotron resonance heated plasmas, TE mode driven impurity transport will likely be important.

In the present study, transport of impurities driven by TE mode turbulence is investigated by NL gyrokinetic simulations using the code GENE, The simulation results are compared to QL gyrokinetic simulations as well as results obtained from a multi-fluid model. The fluid model is employed for the dual purposes of benchmarking a computationally efficient model, suitable for predictive simulations, and interpreting the results. The TE mode results are compared with the more well known results for ITG mode dominated turbulence, obtained from QL gyrokinetic and fluid simulations.

The impurity diffusivity \( (D_Z) \) and convective velocity \( (V_Z) \) are estimated from simulation data, and from these the zero-flux impurity density gradient \( (R/L_{nz} = -RV_Z/D_Z) \), also referred to as the impurity peaking factor \( (P_F) \) is derived. This quantity expresses the impurity density gradient at which the convective and diffusive transport of impurities are exactly bal-
anced. The sign of $PF$ is of special interest, as it determines whether the impurities are subject to an inward ($PF > 0$) or outward ($PF < 0$) pinch. Scalings of peaking factors with impurity charge ($Z$), electron and ion temperature gradients ($\nabla T_e, \nabla T_i$), and electron density gradient ($\nabla n_e$) are studied, giving particular attention to $\nabla T_e$ driven TE mode impurity transport. The important question of how efficient the removal of helium ash will be is also investigated for TE mode turbulence using NL GENE and fluid simulations. The results are compared and contrasted with results from previous studies focused on ITG driven impurity transport. In addition, the impurity peaking relative to the main ion peaking in the plasma core obtained from a self-consistent treatment of the particle fluxes will be discussed. This situation is experimentally relevant in situations with edge particle fuelling where the steady state gradient corresponds to zero particle flux.

The remainder of the paper is structured as follows: first the transport models are reviewed, beginning with of the fluid model employed (Section II A) where the focus is on the impurity dynamics. This is followed by a brief introduction of the gyrokinetic model and the GENE code (Section II B) and a section on the specifics of the simulations (Section III). After this, the main results are covered, including discussion and interpretation of the acquired results (Section IV). The final section of the paper is a summary of the main conclusions to be drawn (Section V).

II. TRANSPORT MODELS

A. Fluid theory

The Weiland multi-fluid model consists of coupled sets of equations for each of the fluid model employed (Section II A) where the focus is on the impurity dynamics. This is followed by a brief introduction of the gyrokinetic model and the GENE code (Section II B) and a section on the specifics of the simulations (Section III). After this, the main results are covered, including discussion and interpretation of the acquired results (Section IV). The final section of the paper is a summary of the main conclusions to be drawn (Section V).

The main ion and electron response is calculated from the following set of equations for ions and trapped electrons. The electron response is given by a trapped electron model, and a free part such that $\delta n_e = f_1 \delta n_{e1} + (1 - f_1) \delta n_{e2}$, i.e., the free electrons are assumed to be adiabatic and thus follow the Boltzmann distribution: $\delta n_{e2}/n_{e2} = e\phi/T_e$.

The equations are closed by the assumption of quasi-neutrality:

$$\frac{\delta n_e}{n_e} = (1 - Z f_Z) \frac{\delta n_i}{n_i} + Z f_Z \frac{\delta n_Z}{n_Z}$$

where $f_Z = \frac{n_Z}{n_{e2}}$ is the fraction of impurities.

Thus an eigenvalue equation for TE and ITG modes is obtained in the presence of impurities. Assuming a strongly ballooning eigenfunction with $k^2_T = (3q^2 R^2)^{-1}$, the eigenvalue equation is reduced to a system of algebraic equations that is solved numerically. The sensitivity of the fluid results to the choice of $k_T$ will be examined in Section IV A below.

The zero-flux impurity peaking factor, defined as $PF = -\frac{\delta n_Z}{\delta n_i}$ for the value of the impurity density gradient that give zero impurity flux, quantifies the balance of convective and diffusive impurity transport. Its derivation relies on the fact that the transport of a trace impurity species can be described locally by dividing the

normalised scale lengths can be assumed to be constant for the flux tube domain considered, and are defined as $\frac{\delta n_Z}{n_i} = -\frac{R}{k_T^2} \frac{\delta n_i}{n_i}$, where $R$ is the major radius of the tokamak and $T_i$ for species $i$. The other parameters are defined as follows: $\tau^*_Z = \frac{R T_i}{T_Z}$, $\frac{\delta n_Z}{n_i}$, $Z = m_Z/m_i$, $Z$ is the impurity mass number and $Z$ is the impurity charge. Further, $s$ is the magnetic shear and $q^* = 2q/\rho_s$, where $q$ is the safety factor, $\rho_s = c_s/\Omega_{ci}$ is the ion sound scale with the ion sound speed $c_s = \sqrt{T_e/m_i}$, which originates from the compression of the $E \times B$ drift velocity, the diamagnetic drift velocity and the diamagnetic heat flow. Curvature effects from the stress tensor enter as $2\tau^*_Z$ at the left hand side of Eq. (1b).

Combining Eq. (1a)–(1c), while neglecting pressure perturbations in Eq. (1b) for simplicity, the relation of the electrostatic potential $\phi$ and impurity density $\tilde{n}_Z$ becomes:

$$\tilde{n}_Z = \left[\frac{\tilde{\omega}^2 + 10\tilde{\tau}_Z^2}{Z^2} + \frac{5\tilde{\tau}_Z^2}{3}\right] \frac{\tilde{\omega} + 5\tilde{\tau}_Z^2}{3} \phi$$

where $\tilde{\omega} = \frac{R}{2L_{ne}} - \lambda$ and $\tilde{\tau}_Z = \frac{R}{2L_{te} - 3\tilde{\omega}^2}$.

The main ion and electron response is calculated from the following set of equations for ions and trapped electrons. The electron response is given by a trapped electron model, and a free part such that $\delta n_e = f_1 \delta n_{e1} + (1 - f_1) \delta n_{e2}$, i.e., the free electrons are assumed to be adiabatic and thus follow the Boltzmann distribution: $\delta n_{e2}/n_{e2} = e\phi/T_e$.

The equations are closed by the assumption of quasi-neutrality:

$$\frac{\delta n_e}{n_e} = (1 - Z f_Z) \frac{\delta n_i}{n_i} + Z f_Z \frac{\delta n_Z}{n_Z}$$

where $f_Z = \frac{n_Z}{n_{e2}}$ is the fraction of impurities.

Thus an eigenvalue equation for TE and ITG modes is obtained in the presence of impurities. Assuming a strongly ballooning eigenfunction with $k^2_T = (3q^2 R^2)^{-1}$, the eigenvalue equation is reduced to a system of algebraic equations that is solved numerically. The sensitivity of the fluid results to the choice of $k_T$ will be examined in Section IV A below.

The zero-flux impurity peaking factor, defined as $PF = -\frac{\delta n_Z}{\delta n_i}$ for the value of the impurity density gradient that give zero impurity flux, quantifies the balance of convective and diffusive impurity transport. Its derivation relies on the fact that the transport of a trace impurity species can be described locally by dividing the
FIG. 1: Impurity flux ($\Gamma_z$) dependence on the impurity density gradient ($-R\nabla n_Z/n_Z = R/L_{n_Z}$), illustrating the impurity peaking factor ($PF$), the diffusivity ($D_Z$) and pinch ($RV_Z$), and the validity of the linearity assumption in Eq. (5) of $\Gamma_Z$ for trace impurities. Parameters of Eq. (5) are estimated from the calculated fluxes, taking the estimated error of the data into account. The flux is acquired as the average of a time series after convergence, as is illustrated in Fig. 2. Data from NL GENE simulations of TE mode driven turbulence with He impurities and parameters as in Fig. 4(a). The error bars indicate an estimated error of one standard deviation.

The effective diffusivity ($D_{Z,\text{eff}}$) into a diffusive and a convective part. In the trace impurity limit, i.e. for $ZJ_z \to 0$ in Eq. 4, the impurity flux $\Gamma_z$ becomes a linear function of $\nabla n_Z$, offset by a convective velocity or “pinch” $V_Z$. The resulting expression is:

$$\Gamma_{n_Z} = -D_{Z,\text{eff}} \nabla n_Z = -D_Z \nabla n_Z + n_Z V_Z \approx \frac{R\Gamma}{n_Z} = D_Z \frac{R}{L_{n_Z}} + \text{slope},$$

(5)

where $n_Z$ is the density of the impurity species and $R$ is the major radius of the tokamak, and both the diffusion coefficient ($D_Z$) and the convective velocity ($V_Z$) are independent of $\nabla n_Z$.

The impurity particle flux at the left hand side of Eq. (5) can be written as:

$$\Gamma_{n_Z} = \langle \delta n_Z v_s B \rangle = -n_Z \rho_s c_s \left\langle \frac{\nabla n_Z}{r} \right\rangle.$$

(6)

The angled brackets imply a time and space average over all unstable modes. Performing this averaging for a fixed

FIG. 2: Time series showing fluctuations in the main ion density ($n_i^2$) and impurity flux ($\Gamma_z$) after averaging over the whole flux tube (see Fig. 3). The averaged impurity flux ($\langle \Gamma_z \rangle$) is calculated from $\Gamma_z$, discarding the first portion to ensure that the linear phase of the simulation is not included. $\langle I_z \rangle$ is used for finding the peaking factor for the impurity species, as is illustrated in Fig. 1. The bursty nature of the transport is seen in the peak around $t \approx 300 R/c_s$. These bursts have been found to affect the average flux little, but to significantly increase the estimated error in $\langle \Gamma_z \rangle$.

Data from NL GENE simulation of TE mode driven turbulence with He impurities. The parameters are the same as in Fig. 4(a), with $-R\nabla n_Z/n_Z = R/L_{n_Z} = 1.5$.

FIG. 3: A cross-section of the flux tube, showing the fluctuation of the electrostatic potential $\phi$. Data from NL GENE simulation of TE mode turbulence, with parameters as in Fig. 4(a) at $t \approx 300 R/c_s$. 

59 (Paper II:3)
length scale $k_θρ_s$ of the turbulence, the following expression is reached:

$$\frac{Γ_{n_z}}{n_2c_s} = \frac{k_θρ_sγ_θ}{|N_1|^2} \left\{ \frac{R}{2L_{n_z}} \left( |\tilde{w}|^2 + \frac{14ρ_0^2}{3} \tilde{ω}_r + \frac{55}\tilde{ω}_r + \frac{25}{9} \right) - \frac{R}{2L_{T_z}} \left( 2ρ_0^2 \tilde{ω}_r + \frac{10ρ_0^2}{3} \tilde{ω}_r + \frac{35ρ_0^2}{9} \right) + \frac{Z}{3A_Zq_0^2|N_1|^2} \right\}$$

where $N_1 = \tilde{w} - 2τ_Z^2$ is introduced.

In the fluid model it is assumed that the turbulence is isotropic in the radial and poloidal directions ($r$ and $θ$ respectively; $k_rρ_s = k_θρ_s$), with a saturated fluctuation level estimate, based on nonlinear fluid simulations, of $|\tilde{ω}| = \frac{1}{\sqrt{r^2+ρ^2}}$. A brief review of the different mechanisms responsible for the impurity transport, as identified in previous studies, is given here. The first term in Eq. (7) corresponds to the diffusive part of Eq. (5), whereas the three subsequent terms correspond to the convective part of the transport of the impurity species. Of this, the $R/L_{T_z}$ term is the thermodiffusion, the sign of which is governed mainly by the real frequency, $\tilde{ω}_r$. For TE modes, $\tilde{ω}_r > 0$, and for ITG modes $\tilde{ω}_r < 0$, resulting the thermodiffusion generally giving an inward pinch for TE modes and an outward pinch for ITG modes. Due to the $Z$-dependence in $τ^2_Z$, this term scales as $V_Z^T \sim (1/Z)(R/L_{T_z})$ to leading order, rendering it unimportant for large $Z$ impurity species, but it is important for lighter elements, such as the Helium ash. Further, the $\langle λ \rangle$ term gives the curvature pinch, which is usually inward, and the final term is the parallel compression term for the impurities. As opposed to the thermodiffusion, the parallel compression pinch is usually outward for TE modes and inward for ITG modes. Its $Z$ dependence is $V_Z^T \sim Z/A_Zk_θ^2 \sim Z/A_Zq_0^2$, but since $A_Z \approx 2Z$ this is expected to be a very weak scaling. Effects of toroidal rotation on the impurity transport have recently been studied, but will not be considered here.

### B. Gyrokinetics – the GENE code

The GENE code is a massively parallel gyrokinetic Vlasov code, solving the nonlinear time evolution of the gyrokinetic distribution functions on a fixed grid in phase space. The gyrokinetic equations are derived from the kinetic equations by performing an average of the particle gyrations around the field lines, so that the equations follow the centre of gyration, rather than the explicit orbits. This reduces the velocity space coordinates from three to two directions: parallel and perpendicular velocity. Following the conventions of GENE, these are referred to as $v$ and $μ$ respectively. In real space, the radial ($z$) and bi-normal ($y$) dependencies are treated spectrally, i.e. those directions are discretised explicitly in $k$-space, whereas the toroidal ($z$) direction is discretised in real space.

In this paper, GENE simulations are performed in a flux tube geometry with periodic boundary conditions in the perpendicular directions. Its application relies on the assumption that the scales of the phenomena of interest are small compared to the length scales associated with the driving gradients. This is usually fulfilled in the core of the plasma. A cross-section of the flux tube is presented in Fig. 3. There the size of the turbulent features can be seen, and a comparison of their size to the flux tube’s perpendicular resolution of $\sim 125 \times 125$ main ion gyro-radii and the overall box size indicates that the resolution and flux tube dimensions are adequate; see Section III for more details on how the resolution was chosen.

The data presented in Fig. 3 is computed from the raw field data. By integrating further, scalar quantities can be obtained; quantities that are useful in comparing both with theoretical, experimental, and other numerical results. In this study, the scalar impurity flux $Γ_{Z}$ is of most interest. Time series showing the fluctuations in the main ion density and the impurity flux for a nonlinear GENE simulation are presented in Fig. 2.

GENE can also be run in quasilinear mode, a method that is considerably less demanding when it comes to computer resources. The method used here only captures the contribution from the most unstable mode, ignoring sub-dominant modes, and only for the particular poloidal length scale $k_θρ_s$ of choice. If the length scale is chosen appropriately, however, the quasilinear simulations are useful for getting a qualitative understanding of the physical processes. The QC model used here does not include a saturation condition to determine the absolute flux. In the QC results presented below, the peaking factor is obtained as a ratio between two fluxes, and is hence independent of the fluctuation level. A more extensive quasilinear kinetic study, accounting for all unstable modes and summing over a wave number spectrum, was presented in Ref. 9.

### III. SIMULATIONS

In this paper, the transport of impurities has been studied numerically, by calculating the impurity peaking factor (PF) for impurities with various impurity charge $(Z)$ and varying values of the driving background gradients. The process of calculating the peaking factor is illustrated in Fig. 1. The impurity particle flux $Γ_{Z}$ is computed for $\nabla N_Z$ in the vicinity of $I_Z = 0$, taking the estimated residuals of the samples’ uncertainty into account (see Fig. 2). The diffusivity $D_Z$ and convective velocity $RV_Z$ are then given by fitting the acquired fluxes to Eq. (5), where after the peaking factor is obtained as
TABLE I: Parameters used in the fluid and gyrokinetic simulations

<table>
<thead>
<tr>
<th></th>
<th>ITG :</th>
<th>TE :</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_i/T_e$:</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$s$:</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>$q$:</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>$\epsilon = r/R$:</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>$k_q\rho_s$:</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$n_{ce}, n_e + Z n_Z$:</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$n_Z$ (trace):</td>
<td>$10^{-6}$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>$R/L_{n_e,x}$:</td>
<td>2.0–3.0</td>
<td>2.0–3.0</td>
</tr>
<tr>
<td>$R/L_{T_i}, R/L_{T_e}$:</td>
<td>7.0</td>
<td>3.0</td>
</tr>
<tr>
<td>$R/L_{T_e}$:</td>
<td>3.0</td>
<td>7.0</td>
</tr>
</tbody>
</table>

* denotes scan parameter

$PF = -\frac{RV_Z}{D_Z}$ (see Section II A).

The instabilities causing the transport are fuelled by the free energy present in gradients in the system, and in general the steeper the gradient the more free energy is available, which is expected to lead to stronger modes and more pronounced transport. Two families of gradients are available that can drive the instabilities: the temperature gradients ($-R\nabla T_j/T_j \approx R/L_{T_j}$) and the density gradients ($-R\nabla n_j/n_j \approx R/L_{n_j}$), where $j = i, e$ for main ions and electrons respectively. Numerical studies have been performed, focused on the dependence of the peaking factor on these gradients.

The main parameters used in the simulations are summarised in Tab. I. The parameters were chosen to represent an arbitrary tokamak geometry at about mid radius, and do not represent any one particular experiment. As can be seen in the table, a TE or an ITG mode dominated plasma was studied by choosing a steep electron temperature gradient ($R/L_{T_e} = 7.0$) together with a moderate ion temperature gradient ($R/L_{T_i} = 3.0$) to prompt TE mode dominated dynamics, and the other way around for ITG mode dominance. It should be noted in this context, that TE modes can also be driven by steep density gradients. This case is omitted here, and left for future study. In order to preserve quasi-neutrality, Eq. (4), $\nabla n_e = \nabla n_i$ was used. The simulations are limited to cases with $T_e = T_i$.

In order to ensure that the resolution was sufficient, the resolution was varied separately for the perpendicular, parallel and velocity space coordinates, and the effects of this on the mode structure, $k_{\perp}$ spectra and flux levels were investigated. The resolution was then set sufficiently high for the effects on these indicators to have converged. For a typical NL simulation for main ions, fully kinetic electrons, and one trace species, a resolution of $n_x \times n_y \times n_z = 96 \times 96 \times 24$ grid points in real space and of $n_v \times n_i = 48 \times 12$ in velocity space was chosen. For QL GENE simulations the box size was set to $n_x \times n_y \times n_z = 8 \times 1 \times 24$ and $n_v \times n_i = 64 \times 12$ respectively.

Simulations have been performed with both deuterons and protons as main ions, but no significant differences in the impurity transport were found between the two cases.

The impurities were included self-consistently as a third species in the simulations, with the trace impurity particle density $n_Z/n_e = 10^{-6}$ in order to ensure that they have a negligible effect on the turbulence.

In the present study, a simple $s-\alpha$ geometry is assumed for the simulation domains. The effects of different tokamak geometries on drift wave turbulence have been studied in both fluid and gyrokinetic descriptions.

IV. RESULTS AND DISCUSSION

For the scalings studied, the charge number $Z$ of the impurities was varied from $Z = 2$ to $Z = 74$, with a mass to charge ratio $A/Z = 2$. The scalings of the peaking factor with the temperature gradients were studied by varying $R/L_{T_e}$ between $R/L_{T_i} = 6.0$ and $R/L_{T_e} = 10.0$ for the TE mode case, and similarly by varying $R/L_{T_{i,z}}$ between $R/L_{T_{e,z}} = 6.0$ and $R/L_{T_{e,z}} = 10.0$ for the ITG mode case. The density gradient scalings were obtained by varying $R/L_{n_e}$ between $R/L_{n_e} = 0.5$ and $R/L_{n_e} = 5.0$.

QL and NL scalings of $PF = -RV_Z/D_Z$ were obtained using GENE and compared to results obtained from the fluid model.

A. Scalings with impurity charge

The $Z$ scalings of the impurity peaking factor for the TE mode dominated case are presented in Fig. 4(a). A good agreement between fluid and NL gyrokinetic results is observed for the value $k_q\rho_s = 0.2$ used in the QL and fluid simulations. The peaking factors are larger and the trends are more pronounced in the QL GENE results, which overestimate the peaking factors by approximately a factor of two for low $Z$ impurities. As expected from the discussion in Section II A above, $PF$ varies the most for low $Z$ impurities where the thermopinch is stronger. For heavier elements, the peaking factor saturates at levels well below neoclassical predictions, as seen in previous gyrokinetic and fluid studies, of both TE and ITG mode dominated impurity transport.

For comparison, the results for the ITG mode dominated case is shown in Fig. 4(b). The two cases show a qualitative difference, with $PF$ falling towards saturation as $Z$ is increased for the TE mode case, while the opposite holds for the ITG mode case. This is in line with previous QL kinetic and fluid results. The peaking factor is close to zero for low $Z$ values in the ITG mode dominated case, however, the sign of $PF$ remains positive for all $Z$ in both the TE and the ITG mode dominated case considered. This indicates that a net inward pinch is the most common situation in both TE and ITG mode driven impurity transport, for the parameters...
The qualitative difference between the $Z$ scalings for the TE and ITG mode dominated cases can be understood from the balance of the thermodiffusion and parallel impurity compression in Eq. (7), the two terms having opposite signs for TE and ITG, as discussed above (Section II A). The parallel impurity compression is almost independent of $Z$, so it can be assumed that the thermodiffusion is the main contributor to the observed trends. The thermodiffusion, on the other hand, has the strongest effect for low $Z$ values, explaining the drop and rise of $PF$ with $Z$ for the TE and the ITG mode respectively. Since this term goes to zero for large values of $Z$, this also explains the observed saturation.

Next, we compare the transport of He in TE and ITG mode driven turbulence. For efficient removal of the helium ash, the ratio between the energy confinement time and the He ash removal time should fulfill $\tau_{eR} / \tau_{He} \geq 0.15$. This confinement time ratio is usually estimated by the $D_{He,eff}/\chi_{eff}$ ratio. Assuming $T_e = T_i$, the effective heat conductivity of the plasma can be defined as

$$\chi_{eff} = \frac{\chi_e R/L_{T_e} + \chi_i R/L_{T_i}}{R/L_{T_e} + R/L_{T_i}}. \quad (8)$$

We note from equation (5), that the convective fluxes will reduce $D_{He,eff}$ to a similar degree for the TE and ITG mode dominated cases since the helium peaking factors ($PF_{He} = -RV_{He}/D_{He}$) are nearly identical, with $PF_{He} \approx 1.2$ for both the NL GENE and fluid model in the TE case, and $PF_{He} \approx 1.3$ for the fluid model in the ITG mode dominated case. The latter is also very near to the NL GENE and fluid peaking factors for helium seen in a previous study. For a simple comparison between the two cases it is therefore sufficient to compare the ratios $D_{He}/\chi_{eff}$. For the TE mode dominated case we find $D_{He}/\chi_{eff} \approx 1.7$ and 1.3 using the fluid model and NL GENE respectively. For the ITG case, the fluid model yields $D_{He}/\chi_{eff} = 1.1$, which is comparable to the ratio 1.0 acquired using NL GENE in a previous study of ITG mode driven impurity transport. The results indicate that TE mode turbulence is at least as efficient as ITG turbulence at removing He ash for the parameters studied.

In the fluid treatment, a strong ballooning eigenfunction is assumed with $k^2_{||,a\phi} = (3\eta^2 R^2)^{-1}$. Since the contribution from the parallel compression pinch depends on the mode structure along the field line, the results are expected to be sensitive to the choice of $k_{||}$. To investigate the sensitivity of the fluid results to the mode structure, a simplified treatment was used, varying $k_{||}$ around its strong ballooning value while keeping the eigenvalues fixed. The results are shown in Fig. 5 for $k_{\rho\theta} = 0.2$ and 0.3 in the TE and ITG mode dominated cases. As observed, the peaking factors for TE mode turbulence are sensitive to the choice of $k_{||}$, with the peaking factor going from $PF \approx 2$ to $PF \approx 0$ when $k_{||}^2$ is varied from 0.5 to 2 times its strong ballooning value.

As is evident from Fig. 4, the value of $PF$ is also dependent on the choice of $k_{\rho\theta}$, the perpendicular length scale. Finding the $k_{\rho\theta}$ that allows the QL gyrokinetic and fluid models to best capture the behaviour of the impurity transport is non-trivial. For the cases considered,
The obtained scalings of $PF$ with the electron temperature gradient are presented in Fig. 7(a). We note that the NL gyrokinetic simulations overestimate the peaking factors by up to $\sim 50\%$. The fluid results are in good agreement with the NL GENE results. Only weak trends were observed, in compliance with previous studies.\textsuperscript{20,22,35} As with the $Z$ scaling in Fig. 4(a), the NL trend is less pronounced, reaching saturation for lower values of $R/L_T$, than the other two models.

For comparison, the results for the ITG mode dominated case are shown in Fig. 7(b). As was observed for the $Z$ scaling in Section IV A above, the trends for the TE and ITG mode dominated case are reversed; $PF$ rises with driving gradient for the TE case, but falls for the ITG case. The difference between the two trends can be understood in part from the thermodiffusion in Eq. (7). This term grows more important as the ion/impurity temperature gradient steepens, providing a strong outward pinch for the ITG mode dominated impurity transport and thus yielding lower values of $PF$ as $R/L_T$ increases (Fig. 7(b)). Since the impurity temperature gradient is constant for the $\nabla T_e$ scaling, however, other effects are behind the TE mode scaling in Fig. 7(a). The eigenvalues, in particular the mode growth rates, grow with $\nabla T_e$, as shown in Fig. 7(c). This will alter the relative contributions of the convective terms in Eq. 7, and hence affect the peaking factor. We note here that the eigenvalues in Fig. 7(c) are normalised to $c_s/R$, giving $\omega_0 < 0$ for TE modes and $\omega_0 > 0$ for ITG modes.

As with the $Z$ scaling, the sign of $PF$ usually remains positive for the $\nabla T_{e,i}$ scalings, though a modest flux reversal is observed when the trends of the scalings with $Z$ and $R/L_T$ for the ITG mode combine. This is the case for He in Fig. 7(b). The flux reversal is observed only for very steep temperature gradients for the considered parameter values with $T_e = T_i$.

### C. Scalings with density gradient

In experimentally relevant situations where the impurity and main ion fuelling originates from the edge, the core impurity and background density peaking factors should be calculated self-consistently for zero particle flux. For this purpose, the equations $I_Z = 0$ and $I_{i,e} = 0$ need
achieved by varying the main ion density gradient to be solved self-consistently. This is in the following achieved by varying the main ion density gradient $R/L_{n_e}$ until $I_e = 0$ is obtained, and using the zero flux background density gradient in the impurity transport calculations. We assume trace levels of impurities and use the fluid model for simplicity. The results are illustrated in Fig. 8 which shows the impurity peaking factor $R/L_{j}$ versus $R/L_{n_e}$ for both the TE and ITG mode dominated cases. The value of $R/L_{n_e}$ for zero background particle flux is marked in the figure. We note that the background density peaking is larger than the impurity peaking with $R/L_{n_e} \approx 2.5$ for both the TE and the ITG case. We emphasise that the result is obtained using a collision-less model. It is known that collisions have a large impact on the background density peaking in both fluid and gyrokinetic models.\textsuperscript{53}

For the $R/L_{n_e}$ scaling, the same trends are observed in both QL GENE and fluid data, with a strong sensitivity for lower $Z$ impurities. This is particularly evident for the ITG mode case in Fig. 8(b), where the peaking factor for the He impurity shows a marked increase as $\nabla n_e$ steepens for both GENE and fluid results, whereas for the heavier elements a nearly flat dependence is observed.

As shown in Fig. 8(c), the eigenvalues vary with the electron density gradient. A reduction of $|\omega_s|$ and an increase of $\gamma$ are observed with increasing $R/L_{n_e}$, which leads to a reduction of the relative amplitude of the thermopinch in Eq. (7). This explains the observed $PF$ scaling for the TE and ITG mode driven cases in Fig. 8(a) and Fig. 8(b) respectively.

As with the $\nabla T_e$ scaling, the combined effect of the $Z$ and $\nabla n_e$ scalings is observed to lead to a flux reversal for the He impurity in the ITG mode dominated case in Fig. 8(b). This happens for flat electron density profiles in the QL GENE results. Outside of this regime the sign of $PF$ remains positive.

V. CONCLUSION AND FUTURE WORK

In the present paper the transport of impurities driven by Trapped Electron (TE) mode driven turbulence has been studied. Non-linear (NL) gyrokinetic simulations using the code GENE were compared with results from quasilinear (QL) gyrokinetic simulations and a computationally efficient fluid model, viable for use in predictive simulations. The main focus has been on model comparisons for electron temperature gradient driven turbulence regarding the sign of the main ion and impurity convective velocities (pinches) and the peaking factors ($R/L_{n_e}$)
8(a): dependence of the impurity peaking factor \((PF)\) on the normalised electron density gradient for the TE case, also indicated is the main ion peaking factor \((PF_e)\) from fluid theory.

8(b): dependence of the impurity peaking factor \((PF)\) on the normalised electron density gradient for the ITG case, also indicated is the main ion peaking factor \((PF_e)\) from fluid theory.

8(c): real frequency \((\omega_r)\) and growth rate \((\gamma)\) for the two cases in Fig. 8(a) and Fig. 8(b).

FIG. 8: Scalings of the impurity peaking factor \((PF)\) with the electron density gradient \((-R\nabla n_e/n_e = R/L_{ne})\), also indicated is the main ion peaking factor \((PF_e)\) from fluid theory. Parameters for the TE and ITG mode cases as in Fig. 4, with \(k_0\rho_s = 0.3\) for both cases. The eigenvalues in Fig. 8(c) are from QL GENE simulations, they are normalised to \(c_s/R\).

The He ash removal was studied through a comparison of the ratio of the particle diffusivity and effective heat conductivity \((D_{He}/\chi_{eff})\), using both NL GENE and fluid simulations. The obtained results indicated that TE mode turbulence is at least as efficient as ITG turbulence at removing He ash for the parameters studied, with \(D_{He}/\chi_{eff} > 1.0\) for both modes of turbulence. A comprehensive investigation, however, would require a predictive global transport simulation with multiple species, including He sources, which is beyond the scope of the present work.

The scaling of impurity peaking with the driving background temperature gradients were found to be weak in most cases. The QL results were also here found to significantly overestimate the peaking factor for low \(Z\) values.

For the scaling of the impurity peaking factor with the impurity charge \(Z\), a weak dependence was obtained from NL GENE simulations, which was reproduced well by the fluid simulations. The QL GENE results showed a stronger dependence for low \(Z\) impurities and overestimated the peaking factor by up to a factor of two in this region. As in the case of ITG dominated turbulence, the peaking factors were found to saturate as \(Z\) increased, at a level much below neoclassical predictions. However, the scaling with \(Z\) was found to be weak or reversed as compared to the ITG case, where the larger peaking factors were obtained for high \(Z\) impurities.
ploying an extended QL model, accounting for all unstable modes and summing over a wave number spectrum. In general, however, only a nonlinear simulation can determine the spectrum that best approximates the transport features for a given set of parameters. Using the fluid model it was further shown that the impurity peaking factors in the TE mode dominated case are sensitive to the mode structure along the field lines ($k_p$) through the parallel compression pinch. Assuming a strong ballooning eigenfunction with $k^2 = \left(3q^2R^2\right)^{-1}$ gave a good agreement with the results from the NL GENE simulations.

The present study is based on low $\beta$ plasmas in a simple $s-\alpha$ circular tokamak equilibrium. Future work will aim to study the effects of more realistic geometries, finite $\beta$, as well as effects of plasma rotation on impurity transport in NL fluid and gyrokinetic descriptions.

ACKNOWLEDGMENTS

The simulations were performed on resources provided on the Lindgren\textsuperscript{54} and HPC-FF\textsuperscript{55} high performance computers, by the Swedish National Infrastructure for Computing (SNIC) at Parallelldatorcentrum (PDC) and the European Fusion Development Agreement (EFDA), respectively.

J. Vincent at PDC and T. Görler at IPP–Garching are acknowledged for their assistance concerning technical and implementational aspects in making the GENE code run on the PDC Lindgren super-computer. A. Strand and L. Strand at Herrgårdskskolan are acknowledged for their help with the nonlinear simulations. The authors would also like to thank F. Jenko, M. J. Piischel, F. Merz and the rest of the GENE team at IPP–Garching for their valuable support and input.

2. Also commonly referred to as the $g_i$ mode.
42. M. A. Beer, GYROfluid Models of Turbulent Transport in Toka-
45The density and temperature gradients of the impurity species can also drive turbulent transport, however, for trace amounts this effect is negligible.
54See http://www.pdc.kth.se/resources/computers/lindgren/ for details on Lindgren.
55See http://www2.fz-juelich.de/jsc/juropa/ for details on HPC-FF.
Particle transport in density gradient driven TE mode turbulence

A. Skyman, H. Nordman, P. I. Strand

Presented at the
13th International Workshop on H-mode Physics and Transport Barriers
Oxford, UK, October 2011

Postprint, see DOI link for the published version

Nuclear Fusion
vol. 52, no. 11, p. 114015


http://publications.lib.chalmers.se/records/fulltext/local_164276.pdf
Particle transport in density gradient driven TE mode turbulence

A. Skyman¹, H. Nordman¹, P. I. Strand¹
¹Euratom-VR Association, Department of Earth and Space Sciences, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Abstract

The turbulent transport of main ion and trace impurities in a tokamak device in the presence of steep electron density gradients has been studied. The parameters are chosen for trapped electron (TE) mode turbulence, driven primarily by steep electron density gradients relevant to H-mode physics. Results obtained through non-linear (NL) and quasilinear (QL) gyrokinetic simulations using the GENE code are compared with results obtained from a fluid model. Impurity transport is studied by examining the balance of convective and diffusive transport, as quantified by the density gradient corresponding to zero particle flux (impurity peaking factor). Scalings are obtained for the impurity peaking with the background electron density gradient and the impurity charge number. It is shown that the impurity peaking factor is weakly dependent on impurity charge and significantly smaller than the driving electron density gradient.

1 Introduction

The compatibility between a reactor-grade plasma and the material walls surrounding the plasma is one of the main challenges facing a magnetic fusion device. The presence of very low levels of high Z impurities in the core plasma may lead to unacceptable levels of radiation losses and fuel dilution. Also low Z impurities, in the form of beryllium or helium-ash, may result in fuel dilution that severely limits the attainable fusion power [1]. Consequently, the transport properties of impurities is a high priority issue in present experimental and theoretical fusion plasma research. This is emphasised by the the new ITER-like wall experiment in JET [2], where a beryllium-clad first wall in the main chamber, combined with carbon and tungsten tiles in the divertor, will be tested for the first time.

The transport of main fuel as well as impurities in the core region of tokamaks is expected to be dominated by turbulence driven by Ion Temperature Gradient (ITG) modes and Trapped Electron (TE) modes. The main drives for the ITG/TE mode instabilities are gradients of temperature and density combined with unfavourable magnetic curvature. Most of the theoretical studies of turbulent particle transport have been devoted to temperature gradient driven ITG and TE modes, using both fluid, and quasilinear (QL) and nonlinear (NL) gyrokinetic models [3–24]. Much less effort has been devoted to particle transport in regions with steep density gradients. The density gradient, which is stabilising for ITG modes, provides a drive for TE modes which may dominate the temperature gradient drive for plasma profiles with $R/L_{Te} > R/L_{ne}$. This may occur in connection with the formation of transport barriers, like the high confinement mode (H-mode) edge pedestal, in fusion plasmas.
In the present article, the turbulent transport of main ion and trace impurities in tokamaks is investigated through nonlinear (NL) gyrokinetic simulations using the GENE code. The main part considers collisionless TE modes driven by density gradients. The impurity density gradient for zero impurity flux is calculated for varying background electron density gradient drive and for a range of impurity species. This study complements recent studies [23, 24] on temperature gradient driven TE and ITG mode impurity transport. The NL GENE results are compared with QL gyrokinetic simulations and a computationally efficient multi fluid model, suitable for use in predictive transport simulations. Of particular interest is the sign of the impurity convective flux and the degree of impurity peaking in the presence of strong background electron density gradients.

The remainder of the article is structured as follows: in section 2 impurity transport is briefly reviewed, with emphasis on topics relevant to the study; this is followed by section 3 on the simulations and a discussion of the main results. The article concludes with section 4, containing a summary of the main conclusions to be drawn.

2 Transport models

The models used have been described in detail elsewhere, see [23] and references therein, only a brief summary is given here.

The NL and QL GENE simulations were performed in a flux tube geometry, in a low $\beta$ ($\beta = 10^{-4}$) s-\(\alpha\) equilibrium [25–28]. The simulations include gyrokinetic electrons (passing and trapped), and gyrokinetic main ions and impurities. Effects of finite $\beta$, plasma shaping, equilibrium $E \times B$ flow shear and collisions have been neglected. The effects of collisions are known to be important for the turbulent fluctuation and transport levels [29], however, their effects on the impurity peaking factor have been shown to be small [12]. In order to ensure that the resolution was adequate, the resolution was varied separately for the perpendicular, parallel and velocity space coordinates, and the effects of this on the mode structure, $k_\perp$ spectra and flux levels were investigated. The resolution was then set sufficiently high for the effects on these indicators to have converged. For a typical NL simulation for main ions, fully kinetic electrons, and one trace species, a resolution of $n_x \times n_y \times n_z = 96 \times 96 \times 24$ grid points in real space and of $n_v \times n_\mu = 48 \times 12$ in velocity space was chosen. For QL GENE simulations the box size was set to $n_x \times n_y \times n_z = 8 \times 1 \times 24$ and $n_v \times n_\mu = 64 \times 12$ respectively. The impurities were included self-consistently as a third species in the simulations, with the trace impurity particle density $n_Z/n_e = 10^{-6}$ in order to ensure that they have a negligible effect on the turbulence.

For the fluid simulations, the Weiland multi-fluid model [30] is used to derive the main ion, impurity, and trapped electron density response from the corresponding fluid equations in the collisionless and electrostatic limit. The fluid simulations include first order Finite Larmor-Radius (FLR) effects for the main ions, and parallel main ion/impurity dynamics. The free electrons are assumed to be Boltzmann distributed. The equations are closed by the assumption of quasineutrality:

$$\frac{\delta n_e}{n_e} = (1 - Z f_Z) \frac{\delta n_i}{n_i} + Z f_Z \frac{\delta n_Z}{n_Z},$$

where $f_Z = n_Z/n_e$ is the fraction of impurities with charge $Z$, and $n_j$ and $\delta n_j$ are the density and the density perturbation for species $j$. An eigenvalue equation for TE and ITG modes is thus obtained in the presence of impurities. A strongly ballooning eigenfunction with $k_\parallel^2 = (3q^2R^2)^{-1}$

\[\text{http://www.ipp.mpg.de/~fsj/gene/}\]
valid for magnetic shear $s \sim 1$ is used [31]. The eigenvalue equation is then reduced to a system of algebraic equations that is solved numerically.

The main ion and impurity particle fluxes can then be written as:

$$
\Gamma_j = \langle \delta n_j v_E \rangle = -n_j \rho_s c_s \left( \tilde{n}_j \frac{1}{R} \frac{\partial \tilde{\phi}}{\partial \theta} \right). \tag{2}
$$

Here $v_E$ is the radial $E \times B$ drift velocity, $\rho_s = c_s / \Omega_{ci}$ is ion sound scale, with $c_s = \sqrt{T_e/m_i}$ being the ion sound speed and $\Omega_{ci} = eB/m_i$ the ion cyclotron frequency. On the right hand side, the perturbations in density and electrostatic potential are defined $\tilde{n}_j = \delta n_j / n_j$ and $\tilde{\phi} = \phi / T_e$ respectively. The angled brackets in equation (2) imply a time and space average over all unstable modes. Performing this averaging, the particle flux can be written:

$$
\frac{R \Gamma_j}{n_j} = D_j \frac{R}{L_{nj}} + D_T \frac{R}{L_{Tj}} + RV_{p,j}. \tag{3}
$$

The first term in equation (3) corresponds to diffusion, the second to the thermodiffusion and the third to the convective velocity (pinch), where $1/L_{nj} = -\nabla n_j / n_j$, $n_j$ is the density of species $j$ and $R$ is the major radius of the tokamak. The pinch contains contributions from curvature and parallel compression effects. The terms of equation (3) have been described in detail in previous work [17–19, 23]. For trace impurities, equation (3) can be uniquely written

$$
\frac{R \Gamma_Z}{n_Z} = D_Z \frac{R}{L_{nz}} + RV_Z, \tag{4}
$$

where $D_Z$ is the impurity diffusion coefficient and $V_Z$ is the total impurity convective velocity with the thermodiffusive term included, and neither $D_Z$ nor $V_Z$ depend on $1/L_{nz}$. The sign of the thermodiffusive, or “thermopinch”, term is decided mainly by the real frequency, $\tilde{\omega}_r$. For electron modes $\tilde{\omega}_r = R \omega_r / c_s < 0$, resulting in the thermodiffusion generally giving an inward contribution to the pinch for TE modes. For an impurity with charge number $Z$, this term scales as $D_{Tz} \sim (1/Z)(R/L_{Tz})$ to leading order, rendering it unimportant for large $Z$ impurity species, but it is important for lighter elements, such as the He ash.

The zero-flux impurity density gradient (peaking factor) is defined as $PF_Z = -RV_Z/D_Z$ for the value of the impurity density gradient that gives zero impurity flux. The peaking factor thus quantifies the balance between convective and diffusive impurity transport. Solving the linearised equation (4) for $R/L_{nz}$ with $\Gamma_Z = 0$ yields the interpretation of $PF_Z$ as the gradient of zero impurity flux. It is found by first computing the impurity particle flux $\Gamma_Z$ for values of $R/L_{nz}$ in the vicinity of $\Gamma_Z = 0$. The diffusivity ($D_Z$) and convective velocity ($V_Z$) are then given by fitting the acquired fluxes to equation (4), whereafter the peaking factor is obtained through their quotient. This is illustrated in figure 1.

### 3 Simulation results

The main parameters used in the simulations are summarised in table 1. The parameters where chosen to represent an arbitrary tokamak geometry at about mid radius, and do not represent any one particular experiment. A moderately steep electron temperature gradient ($R/L_{Te} = 5.0$) together with a flatter ion temperature gradient ($R/L_{Ti, Z = 2.0}$) was used to promote TE mode dominated dynamics. Following [32], the background density gradient for the base scenario was set higher than the temperature gradient, to ensure density gradient driven dynamics. In order to preserve quasineutrality $\nabla n_e = \nabla n_i$ was used. The quasilinear gyrokinetic and fluid results
were calculated for a single poloidal mode number with $k_\theta \rho_s = 0.2$; see [23] for a discussion on the choice of $k_\theta \rho_s$.

First, the main ion particle flux ($\Gamma_p$) is studied. Time averaged fluxes are calculated from time series of NL GENE data after convergence, as illustrated in figure 2a. The scalings of $\Gamma_p$ with the electron density gradient obtained from NL GENE and fluid simulations are shown in figure 2b. The fluid and nonlinear gyrokinetic model show similar scalings for the main ion flux, but the gyrokinetic transport exhibits a stronger dependence on $R/L_n$. This is in line with the trends seen for the linear eigenvalues, as show in figure 2c. The NL GENE and fluid results presented in figure 2b indicate that for the present parameters, neither model gives a main ion flux reversal for TE mode driven turbulence.

Next, the scaling of the impurity transport with the background density gradient ($R/L_n$) is investigated. The results for the impurity peaking factor are shown in figure 3a. We note that the impurity peaking increases with $R/L_n$, saturating at $PF_Z \approx 2.0$ for large values of the electron density gradient. The QL GENE results tend to consistently overestimate the peaking factors compared to the NL GENE results, while the fluid model gives results that are somewhat below the NL GENE results for the steeper gradients. The fluid results show a considerably less dramatic dependency of the peaking factor than the QL and NL gyrokinetic results, both of which show a strong decrease in $PF_Z$ as the electron density profiles flatten. This is observed for all values of the impurity charge number. As the background density profile becomes more peaked, a corresponding increase in impurity transport is expected. This is illustrated in figure 3b, where scalings, obtained from NL GENE simulations, of the diffusivity ($D_Z$) and convective velocity ($RV_Z$) with $R/L_n$ are shown. Although the magnitudes of $D_Z$ and $RV_Z$ both show a strong increase with $R/L_n$, in accordance with the scaling of the growth rate seen in figure 2c, the impurity peaking ($PF_Z = -RV_Z/D_Z$) is only weakly sensitive to the electron density gradient. For $R/L_n \lesssim 2.0$ the impurity peaking factor is not well defined, since both $D_Z$ and $RV_Z$ go to zero. The fluid and gyrokinetic results are in qualitative agreement, showing a growth rate that increases uniformly with $R/L_n$. For the studied parameters, there are no clear signs of a transition from density gradient driven to temperature gradient driven TE mode turbulence, which has been reported to dominate for $R/L_n \lesssim R/L_T$ [32].

The scaling of the impurity peaking factor with impurity charge ($Z$), with $R/L_n$ as a parameter, is illustrated in figure 4. The impurity charge was varied from $Z = 2$ (He) to $Z = 42$ (Mo). The models show only a very weak scaling, with $PF_Z$ falling toward saturation for higher $Z$. The results are similar to those for the temperature gradient driven TE mode reported in [24]. Notably, the QL GENE simulations overestimate the peaking factors compared to the NL GENE results, whereas the fluid results are lower than the NL GENE results. The scalings observed for low $Z$ impurities ($Z \lesssim 10$) is weak or reversed compared to results for the ITG mode driven case, reported in e.g. [23], where a strong rise in $PF_Z$ with increasing $Z$ was obtained. The qualitative difference between the TE and the ITG mode dominated cases can be understood from the $Z$-dependent thermodiffusion in equation (3), which is outward for ITG modes and inward for TE modes.

4 Conclusions

In summary, the turbulent transport of main ion and trace impurities in regions of steep density gradients has been investigated through nonlinear (NL) gyrokinetic simulations using the GENE code. The simulations included gyrokinetic electrons (passing and trapped), and gyrokinetic main ions and impurities in a low $\beta$ s-\alpha equilibrium. The main part has considered collisionless TE modes driven by steep density gradients, a parameter regime of relevance for the formation
of transport barriers in fusion plasmas. The NL GENE results for the density gradient of zero impurity particle flux (peaking factor) have been compared with QL kinetic simulations and a reduced and computationally efficient multi-fluid model, suitable for use in predictive transport simulations. In the simulations, the magnetic shear and safety factor were held fixed at $s = 0.8$ and $q = 1.4$. For the parameters studied, qualitative agreement between gyrokinetic and fluid results has been obtained for the scaling of the impurity peaking factor with both the background density gradient and the impurity charge. An inward impurity convective velocity, corresponding to positive peaking factor, was found in all cases considered. In the region of steep electron density gradients, it was shown that the impurity peaking factor saturates at values significantly smaller than the driving electron density gradient. In general, a good qualitative agreement between the considered models was found. It was, however, noted that for the chosen length scales ($k_0 \rho_s = 0.2$), the QL GENE, in comparison with the NL GENE results, tended to overestimate the peaking factors, whereas the fluid results were close to or lower than the NL GENE results. The scaling of the peaking factor with impurity charge was observed to be weak, with a slight increase in the impurity peaking factor observed in the gyrokinetic results for low impurity charge numbers.

Acknowledgements

The simulations were performed on resources provided on the Lindgren\(^2\) and HPC-FF\(^3\) high performance computers, by the Swedish National Infrastructure for Computing (SNIC) at Parallelatorcentrum (PDC) and the European Fusion Development Agreement (EFDA), respectively. The authors would like to thank Frank Jenko, Tobias Görler, M. J. Puschel, and the rest of the GENE team at IPP–Garching for their help with the gyrokinetic simulations.

References


\(^2\)http://www.pdc.kth.se/resources/computers/lindgren/

\(^3\)http://www2.fz-juelich.de/jsc/jupopa/


[27] Dannert T and Jenko F 2005 Phys. Plasmas 12 072309


Table 1: Parameters used in the fluid and gyrokinetic simulations, † denotes scan parameters

<table>
<thead>
<tr>
<th></th>
<th>$R/L_{n_e}$-scaling:</th>
<th>$Z$-scaling:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_i/T_e$:</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$s$:</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>$q$:</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>$\beta$:</td>
<td>$10^{-4}$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>$\varepsilon = r/R$:</td>
<td>0.14</td>
<td>0.14</td>
</tr>
<tr>
<td>$k_0 \rho_s$:</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$n_e, n_i + Z n_Z$:</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$n_Z$ (trace):</td>
<td>$10^{-6}$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>$R/L_{T_i}, R/L_{T_Z}$:</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>$R/L_{T_e}$:</td>
<td>5.0</td>
<td>5.0</td>
</tr>
<tr>
<td>$R/L_{n_i,e}$:†</td>
<td>1.0–13.0</td>
<td>5.0–13.0</td>
</tr>
<tr>
<td>$Z$:†</td>
<td>2, 28</td>
<td>2–42</td>
</tr>
</tbody>
</table>
Figure 1: Impurity flux ($\Gamma_Z$) as a function of the impurity density gradient ($-R\nabla n_Z/n_Z = R/L_{n_Z}$), illustrating the process of finding the impurity peaking factor ($PF_Z$), diffusivity ($D_Z$) and convective velocity ($V_Z$). NL GENE data of TEM turbulence in a proton plasma with He impurities, and background density gradient $R/L_n = 5.0$. 

78 (Paper III:8)
(a) time series and time averages of the main ion flux ($\Gamma_p$) from NL GENE simulations

(b) main ion flux ($\Gamma_p$) dependence on the background density gradient ($R/L_{ne}$).
Figure 2: Main ion flux ($\Gamma_p$) dependence on the background electron density gradient $(-R\nabla n_e/n_e = R/L_{ne})$. NL GENE and fluid data with protons as main ions. Parameters are $q = 1.4$, $s = 0.8$, $\varepsilon = \tau/R = 0.14$, $R/L_{T_i,Z} = 2.0$, $R/L_{T_e} = 5.0$, and $\tau = T_e/T_i = 1.0$. The fluid data was obtained for $k_0 \rho_s = 0.2$. The fluxes are normalised to $v_{T_i} n_e \rho_i^2 / R^2$. The error bars indicate an estimated uncertainty of one standard deviation. The eigenvalues in figure 2c are from fluid and GENE simulations, and are normalised to $c_s / R$. 

(c) scaling of real frequency ($\omega_r$) and growth rate ($\gamma$) with the background density gradient
(a) dependence of the impurity peaking factor ($PF_Z$) on the background density gradient
(b) dependence of the impurity diffusivity and convective velocity \((DZ\) and \(RVZ\)) on the background density gradient.

Figure 3: Scalings of the impurity peaking factor \((PF_Z = -RVZ/DZ)\) with the background electron density gradient \((R/Lne)\), with parameters as in figure 2. QL and fluid data have been acquired using \(k_0\rho_s = 0.2\). Figure 3b shows the diffusivities and pinches corresponding to the NL GENE impurity peaking factors \((PF_Z)\) in figure 3a. \(DZ\) and \(RVZ\) are normalised to \(vT,i\rho_i^2/R\). The error bars indicate an estimated uncertainty of one standard deviation.
Figure 4: Scaling of the impurity peaking factor ($PF_Z = -RV_Z/D_Z$) with impurity charge $Z$, with parameters as in figure 2; $k_θρ_s = 0.2$ was used in the QL and fluid simulations. The error bars indicate an estimated uncertainty of one standard deviation.