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**AN IMPROVED NEUTRAL DIFFUSION MODEL AND
NUMERICAL SOLUTION OF THE TWO DIMENSIONAL EDGE
PLASMA FLUID EQUATIONS**

FINAL REPORT

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Chapter 1

Introduction

The availability of a relatively unlimited source of energy through nuclear fusion has been long awaited. With the present physical/engineering status, it is very unlikely that a commercial fusion reactor will be in operation within the next decade. This is due to the fact that numerous physical and engineering problems must be clearly understood and resolved in order to realistically build such reactor. Despite these difficulties, the research effort has never stopped. Just recently, early December 1993, Princeton's tokamak reactor (TFTR-Tokamak Fusion Test Reactor), produced about 6.2 MW energy for about 1 second, a significant improvement since JET (Joint European Tokamak) in 1991. The output energy is still far from break-even (compared to 24 MW input), but it indicates that fusion is moving toward the desired goal at its own pace. Currently there is an extensive collective research effort by the USA, Russian, European Community and Japan to build a prototype of a commercial fusion reactor (ITER - International Thermonuclear Experimental Reactor). ITER owes its inception to the joint communique by President Reagan of the USA and General Secretary Gorbachev of the USSR issued at the November 1985 Geneva Summit. In its terms of reference agreement, ITER is expected to demonstrate a confinement capability to reach controlled ignition for a duration sufficient to achieve steady state conditions and to demonstrate the technology essential for a fusion reactor. Ultimately ITER is expected to demonstrate the scientific and technological feasibility of

fusion power [1].

1.1 Brief Review of Nuclear Fusion

Nuclear fusion is the process of the joining together or fusing of two nuclei of light atoms (Deuterium and Tritium) to form the nucleus of a heavier atom (Helium) (see figure 1.1). There are other reactions (D-D or D-He) that may occur, but the D-T reaction is more favorable due to the low range temperature at which the fusion reaction can be harnessed. The D-T reaction is associated with an enormous energy release of about 17.6 MeV. However, due to the Coulomb force interaction, the reaction is difficult to bring about. To overcome the Coulomb force, the nuclei must be made sufficiently energetic (10-100 keV). At these temperatures, light atoms are completely stripped of their orbital electrons. This macroscopically neutral gas of positively charged light atomic nuclei and electrons is a thermonuclear plasma [2]. To sustain the reaction the plasma is confined by using an intense magnetic field in a doughnut-shaped vacuum vessel, i.e., a torus or a tokamak, a name derived from the Russian word for toroidal magnetic chamber. The vessel/reactor is set up as an axisymmetric configuration that is characterized by poloidal and toroidal fields. The toroidal field is stronger than the poloidal field, such that ideally the plasma can be held and confined as long as necessary. However, there is always a possibility that the plasma "leaks" out of the confining magnetic fields due to fluid instabilities and hits the confining wall. As a consequence, the leaking plasma cools off and impurities (from the interactions of plasma particles and the wall material) enter the core plasma, collapsing the plasma confinement. To alleviate this problem a separate chamber is added such that plasma particles are diverted away from the confining wall. This chamber is known as a poloidal divertor.

The overall plasma performance in the tokamak reactor is greatly influenced by the characteristics of the scrape-off layer (SOL) or edge plasma region. The term "SOL" and "edge plasma" terms will be used interchangeably throughout this study.

Reactants	Products
D-D	T (1 MeV) + p (3 MeV)
D-D	He ³ (0.8 MeV) + n (2.5 MeV)
D-T	He ⁴ (3.5 MeV) + n (14 MeV)
D-He ³	He ⁴ (3.7 MeV) + p (14.7 MeV)

Figure 1.1: Nuclear Fusion Reaction

The scrape-off layer is defined as that part of the plasma which lies outside the separatrix (figure 1.2), and where the occurrence of plasma particle creation, plasma-wall interaction processes (impurities generation), large energy losses and hydrogen recycling could have significant effects on the plasma particle and the energy confinement of the tokamak plasma. The plasma behavior in this region is the subject of this dissertation and it is studied through the development of a robust and efficient computational tool that can be used for routine optimization studies of poloidal tokamak divertors.

1.2 ITER and its Poloidal Divertor

A unique element of the ITER reactor is its size (figure 1.3). Unlike other existing experimental reactors, ITER's dimensions are much larger. The major and minor radii are designed to be approximately 7 and 3 meters respectively with an expected power delivery in the range of 2-3 GW. Although ITER has most of the other physics and physical reactors' characteristics, the extrapolation from existing reactors to the desired ITER conditions is by no means straightforward. This is due mainly to the fact that the current physical data base on the existing reactors is not exact. The basic physical assumptions however are similar to existing ones. As indicated earlier, ITER is expected to be operating with a divertor to divert particles and energy away from the vessel wall. Several existing tokamak reactors have been performing experiments to simulate the divertor dynamics with a certain degree of success. The

Figure 1.2: Poloidal Cross-Section of a Tokamak (ITER-International Thermonuclear Experimental Reactor)

primary objective of these experiments is mainly directed toward understanding the divertor material longevity as a result of plasma particle bombardment. In terms of the material choice the divertor is the most challenging problem of ITER design. Our present work is an attempt to understand the effect of impinging particles on ITER divertor plates by providing a reliable computational tool consisting of basic governing equations.

A consequence of using a poloidal divertor is a high peak heat flux that the plate must endure. Depending upon the scenario, the peak heat flux can vary between $40 - 200 \text{ MW/m}^2$, imposing stringent limitation on the thermo-physical and thermo-mechanical properties of the divertor material. The ITER divertor is expected to operate under a high recycling regime resulting in low temperature and high plasma density. In the high recycling scenario a large fraction of neutral particles of the working gas are entered back into the divertor plasma where they are ionized, thus increasing the plasma density accompanied by a decrease of temperature in the region near the divertor plate. The low temperature will significantly reduce the flux of impurities from the divertor to plasma core [3]. This option is not without disadvantages. Although the recycling process causes a desired steep poloidal temperature gradient near the plate, the area of flow reversal increases substantially. Consequently, this condition will cause impurities to flow out of the divertor region and contaminate the core plasma.

The high recycling process which results in a high plasma density condition can also be triggered by deuterium gas injection near the divertor plate (gas puffing). Earlier studies indicated that extremely large quantities of injected gas ($\sim 10^{24}$ particles/second) may be necessary to achieve a desirable divertor operation. Intense gas puffing allows energy loss from plasma electrons through excitation, dissociation or ionization, as well as energy extraction from plasma ions through charge exchange and elastic/ion neutral collisions [4]. Another possibility is to inject an acceptable amount of impurities into the divertor chamber. By radiating away some of the incoming power toward the divertor, the divertor peak heat load can be reduced. The

A computer-generated model of the ITER device.

Figure 1.3: Proposed ITER Reactor Configuration

existence of impurities can be viewed from two perspectives. The accumulation of impurities and the accompanying radiation losses in the core plasma can have severe consequences in the achievement of viable reactor grade plasma. This is mainly due to the degradation of the energy confinement as a result of radiation losses and the reduction of reaction rates caused by impurities in the core plasma dilution. On the other hand, as stated earlier, it can be advantageous in the periphery of the reactor. The latter scenario is often referred to as a gaseous-radiative divertor operation.

1.3 General Philosophical Goal

It has been established without doubt [5], [6] that the key to successfully model the physics of ITER edge plasma relies on the availability of a robust computational scheme. Edge plasma study is a very complex problem and it is still searching its established form. During the development, as indicated earlier, numerous new physical models are being developed as well as refinements of the currently used physical models, particularly near the divertor plate. The atomic physics of the plasma-neutral interactions is rich and strongly influences the dynamics of the edge plasma or SOL. Results from experiments with other (non-ITER) tokamak machines as well as ITER simulations are used and evaluated interchangeably to optimize current ITER design. The intention of this research is to develop a complete basic edge plasma physics model with a robust numerical scheme such that a routine ITER optimization study can be performed. Numerical limitations such as slow convergence, number of computational cell inflexibility, memory shortage and others that have been encountered, especially NEWEDGE (Newton Edge Plasma), will be used as a guidance to improve existing numerical approach. NEWEDGE [5] can be considered as the pioneer to simulate edge plasma by employing a fully implicit technique. The code has shown successes on non-ITER geometry and therefore it will be used as the basis of our research. All of the NEWEDGE attractive features that are currently demonstrated will be kept and further enhanced.

The current code is intended to provide a solid numerical foundation on which any future extensions or modifications would can be added with minimum effort. The foundation of this work is based on a basic yet sound set of governing equations in which future expansion can be performed in a relatively easy fashion. Thus, within the framework of this work, treatment for fluid drifts and multispecies impurities are not included in the governing equations. Code robustness on our basic edge plasma physics model is determined by allowing only a minimum work for future modifications. The implication is that the chosen numerical scheme must not be changed fundamentally. It is well-known in the computation community, that as physical complexities increases, without a solid and appropriate numerical scheme, the problem of convergence becomes a dominant factor that may inhibit success. In edge plasma physics, for instance, the plasma-neutral interaction near the divertor plate that will cause a sharp gradient profile in density, temperature or velocity will certainly require a stable numerical scheme to be employed. Without it, we believe that further physics expansion, as indicated by the current dynamic development of atomic physics near divertor plate, would not be succesfull or maybe unjustified in complementing ITER divertor design. The development stages of this research then can be characterized as follows.

1. The extension of the original NEWEDGE computational geometry (noncurvilinear) [7] to ITER geometry (curvilinear plate-plate) simulation which translates into a multiply connected domain computation. Originally, NEWEDGE was intended to simulate ASDEX (Axysymmetrical Divertor Experiment) in Garching, Germany, where, due to the geometric symmetrical configuration, the analysis is done from a symmetry point to divertor plate.
2. The restructuring of NEWEDGE to include multigrid method to allow a very fine computational grid simulation. Concurrently, a continuation method is added into the coarsest grid simulation to expand the capability of NEWEDGE to handle a wide range of key transport parameters. At this stage the earlier version of NEWEDGE plus continuation serves as the lowest cycle of the multigrid cycle.

These two methods are implemented in a modular fashion and are not expected to change except for a minor possible future modifications.

3. Through continuation process, intense gas puffing and impurity radiation are included to simulate the possibility of reducing heat flux incident into the divertor plates.

It is appropriate then that by keeping the earlier version of NEWEDGE as the important starting point and the inclusion of multigrid method, the revised code is called NEWEDGE-MG.

Chapter 2

Two-Dimensional Scrape-Off Layer Modeling

The Scrape-off layer (SOL) region has undoubtedly become one of the most important foci of analysis in the quest to sustain a desirable plasma condition for power production through nuclear fusion. Numerous experimental and simulation studies on SOL have been done and are continually being performed to seek a clear description of SOL dynamics. The complexity of particle transport is challenging to say the least, yet major improvements have been obtained consistently in the last decade. To describe the particle transport within the SOL and divertor regions, a two-fluid treatment of electrons and ions is employed (Braginskii equations [8]). This approach essentially treats the plasma as a continuous medium and it can also be viewed as a fluid description of a collisional plasma. This approach analyzes particle transport in the directions parallel and transverse to the magnetic field. The use of Braginskii equations is consistent with the current practice in analyzing the SOL. From a numerical perspective, the form of the plasma fluid equations is similar to that of the Navier-Stokes equations, which have been numerically intensively studied. This fluid approach is far from accurate, especially immediately adjacent to the divertor plate, yet it is relatively easy to model and simulate and it may lead to a better understanding of the SOL.

2.1 Physics of the SOL and Braginskii Equations

The SOL region is typically characterized by plasma densities of approximately 10^{17} to 10^{21} m^{-3} and temperatures of near 1 eV to 300-400 eV [3]. Typically, the mean free path is sufficiently shorter than the system length, a condition under which the fluid approach is reasonably valid. Consequently, for a fully ionized hydrogen plasma, the analysis of the SOL region by a fluid-like approach involves classical fluid governing equations (continuity, momentum and energy). Each equation can be derived by taking the zeroth (continuity), first (momentum) and second (energy) moment of the Boltzmann equation [8]. None of these mathematical steps will be performed, but we will merely present the equations and we will explore their physical meaning. The major assumptions made to attain the desired equations are ambipolar flow, steady state and symmetry in the toroidal direction. The momentum equation consists only of the parallel momentum, the divergence of which covers both the poloidal and radial components. The effects of viscous heating in the energy equations are also ignored. Other assumptions relating to thermal conductivity and viscosity will be further explored in the next section. As expected, due to the different nature of collisionality between plasma particles and fluid, especially near the divertor plates, the boundary equations need to be adjusted. Typically, in this region, the plasma deviates strongly from the Maxwellian norm, a key assumption for the fluid approach. This will be elaborated on in the boundary conditions section.

2.1.1 Continuity, Momentum and Energy Equations

In vector form the two-dimensional fluid edge plasma equations (plasma continuity (n), momentum (u), ion (T_i) and electron (T_e) energy) can be represented as (x poloidal and y radial) :

$$\frac{\partial}{\partial x}(\vec{C}_x - \vec{D}_x \frac{\partial \vec{\Psi}}{\partial x}) + \frac{\partial}{\partial y}(\vec{C}_y - \vec{D}_y \frac{\partial \vec{\Psi}}{\partial y}) = \vec{S} \quad (2.1)$$

where :

$$\vec{C}_x = \begin{bmatrix} nu \\ \frac{3}{2}nuT_i \\ \frac{3}{2}nuT_e \\ mnvu_{\parallel} \end{bmatrix}, \vec{C}_y = \begin{bmatrix} nv \\ \frac{3}{2}nvT_i \\ \frac{3}{2}nvT_e \\ mnvu_{\parallel} \end{bmatrix}, \vec{\Psi} = \begin{bmatrix} n \\ T_i \\ T_e \\ u_{\parallel} \end{bmatrix} \quad (2.2)$$

and,

$$\vec{D}_j = \begin{bmatrix} 0 \\ k_j^i \\ k_j^e \\ \eta_j \end{bmatrix}, \vec{S} = \begin{bmatrix} nn_o < \sigma v >_{ie} \\ -P_i(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) + k_{eq}(T_e - T_i) + \epsilon_i nn_o < \sigma v >_{ie} \\ -P_e(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}) - k_{eq}(T_e - T_i) - \epsilon_e nn_o < \sigma v >_{ie} \\ \cancel{\frac{B_x}{B}}(\frac{\partial P_i}{\partial x} + \frac{\partial P_e}{\partial x}) \end{bmatrix} \quad (2.3)$$

where : $j = (x, y)$

Note that, as in the fluid Navier-Stokes equations, the components of equation 2.1 are characterized by the existence of advection-diffusion and source terms, an assuring effect for numerical study. For closure, a deterministic neutral equation which is based on modified neutral diffusion model will be employed. However, due to the inherent interesting and important nature of neutral particles, this will be explained in detail separately.

The source term of the plasma continuity equation accounts for the neutral plasma interaction through electron impact ionization, resulting in density gain due to the neutral recycling. To include collisional radiative corrections, the electron impact ionization rate, $< \sigma v >_{ie}$, is defined as a function of electron temperature and plasma density [9].

With the assumption that the cross-field particle flow is transported diffusively, the radial velocity, v , is determined from the radial density gradient and the diffusion coefficient.

$$v = -\frac{D_{ni}}{n} \frac{\partial n}{\partial y} \quad (2.4)$$

where D_{ni} is anomalous (empirically defined). This implies that only the parallel

component of the momentum equation is needed. Physically, this is consistent with the fact that most of the particles will move in the direction of the magnetic field lines toward the divertor plates. The poloidal velocity, u , itself is a vector projection of the parallel velocity onto the poloidal plane. Note that both velocity equations ignore fluid drifts caused by the crossing of the poloidal and radial body forces with the toroidal magnetic field. The poloidal velocity, the poloidal and radial viscosity (modeled anomalously) and pressure equation of state in the momentum equation are given as :

$$\begin{aligned}
 u &= \frac{B_x}{B} u_{\parallel} \\
 \eta_x &= 0.96 n T_i \left(\frac{3 m_i^{1/2} T_i^{2.5}}{4 (2\pi)^{1/2} e^4 \ln \Lambda} \right) \\
 \eta_y &= \eta_{\perp} n m_i \\
 P_i &= n k T_i \\
 P_e &= n k T_e
 \end{aligned}$$

where k is the Boltzmann constant and $\eta_{\perp}$ is a constant. Here, m_i is the ion mass, e is the electronic charge, and $\ln \Lambda$ is the Coulomb logarithm, which is set to be 10.

In general, the transport coefficients in the energy equations are the classical ones for transport along a magnetic field [8]. The parallel thermal conductivity, k_x , is assumed to be flux-limited. The limiting case is needed to consider that the continuum formulation of the diffusive energy flux may predict an excessive and unrealistic flux. The diffusive flux is limited to 20 percent of the free streaming value, as commonly used by others [6], [7], [10]. Thus, k_x is expressed as :

$$k_x = \left(\frac{B_x}{B} \right)^2 k_{sh} \left(1 + \frac{q_{sh}}{q_{fl}} \right)^{-1} \quad (2.5)$$

where k_{sh} is the classical (Spitzer-Harm) electron heat conduction coefficient, q_{sh} is the classical conductive electron energy flux density and q_{fl} is the flux limit. The fluxes are defined as follows.

$$q_{sh} = -k_{sh} \frac{\partial T}{\partial x} \quad (2.6)$$

$$q_{fi} = 0.2nkT_e \sqrt{\frac{T_e}{2m_i}} \quad (2.7)$$

The radial conductivity is assumed to be anomalous and given as constants (χ_e and χ_i).

$$k_y^e = \chi_e n, k_y^i = \chi_i n \quad (2.8)$$

Another important term is the thermal relaxation which represents the energy transfer from electrons to ions and is expressed as :

$$k_{eq} \propto \frac{n^2}{T_e^{1.5}} \quad (2.9)$$

Detailed description of all classical transport coefficients in use can be found in the work of Braginskii [8]. Historically, the radial transports in edge plasma modeling have been treated as constants or constants times plasma density. These constants are usually determined empirically (anomalous), i.e., fitting experimental data. This is a common practice in fluid edge plasma modeling in which fluid level models are strongly influenced by microscopic physics (plasma turbulence) that is not fully understood. For ITER their exact numbers are still comprehensively studied and continually corrected. An important indication from these coefficients is their temperature dependency. The flux limit for example, is a function of $T_e^{2.5}$, a relatively steep dependency. This is rarely found in fluid dynamics computations.

2.1.2 Boundary Conditions

The two-dimensional domain requires boundary conditions in the **core**, **first wall**, **divertor plates** and **private flux** regions. As indicated earlier, near the **divertor plate** the fluid approach falls apart. Here the plasma can deviate strongly from its Maxwellian property. It is known that when plasma (ions and electrons) hits the wall,

it will recombine and is lost. Since electrons are much lighter than ions, they have much higher thermal velocities than ions. As a consequence, they are lost faster and the divertor plate will develop a negative electric charge which will repel electrons and attract ions. A floating potential (sheath) develops in which the ion and electron flows are equal. For stable (steady state) conditions the ion velocity at the sheath boundary then must be greater than or equal to the local ion speed (C_s), a condition known as the Bohm sheath criterion [11], where :

$$C_s = \sqrt{\frac{k(T_e + T_i)}{m_i}} \quad (2.10)$$

The sheath also acts as an energy filter for the electrons, i.e., only the very energetic electrons can escape from the plasma to the divertor plate. The electrons that do not have enough energy to penetrate the sheath have to give up their energy. This energy is gained by ions and as a consequence the impact energy of the ions on the plate is substantially increased over the average ion energy in the plasma [11]. This means that the power removal rate from ions is higher than when there is no sheath present. Although only high energy electrons can penetrate the sheath, the power removal rate from the population of electrons in the plasma exceeds that of the ions. This is due to the fact that for a given time interval, despite the fact that more ions than electrons can penetrate the sheath, only high energy electrons do penetrate the sheath. Thus the total energy carried by electrons per time is higher than that of the ions. The increase of the power removal rate of both ions and electrons from the plasma is denoted by δ , the heat transmission factor. Their relationship to the heat flux is given as :

$$q_i = \delta_i \frac{B_x}{B} n C_s T_i \quad (2.11)$$

$$q_e = \delta_e \frac{B_x}{B} n C_s T_e \quad (2.12)$$

where $\delta_i = 1.5$ and $\delta_e = 5.5$.

Table 2.1: Edge Plasma Boundary Conditions

<i>Location</i>	<i>Plasma</i>	<i>Momentum</i>	<i>Ion</i>	<i>Electron</i>
Divertor Plate	$nu_{\parallel} = nC_s$	$u_{\parallel} = C_s$	$q_i = \delta_i n T_i C_s$	$q_e = \delta_e n T_e C_s$
Core-SOL	fixed n	$u_{\parallel} = 0$	fixed T_i	fixed T_e
First Wall	$\frac{\partial n}{\partial y} = 0$	$\frac{\partial u_{\parallel}}{\partial y} = 0$	$\frac{\partial T_i}{\partial y} = 0$	$\frac{\partial T_e}{\partial y} = 0$
Private Flux	$\frac{\partial n}{\partial y} = 0$	$\frac{\partial u_{\parallel}}{\partial y} = 0$	$\frac{\partial T_i}{\partial y} = 0$	$\frac{\partial T_e}{\partial y} = 0$

The boundary at which the plasma enters the SOL region from the core is considered fixed (plasma density and electron/ion temperature). In actuality this can not be true, since the recycling of neutrals near the divertor will change the flow and amount of plasma particles to and from the core plasma. However, to account for the change, a coupling with a core plasma simulation is needed. Our current work does not intend to perform such a task, due to its extreme complexity. Since particles in this region tend to flow cross-field, thus leading to a situation where the parallel velocity is set to be zero. In the region below both the null point and the strike point at the divertor plate (**private flux**) the boundary must be treated carefully. Gas puffing is intended to be introduced here and a specified rate of neutral gas is used. The neutral gas rate is determined by the desired heat flux impinging on the divertor plates. In addition, the flux gradient of plasma, momentum and energy in this region is assumed to be adiabatic. The intention is to model the net loss of energy in the private flux region, with no net loss of particles [5]. The last part of the boundary conditions is the **first wall** or confinement wall. The flux in the confinement wall boundary is assumed to be small compared to the parallel flow and its gradient is assumed to be zero. In summary the boundaries are tabulated in table 2.1. Throughout this study, the foregoing boundaries, with the appropriate constants will be used to simulate the edge plasma region. Neutral boundary conditions will be described in the next section.

2.2 Neutral Particles Transport

As previously stated, the confinement of plasma particles and energy in a tokamak reactor is degraded in an area close to the wall. The plasma ions recombine at the wall and divertor plates and return to the plasma core as neutral particles. Depending on the energy of the ions, most of the particles are reflected back with a significant fraction of their incident energy. This is usually the case for low energy hydrogen plasma. At high energy most of the incoming ions are absorbed by the divertor wall material, diffuse back from inside the wall to the surface and are recycled back into the plasma as wall temperature molecules. If most of neutrals are recycled back into the plasma and ionize, the plasma close to the plate would be cooled significantly. This would reduce the impurity generation from the divertor [12, 7] accompanying with large poloidal temperature gradient near the plate. From numerical perspectives this can result in convergence problem. Hence, the role of neutral recycling (transport) is important in lowering plasma temperature and in radiating part of intense heat flux. Neutral transport includes both neutral atoms and molecules.

2.2.1 First Flight Corrected Diffusion Model

Unlike previous work, where neutrals that are generated at the divertor plate are modeled with a single energy diffusion equation, the transport of neutral atoms from the boundary to the first interaction with the plasma (the first flight or generation) is treated separately and exactly, while the diffusion approximation is applied to all higher generations [13]. The standard diffusion model is unable to describe neutrals originating at the divertor boundary through recycling. These neutrals are, in general, far from equilibrium with the plasma and would have to undergo a charge exchange interaction before a diffusive description becomes valid. Thus, a boundary layer exists, of dimension approximately one mfp, in which the diffusion approximation breaks down. Clearly if the plasma is sufficiently dense so that the mfp is short, the standard model may be acceptable, but such conditions are uniformly encountered in

the divertor.

This first flight corrected diffusion model or FFCD represents part of the boundary layer at little extra computational cost. Significantly this model allows a detailed angle and energy spectrum of recycling neutrals, as well as different species (e.g H_2), to be considered, although these features are not fully exploited here. The molecules will be treated as first flight also and a similar approach as will be taken for neutrals will be used for the molecules.

The kinetic equation for the neutral particle distribution function, $f(\vec{r}, \vec{v})$ is given by [14].

$$\vec{v} \cdot \nabla f + n \langle \sigma v \rangle_i f = n \langle \sigma v \rangle_{ex} f_m n_o \quad (2.13)$$

where $f_m(\vec{r}, \vec{v})$ is the Maxwellian ion distribution function in an inhomogeneous plasma, $n_o(\vec{r})$ is the neutral atom density, and the other terms have their usual meaning. The construction of the standard diffusion model proceeds by first assuming that $f(\vec{r}, \vec{v})$ can be represented as a weak perturbation from the Maxwellian at local ion temperature. A detailed asymptotic analysis [15] from which it can be shown that

$$f(\vec{r}, \vec{v}) \approx f_m(\vec{r}, \vec{v}) n_o(\vec{r}) - \frac{\vec{v} \cdot \nabla (f_m n_o)}{n(\vec{r}) \langle \sigma v \rangle_i} \quad (2.14)$$

for a weakly ionizing plasma with weak gradients and outside the boundary layer. A diffusion equation for the n_o is then obtained from equation 2.13 and 2.14.

$$-\nabla \cdot [D \nabla n_o] + \nabla \cdot (n_o \vec{V}_d) + n \langle \sigma v \rangle_{ie} n_o = 0 \quad (2.15)$$

where the diffusion coefficient is given by

$$D(\vec{r}) = \frac{V_{th}^2(\vec{r})}{2n(\vec{r}) \langle \sigma v \rangle_i} \quad (2.16)$$

and the thermal drift by

$$\vec{V}_D = -\frac{1}{2n(\vec{r}) <\sigma v>_t} \nabla V_{th}^2 \quad (2.17)$$

The drift is seen to depend on the ion temperature gradient and can thus be important near the plate. However, this drift as well as the plasma drift will be ignored for now.

A boundary condition can be constructed by requiring that the neutral flux entering the plasma be equal to the recycling plasma flux, Γ_i , i.e.,

$$\int_{\vec{n} \cdot \vec{v}} d\vec{v} \vec{n} \cdot \vec{v} f_o(\vec{r}_s, \vec{v}) = \Gamma_i \quad (2.18)$$

where $\vec{n}$ is an outward directed unit normal at boundary point $\vec{r}_s$. Inserting equation 2.14 into equation 2.18 and simplifying then yields an appropriate boundary condition for equation 2.15.

In the FFCD model, the first flight distribution, $f^{(o)}(\vec{r}, \vec{v})$, is subtracted from equation 2.13 and treated separately. The relevant equation is given by

$$\vec{v} \cdot \nabla f^{(o)} + n <\sigma v>_t f^{(o)} = 0 \quad (2.19)$$

with

$$f^{(o)}(\vec{r}_s, \vec{v}) = \Gamma(\vec{r}_s, \vec{v}), \quad \vec{n} \cdot \vec{v} < 0 \quad (2.20)$$

where Γ describes the energy and angle spectrum of recycled neutrals. The higher generations satisfy the so-called collided distribution equation, given by

$$\vec{v} \cdot \nabla f^{(c)} + n <\sigma v>_t f^{(c)} = n <\sigma v>_{cx} f_m n_o^{(c)} + n <\sigma v>_{cx} f_m n_o^{(o)} \quad (2.21)$$

with :

$$f^{(c)}(\vec{r}_s, \vec{v}) = 0, \quad \vec{n} \cdot \vec{v} < 0 \quad (2.22)$$

In this scheme, equation 2.19 for the first flight is solved exactly, while the diffusion approximation is developed for the collided density given by equation 2.21. Proceeding as before, we obtain finally, for the collided density equation

$$-\nabla \cdot [D\nabla n_o^{(c)}] + \nabla \cdot (n_o^{(c)} \vec{V}_d) + n \langle \sigma v \rangle_{ie} n_o = n \langle \sigma v \rangle_{ex} n_o^{(o)} \quad (2.23)$$

By requiring that all collided neutrals and plasma ions recycle as first flight neutrals, a pair of coupled equations is constructed of which equation 2.19 is a kinetic equation while equation 2.23 is a moment of fluid equation. It is convenient to reduce equation 2.19 also to a moment equation as only the first flight density is required in equation 2.23. For simplicity equation 2.19 is reduced to a locally 1D equation for the first flight density, namely

$$-\frac{\partial n^{(o)} V_o}{\partial x} + n \langle \sigma v \rangle_t n_o^{(o)} = 0 \quad (2.24)$$

where V_o is a function of local ion and electron temperature [12]. The boundary condition at $x=L$ (the divertor plate) for arbitrary y becomes

$$V_o n_o^{(o)} = \alpha_i n C_s + \frac{\alpha_o}{\sqrt{\pi}} n_o^{(c)} V_{th} \quad (2.25)$$

where α_i and α_o are the local plasma and neutral recycling coefficients (α_o is assumed to be 1). The corresponding collided density diffusion equation becomes :

$$-\frac{\partial}{\partial x} D \frac{\partial n_o^{(c)}}{\partial x} - \frac{\partial}{\partial y} D \frac{\partial n_o^{(c)}}{\partial y} + n \langle \sigma v \rangle_{ie} n_o^{(c)} = n \langle \sigma v \rangle_{ex} n_o^{(o)} \quad (2.26)$$

with boundary condition :

$$\left[\frac{n_o^{(c)} V_{th}}{\sqrt{\pi}} + D \frac{\partial n_o^{(c)}}{\partial x} \right]_{x=L} = 0 \quad (2.27)$$

where we have ignored the thermal drift. Equations 2.24-2.27 define the FFCD model of neutral transport. The standard diffusion model is obtained by setting the RHS to zero in equation 2.26 and using the boundary condition at $x = L$:

$$\frac{(1 - \alpha_o)}{2\sqrt{\pi}} n_o V_{th} + \frac{(1 + \alpha_o)}{2} D \frac{\partial n_o}{\partial x} \Big|_{x=0} = \alpha_i n C_s \quad (2.28)$$

Thus, we are readily able to compare the result of using the two different neutral transport models.

An important advantage of the FFCD model is that molecules can be treated exactly, unlike the standard diffusion model where each molecule is assumed dissociated before leaving the solid boundary. In the refined model, the molecules are simply regarded as uncollided particles and followed until their first interaction with the plasma. Subsequently, the molecules are assumed to be ionized and/or dissociated via the normal channels, yielding an ion and a neutral atom, two ions or two neutral atoms, depending on the local electron temperature. Although it is trivial matter to implement all these reaction pathways, we have assumed for now that at a collision site each molecule immediately dissociates into an ion and a neutral atom, i.e., the Franck-Condon pair (we emphasize, this does not represent a loss of generality). While the ion represents a source in the plasma continuity equation, the neutral atom must strictly be followed exactly (i.e. a second flight) until it experiences a charge exchange reaction following which it can be subsumed into the collided distribution. Although this can be accomplished within the framework of our model, the additional complexity of the algorithm is not justified for this second order effect. Thus, noting that these low energy (3-5 eV) atoms may not travel far before colliding again, we have, as a practical matter, simply incorporated the Franck-Condon atoms into the collided, diffusive species. The first flight equation for the neutral molecule density is given by :

$$-V_2 \frac{\partial n_2}{\partial x} + n_e \langle \sigma v \rangle_2 n_2 = 0 \quad (2.29)$$

where V_2 , the molecule speed, is evaluated at a wall temperature (taken to be 0.1 eV) and $\langle \sigma v \rangle_2$ is the total reaction rate at the local electron temperature. The equation for the collided density becomes :

$$-\nabla \cdot (D \nabla n_o^{(c)}) + \nabla \cdot (n_o^{(c)} \vec{V}_d) + n_e = S_{n_o^{(c)}} \quad (2.30)$$

where : $S_{n_o^{(c)}} = n_i < \sigma v >_{cr} n_o^{(o)} + n_e < \sigma v >_2 n_2 - n < \sigma v >_{ie} n_o^{(c)}$.

The fraction of ions and atoms reflected from the solid boundary (e.g. divertor plate) as fast atoms and slow molecules is given by the reflection coefficient appropriate to the material type and energy of the incident particle, compiled by Ito et.al [16]. The average energy of the reflected fast atoms is computed using the particle and energy reflection coefficients. Note that a complete energy spectrum of reflected atoms, if known, can be readily incorporated in this model by discretizing the energy variable and performing an exact first flight calculation for particles in each energy bin.

Neutral boundary conditions from the vessel wall are treated in two ways. Next to the divertor plate, where neutral pumping is to occur, an albedo boundary condition is utilized which is consistent with other works [7], [17]. On the other hand, at the vessel wall and private flux, the boundary is treated as an adiabatic condition. Both boundaries are expressed as :

- Neutral pumping

$$-D_{no} \frac{\partial n_o}{\partial y} = \frac{(1 - \alpha) n_o V_{th}}{(1 + \alpha) 4\pi^{3/2}} \quad (2.31)$$

- Vessel wall

$$\frac{\partial n_o}{\partial y} = 0 \quad (2.32)$$

where α is an albedo coefficient ($0 \leq 1$).

The locally 1D model does not describe the transport of first flight neutral particles exactly, because, as indicated earlier, neutrals can move in all possible directions (angles) and with a wide energy spectrum. However, it is a major improvement over the single energy model that is currently used. FFCD also serves as an alternative deterministic neutral scheme to the more computationally expensive Monte Carlo scheme. Finally, the numerical implementation of the FFCD model within the framework of the schemes to be described later is straightforward.

2.3 Gaseous and Radiative Divertor

Control of divertor thermal loading has been a major issue in divertor physics studies in which the heat flux striking on the plate can be as high as 200 MW/m^2 . Most of the incoming heat is focused in a narrow region around the divertor strike point. The obvious consequence is damage to the divertor plate accompanied by an increase of the erosion rate of the divertor material. The concept of a radiative or gaseous divertor has been proposed to alleviate this severe condition by injecting neutral deuterium and/or impurities near the divertor plates. The essence of this proposed method is to increase radiative power loss in the divertor area. Each of these options are explored in the next sections.

2.3.1 Gas Puffing

The key feature of the gaseous divertor is to dump the energy into a quantity of deuterium gas, i.e., spreading the heat flux over a larger divertor surface area. Experiments have indicated that at low temperatures the main heat loss process was found to be elastic ion-neutral collisions [18] at which neutral atoms injected near the plate will undergo charge exchange (CX) or be ionized with plasma ions. During the CX process the new neutral atoms may have a higher energy and a longer mean-free-path for either ionization or CX. Thus allowing the neutral atoms to penetrate deeply into the plasma before being either ionized or CX'd. This deep penetration causes the plasma to cool down. The neutral effect extends into the region in which the neutral density has dropped to a level where the effect of ionization is too small to cause the heat imbalance or ion production. As a result, a shock-like plasma temperature profile occurs. In this work, the effect of charge exchange is not fully exploited, thus the cooling down effect of plasma particles is due mainly through ionization.

Although there is no definite plan on where neutrals are to be puffed into the ITER reactor, several experimental and simulation works on DIII-D (at General Atomic San Diego) [19], [20], [21] have indicated that among others the private flux region is one

of the leading candidates for gas puffing. The injection from private flux is treated by expressing the private flux neutral boundary conditions as :

$$\Gamma_{n_o} = Constant \quad (2.33)$$

where Γ_{n_o} is a specified constant rate (*particles/s*). This replaces the adiabatic boundary condition at the private flux region when no gas puffing is done (table 2.1).

In the present work, the neutrals are injected uniformly throughout the region of interest in the simulation, at a variable puff rate and the impact on the numerical and physical performance will be addressed.

2.3.2 Impurity Puffing

As stated earlier, the occurrence of impurities produced from the erosion of the divertor plates due to ion bombardment can be a dilemma. Excessive impurity production may lead to excessive radiative cooling of the core plasma and extinguish the fusion reaction. However, at a certain level, impurities can be a blessing in disguise. The radiative cooling produced by the presence of impurities, depending on the location and the rate of power loss, can be beneficial. The cold impurities released from the divertor wall may absorb and radiate a significant portion of the incoming plasma energy, thus lowering the peak divertor heat load. This temperature may well be on a level below the threshold for physical sputtering of the divertor plate material [9]. In principle, this condition can be thought of as one in which plasma contamination is self-limited by the conversion of the incoming heat flux into impurity radiation. This analysis can be traced back to the proposal of a 'cold plasma mantle' presented by Gibson and Watkins [22]. In this work, we do not intent a full scale analysis of all possible impurities generated from the first wall and the divertor plates. The aim is to show plasma and numerical performance in the presence of impurities deliberately injected into the SOL region. The impurities are introduced into the SOL by assuming impurity density as a fraction of plasma density. Prior to the description of the effect

of impurities on the plasma equation (electron energy equation) we will present a brief review on how impurities actually affect the plasma. This presentation is limited to the most dominant atomic and molecular processes that must be considered in impurity analysis.

When impurity ions enter the plasma, they will cause energy losses through radiation. For fusion plasmas, the most elementary processes are electron collisional excitation followed by radiative decay, electron ionization and radiative recombination [2]. Thus for a given input of impurities, the radiative energy loss per unit volume is expressed as :

$$P_{rad} = nn_z L_z \quad (2.34)$$

where n is the plasma density, n_z is the impurity density and L_z is the impurity cooling rate. The expression of L_z is presented later in this section.

To model the impurity dynamics completely, typically, a set of impurity continuity, momentum and energy equations for each impurity specie are needed (fluid approach). The fluid approach is valid when the impurity density is 'low' enough, i.e. [23]

$$\sum_z (Z^2 n_z) \leq n_e \simeq n_i \quad (2.35)$$

However, due to the wealth of molecular and atomic processes and the number of ionization stages, usually, some simplifications are made. In this work, we do not intend to develop a complete multi-species impurity model as this would represent a substantial effort in its own right. Rather, a simple model will be used as a starting point to understand the impurity effect on plasmas, and more importantly, to analyze the numerical ramifications of intensely radiating plasma not achieved so far in any code.

A first simplification is the stationary condition, consistent with the steady state mode for the plasma equations. The second simplification is the assumption that the

impurity temperature is tightly coupled to that of the ions [3]. This allows the energy equation to be neglected ($T_z = T_i$).

At any time during the course of fusion reaction, the concentration of impurities depends upon their ionization stages. Thus, the distribution of impurities is expressed as :

$$\frac{\partial n_z u_z}{\partial x} + \frac{\partial}{\partial y}(-D_z) \frac{\partial n_z}{\partial y} = S_{n_z} \quad (2.36)$$

where S_{n_z} is defined as :

$$S_{n_z} = n n_{z-1} I_{z-1 \rightarrow z} + n n_{z+1} R_{z+1 \rightarrow z} - n n_z (R_{z \rightarrow z-1} + I_{z \rightarrow z+1})$$

The coefficients I and R represent the ionization and recombination rates. Assuming that : (a). spatial and transport effects are neglected, (b). the total impurity density n_z is given as : $n_z = \sum_q n_q$, and (c). ions are fully-stripped, one gets the so-called 'Coronal-Equilibrium'.

$$n_{z-1} I_{z-1 \rightarrow z} = n_z R_{z \rightarrow z-1} \quad (2.37)$$

Under this assumption, the radiative cooling rate L_z of equation 2.34 is a function only of electron temperature.

As a starting point, instead of implementing a full scale impurity continuity model, the impurity density is assumed to be a fraction of plasma density, i.e., $n_z = f_{imp} n$. In this work, the value of f_{imp} is typically set between 0 – 8%. At high f_{imp} it is expected that most of the incoming plasma energy is radiated. The distribution of impurity density is by no means physically correct, yet it serves as a preliminary step toward full impurity model as well as a resiliency test of the numerical schemes. The impurity cooling rate is approximated as follows [24].

$$L_z = \frac{A_e \sqrt{T_e} e^{(-E/T_e)}}{1 + B_e \sqrt{T_e} + C_e T_e} \quad (2.38)$$

For ITER, where the divertor is planned to be made from a carbon-like material, the analysis in this work is concentrated on carbon. As a low Z impurity, carbon is also loosely bound on the surface and it is easily released by minimal radiation, or low energy particle fluxes. For carbon (C^{2+}), the activation energy E and coefficients A_e , B_e and C_e are given as : $E = 7.59 \text{ eV}$, $A_e = 7.27 \times 10^{-7} \text{ eV}^{1/2} \text{ cm}^3 \text{ s}^{-1}$, $B_e = 0.265 \text{ eV}^{-1}$ and $C_e = 23 \times 10^{-3} \text{ eV}^{-1}$. The functional relationship between the cooling rate and electron temperature is graphically shown in figure 2.1.

Figure 2.1: Temperature dependence of the cooling rates of ions

With the inclusion of radiative cooling, the electron energy equation now takes the form of :

$$\frac{\partial}{\partial x} \left(\frac{3}{2} n u T_e - k_x^e \frac{\partial T_e}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{3}{2} n v T_e - k_y^e \frac{\partial T_e}{\partial y} \right) = S_e \quad (2.39)$$

where S_e is the source term and expressed as :

$$S_e = -P_e \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - k_{eq}(T_e - T_i) - \epsilon_e n n_o < \sigma v >_{ie} - L_z(T_e) n n_z \quad (2.40)$$

The above approaches (coronal) are adequate when the plasma is relatively stable in time and the impurity particle transport (momentum) across the plasma is slow compared with ionization and recombination times [9]. It is understood that near the divertor plates this condition is not true. At this latter region the neutral hydrogen atoms produced by recycling plasma or other processes can charge exchange with impurity ions resulting in a substantial net recombination rate. Moreover, the balance of ionization and radiative recombination that is required by coronal equilibrium is not valid anymore. However, the above approximation will provide a useful first indication of the flexibility of radiating significant amounts of power within the divertor chamber, and establish the robustness of the numerical scheme.

Chapter 3

Review of Existing Numerical Approaches to Solving the Edge Plasma Equations

3.1 Existing Numerical Approaches

The development of a robust coupled plasma-neutral transport code is an evolving process. The robustness depends on the level of understanding of the physics of plasma-wall interactions, which is by no means complete yet. Currently, there are several edge plasma Braginskii fluid based codes in use in the U.S (B2, PLANET, UEDGE, EPIC and NEWEDGE) which all have demonstrated various degrees of success. B2 can be considered the pioneer of comprehensive 2-D edge plasma simulations and was originally developed by B.J. Braams [6]. Beside B2, PLANET by Petravic [25], EPIC by Vold [10], UEDGE by Roenglien et.al [26] and NEWEDGE by Knoll [5] were developed as alternative edge plasma codes. Except for PLANET, all these codes use a finite volume method as developed by Patankar [27]. The numerical scheme used in the original PLANET is not clearly known, but appears to be alternating direction implicit (ADI) method [28, 25]. The finite difference method

is relatively easier to implement, but as nonlinearity increases, the method must be patched up to the degree that physical conservation may be lost. B2 and EPIC use a Power law discretization scheme [27] and a relaxation scheme based on the SIMPLE (Semi Implicit Pressure Linked Equations) algorithm [27] while UEDGE and NEWEDGE employ a Newton-Raphson iterative scheme.

In its inception, B2 simulated the Braginskii equations plus elementary neutral equation which was simply assumed to be attenuated along the field lines. However, as the physics models were made more sophisticated, or applications to high power tokamaks was involved, the code performance deteriorated markedly. This is due to the fact that SIMPLE assumed that the change in the pressure of a computational cell is due only to a change in the density. In edge plasma, due to its high nonlinearity, the change of any unknown can be due to a change of more than one of the other unknowns. The change of plasma pressure for example is due to a change in plasma particles and temperatures. Likewise, in the case when puffing is applied, it is expected that the ion/electron temperature drops significantly such that a shock-like profile may appear. Since $P = nT$, we have $\Delta P = \Delta n(T) + n(\Delta T)$, indicating that the temperature change is equally important as the density change. Another example is in the transport coefficients. Thermal relaxation and conductivity are both strongly dependent on plasma density and temperature. The SIMPLE method has also been found to perform poorly in some compressible fluid dynamics problems, typically for complex reactive flow. Numerous modifications of SIMPLE are available currently and most are problem dependent. This leads to the conclusion that future physics expansions such as puffing or others in this code may impose major hurdles for B2 to perform satisfactorily. Knoll [5] evaluated the strength and weaknesses of B2 in great details and came up with identical conclusions.

The current effort to improve B2 performance is to include the Monte Carlo method for neutral treatment. This coupling may not be time efficient, since a Monte Carlo run can be very time consuming. The neutral model of B2 was significantly modified on EPIC, by solving neutrals diffusively (single energy group). There are

two advantages in using this type of approach [10]. First is the simplicity of the equations, allowing more analysis on the physics. Second is that the neutral equation can be solved in a consistent manner with the fluid equations. However, the same SIMPLE approach that EPIC uses poses an unattractive future development.

NEWEDGE and later on UEDGE approached the edge plasma problem with a motivation to solve all of the unknowns simultaneously by Newton's method, avoiding the problems encountered by B2 and EPIC. As of the present time, NEWEDGE and UEDGE have performed relatively well compared to others but they are not without problems. A typical and classical requirement of Newton's method is the initial guess which has to be relatively close to the solution (small radius of convergence). Due to the wide range of ITER parameters, such as core boundaries, transport coefficients or others, a good initial guess sometimes can be extremely difficult to make. Another difficulty arises from the size of the Jacobian matrix that must be constructed. As more computational cells are needed and more physical models are introduced, the Jacobian matrix size can be unmanageably large, a well known aspect of the weakness of Newton's method. However, the quadratic convergence that Newton's method possesses is an attractive feature and for relatively coarse computational cells this method is extremely efficient. To alleviate the aforementioned difficulties an alternative method which may be an extension of Newton's method then must be developed. In this work we develop an extension of the Newton method as well as an implementation of the multigrid method. Prior to describing these improvements, a short description of Newton's method as used in the codes NEWEDGE or UEDGE and its weaknesses will be reviewed.

3.2 NEWEDGE-Newton Edge Plasma Solver

Newton's method is an effective iterative technique to solve a nonlinear system of equation(s). It can also be used to solve a single equation. Consider a system of n non-linear equations :

$$f(\vec{\Psi}) = 0 \quad (3.1)$$

where $\vec{\Psi} = \Psi(n, T_i, T_e, n_o, u_{\parallel})$.

Newton's method comes about from linearizing $f(\vec{\Psi})$, i.e., replacing $f(\vec{\Psi})$ by a linear approximation $f(\vec{\Psi}^*)$ consisting of the first two terms in its Taylor expansion about $\vec{\Psi}^k$, and solving $\Psi^{k+1} = 0$. Thus,

$$f(\vec{\Psi}^*) = f(\vec{\Psi}^k) + J(\vec{\Psi}^k)(\vec{\Psi}^* - \vec{\Psi}^k) \quad (3.2)$$

where

$$J(\vec{\Psi}^k) = \frac{\partial f_i}{\partial \Psi_j} = \begin{bmatrix} \frac{\partial f_1}{\partial \Psi_1} & \cdot & \cdot & \cdot & \frac{\partial f_1}{\partial \Psi_n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \frac{\partial f_n}{\partial \Psi_1} & \cdot & \cdot & \cdot & \frac{\partial f_n}{\partial \Psi_n} \end{bmatrix} \quad (3.3)$$

is known as the Jacobian matrix of $f(\vec{\Psi})$. Thus, given an initial approximation $\vec{\Psi}^o$, the Taylor expansion form can be written as :

$$J(\vec{\Psi}^k)(\vec{\Psi}^{k+1} - \vec{\Psi}^k) = -f(\vec{\Psi}^k) \quad (3.4)$$

or,

$$J(\vec{\Psi}^k)\delta\vec{\Psi}^k = -f(\vec{\Psi}^k) \quad (3.5)$$

and the new solution is approximated by :

$$\vec{\Psi}^{k+1} = \vec{\Psi}^k + \alpha_N \delta\vec{\Psi}^k \quad (3.6)$$

Equation 3.4 is solved iteratively until $\vec{\Psi}^{k+1} - \vec{\Psi}^k$ falls below some prescribed tolerance level (usually within the range of machine accuracy). The scalar α_N is used to damp the update and its value is set to prevent the calculation of negative thermodynamic variables, and to scale large variable updates when the solution is far from

the converged solution. The convergence of the iteration scheme in equations 3.5 and 3.6 is very sensitive to the initial guess. Since a good initial guess is not always available some means of improving the convergence rate becomes necessary. In the NEWEDGE code, convergence is accelerated by first performing the calculation on a coarse grid and then interpolating the solution to a fine grid for which it can serve as a good initial guess. This is known as mesh sequencing. The difference is a banded Gauss elimination that is used to solve the linearized problem instead of an iterative method. The interpolation to the finer grid is performed through a bilinear interpolating routine and the fine grid is generated by doubling the coarse grid in both spatial directions. Other features are added that further enhance robustness and efficiency. For instance, the linearization process generates a Jacobian matrix that must be factored when solving the unknown variables at each iteration. On the fine grid the matrix dimension can become very large so that each factorization is computationally expensive. To minimize this cost, factorization frequency is reduced whenever possible according to a prescribed criterion. Under certain conditions factorization can be completely frozen.

It has been shown that Newton's method possesses a quadratic convergence [29], provided that $\vec{\Psi}^o$ is sufficiently close to $\vec{\Psi}^*$. The convergence can be stated by the following basic theorem without proof [30].

Theorem 1 *If f is twice continuously differentiable in a neighborhood of a solution $\vec{\Psi}^*$ of $f(\vec{\Psi}) = 0$ and $f'(\vec{\Psi}^*)$ is nonsingular, the Newton iterates of (3.4) will converge to $\vec{\Psi}^*$ provided that $\vec{\Psi}^o$ is sufficiently close to $\vec{\Psi}^*$, and they will have the property of quadratic convergence ;*

$$\|\vec{\Psi}^{k+1} - \vec{\Psi}^*\|_2 \leq c \|\vec{\Psi}^k - \vec{\Psi}^*\|_2^2 \quad (3.7)$$

for some constant c .

However, as indicated earlier, the initial guess may not be sufficiently good to ensure convergence, even when a solution exists and the Jacobian is well-conditioned.

For example, in applications to edge plasma simulation, success was limited to a class of problems characterized by relatively 'benign' conditions : L-mode type transport coefficients, small problem domain, low incident heat and particle fluxes etc (ASDEX). In particular, convergence for ITER divertor configurations was not achieved within the constraints of the original code, even on a crude grid. At the earlier stages of this research a set of parameters, typically used for non-ASDEX configurations was used to no avail. The convergence rate for each unknown becomes essentially stalled and no converged solution was obtained (see figure 3.1).

Figure 3.1: Convergence Behavior for Condition : $T_{core} = 300$ eV, $n_{core} = 3.0 \times 10^{19}$, $D_{\perp} = 1.333$ m^2/s , $\chi_i = 1.333$ m^2/s and $\chi_e = 4.0$ m^2/s on 32×6 grid size.

Various other sets of parameters were used and the results were the same (nonconvergence).

Another important factor to consider are the characteristics of the Jacobian matrix. For our problem, the Jacobian matrix is usually sparse and for a simple geometry, such as ASDEX in Garching, Germany, where the analysis was performed from the symmetry point to a divertor plate, the bandwidth of the Jacobian matrix is relatively small. This allows for the use of any available bandwidth solver routine. However, for ITER, due to the asymmetrical geometry, the analysis has to be done from plate

to plate. As a consequence, the bandwidth increases, which comes from the across domain (multiply connected) communication (describe in the next section). Thus, a direct banded solver as was used in the original NEWEDGE will be very inefficient and must be abandoned. With the inclusion of multiply connected domains and an increasing grid density, an alternative option must be looked for. Our approach is to keep the banded solver on a coarse grid and to employ the multigrid cycle on the finer grids. The choice of multigrid, among others, was motivated by the fact that the effect of grid density virtually has no memory cost. This method has been known to be very efficient ($\mathcal{O}(\mathcal{N})$ space and time) for various linear and nonlinear fluid dynamics problems. The sole drawback is the amount of time needed for programming, which is quite difficult and complex.

3.3 Multiply Connected Domain

The discretized equations are most efficiently solved in a rectangular domain. Unfortunately, the edge plasma physical domains, as in the majority of physical domain encountered in scientific problems are nonrectangular (usually curvilinear) in shape. Thus, it is necessary to transform the curvilinear physical domain to a rectangular computational domain.

Prior to the transformation, for a plate to plate simulation, a branch cut must be taken from the null point across the private flux region (figure 3.2) such that a 2-D like physical domain suitable for simulation becomes available. The cut is intended to maintain the connectivity of the transformed domain in the same way as for that of the physical domain. As a consequence, a 2-D multiply connected domain approach in the coding structure is required. Note that, in the transformed domain (figure 3.3), the region EFIH (core) communicates to region BEHKLA only. Thus, the 'coincident' lines EF-ED and HI-HG act as a communication barrier between the private flux and the core. Points on lines ED and HG (on the private flux side) are identical, i.e., during computation they must be updated simultaneously (periodic or re-entrant boundary

Figure 3.2: Computational Cut on the Physical Domain

conditions). This allows for transport across the cut (T_i at the inner divertor side is equal to T_i at the outer divertor side, etc). The numerical implication as stated earlier, is the increase of the matrix bandwidth in the Jacobian matrix of Newton's method. For simple (half domain) geometry (ASDEX), the neighboring control volumes that need to be included for the discretization of a particular control volume are mainly next neighbor control volumes in all spatial directions. This is not true for multiply connected domain because the cut which has been imposed between the inboard and outboard would force across domain communication (figure 3.4). This is one of the primary facts that an alternative method to solve the discretized equations must take into account.

The computational domain for our work is generated by a magnetic flux code from the Lawrence Livermore National Laboratory (LLNL). The curvilinear grid is orthogonal and the data generated include the location and size of each transformed computational cell including its metric coefficient. The metric coefficient measures the relative contribution of changes in the physical domain to the computational domain. In a 2-D system for example, this can be related to the grid cell area or face. As of the current date, a grid generated by M. Rensink is used [31].

3.4 Summary

As stated previously, the weakness of Newton's method is its dependency on the initial guess. For Newton's method to converge the initial guess must be well within the radius convergence. However, finding an initial guess for a wide range of ITER transport parameters is a very difficult task, even on a coarse grid. Our experiences indicated that Newton's method converged only for small set of transport parameters, typically for a 'benign' conditions, and extension to a wider set of parameters has been unsuccessful. Another problem of the Newton method is the size of the Jacobian matrix that needs to be constructed as the grid size increases. For a very fine grid, which may be needed for ITER simulation, the memory storage for the Jacobian

Figure 3.3: Edge Plasma Computational Domain

Figure 3.4: Bandwidth difference of the Jacobian matrix between multiply connected domain and simple domain

matrix is unmanageable. The latter problem is solved by using a multigrid method. However, in order for the multigrid method to succeed, for our case, a converged coarse grid solution must be obtained. An alternative to overcome the difficulty in finding initial guess for Newton's method is described as follows.

A choice of system parameters (most likely not the desired set) is used on an appropriate crude grid to generate a converged solution. This solution to the 'pseudo-problem' is then used to generate successive solutions for parameter sets (e.g. transport coefficients) that gradually approach the desired parameters, i.e., until solution to the real problem is obtained. This procedure, which works extremely well, is known as a *continuation method*, belonging to the family of *homotopy methods*.

The continuation and multigrid approaches are described in great detail in chapter 4.

Chapter 4

Numerical Method

Edge plasma physics analysis has been somewhat revolutionized in the last decade by the advent and rapid evolution of powerful computers. These machines, along with state-of-the-art numerical packages, now have the capability of simulating various edge plasma problems. The similarity of the fluid plasma approach to the fluid flow analysis, despite its limitations, helps the SOL investigation by employing methods common to fluid flow analysis. This, in general, is done by discretizing the edge plasma domain, applying algebraic approximations of the fluid Braginskii equations to each computational volume and enforcing physically realistic boundary conditions. Generally, this process results in the need for an efficient algorithm to solve a relatively large number of coupled nonlinear equations. Presently, there are abundant numerical methods available to simulate edge plasma problems. However, most, if not all, existing methods were originally developed for simple, usually one dimensional problems. As the physical models becomes more sophisticated, many modifications must also be included, as can be seen in many fluid dynamics simulation problems. Edge plasma problems, as described in chapter 2 are complex problems. Thus, the selection of numerical methods to be used must be done judiciously. As a precaution, the selected method(s) in this work will not guarantee their general applicability to any future edge plasma problems, but it will definitely narrow down future scheme selection and optimistically it will only require minimum modifications.

4.1 Two Dimensional Discretization Scheme

The spatial variations of the simplified Braginskii equations are represented by the advection and diffusion terms. Within its computational domain, the governing equations are discretized by employing a cell-centered finite volume approach. Here, the domain of the solution is divided into small volumes (areas for 2-D edge plasma). Subsequently, the conservation law in its integral form (finite volume) are applied in these control volumes, and divergence terms are transformed into surface integrals by using a divergence theorem. The choice of finite volume over common finite difference is based on the independence of the finite volume method from the nonuniformity of the physical domain. For a finite volume, the computational domain complexities, i.e., coordinate transformation, are handled separately through the grid generation [27].

By taking into account the shape of the control volume (CV), for a given CV, the governing equations to be discretized can be written as

$$\int_V \left(\frac{\partial}{\partial x} (\vec{C}_x - \vec{D}_x \frac{\partial \vec{\Psi}}{\partial x}) + \frac{\partial}{\partial y} (\vec{C}_y - \vec{D}_y \frac{\partial \vec{\Psi}}{\partial y}) - \vec{S} \right) dV = 0 \quad (4.1)$$

with three distinctive parts : advection, diffusion and source. The evaluation of each term will be described next. The cell-centering requires that the unknown variables n , n_o , T_i and T_e are located in the center, while u is defined at the control volume interfaces (figure 4.1).

4.1.1 Advection Fluxes

The advection terms on each equation represent the field variable fluxes through the CV faces. After integration, for example, the poloidal spatial discretized form of the plasma continuity equation is written as :

$$(nu)_i dy(i, j) - (nu)_{(i-1)} dy(i-1, j) = nn_o < \sigma v >_{ie} \quad (4.2)$$

where the subscript i denotes the CV face. Note that the metric coefficient from the coordinate transformation is embedded in dy . In our work, the advection flux, nu , is expressed through an upwind method, also called the first order donor-cell method, given by

$$n^*u(i, j) = \begin{cases} n(i, j)u(i, j) & u(i, j) > 0 \\ n(i + 1, j)u(i, j) & u(i, j) < 0 \end{cases} \quad (4.3)$$

The first order upwind method is selected based on the fact that it is numerically stable and simple. There are several other versions of upwind methods, but they are commonly problem dependent and complicated. The upwind method also assures positivity in the diagonal term of the Jacobian matrix for Newton's method. Although this is not a critical requirement for diagonal dominance of the Jacobian matrix, it reduces the possibility of error from the convection discretization scheme.

4.1.2 Diffusion Fluxes

The diffusion term is centrally (second order) differenced and this scheme is known to produce numerical oscillations [30]. However, combined with first order upwind differencing of the advection term, the overall scheme is known to be stable. Thus, for example, the poloidal spatial discretized form of the ion energy equation is expressed as follows (Patankar's notation is followed [27]).

$$\begin{aligned} Q_i = & \left\{ \frac{3}{2}(nT_i)_i^* u_{\parallel}(i, j) pit(i, j) - 0.5k_x \frac{T_i(i + 1, j) - T_i(i, j)}{dx(i, j) + dx(i + 1, j)} \right\} dy(i, j) \\ & + \left\{ \frac{3}{2}(nT_i)_{i-1}^* u_{\parallel}(i - 1, j) pit(i - 1, j) \right. \\ & \left. - 0.5k_x \frac{T_i(i, j) - T_i(i - 1, j)}{dx(i, j) + dx(i - 1, j)} \right\} dy(i - 1, j) \end{aligned} \quad (4.4)$$

where $pit(i, j)$ is the magnetic field pitch (known for each control volume) and the upwind ion energy expression is :

$$(nT_i)^*u(i,j) = \begin{cases} n(i,j)T_i(i,j)u(i,j) & u(i,j) > 0 \\ n(i+1,j)T_i(i+1,j)u(i,j) & u(i,j) < 0 \end{cases} \quad (4.5)$$

Again following Patankar's notation the first term of the equation 4.4 can be written as :

$$T_i(i,j)n(i,j) \parallel F_e, 0 \parallel -T_i(i+1,j)n(i+1,j) \parallel -F_e, 0 \parallel -D_e(T_i(i+1,j) - T_i(i,j)) \quad (4.6)$$

where : $F_e = \frac{3}{2}u_{\parallel}(i,j)pit(i,j)dy(i,j)$ and $D_e = \frac{2k_x dy(i,j)}{dx(i,j)+dx(i+1,j)}$ and the notation $\parallel A, B \parallel$ indicates the maximum between A, B . The extension to the Power-law scheme as indicated in a previous study [7], does not appear to offer a significant improvement in accuracy. Thus, based on CPU time savings the above scheme is used throughout the simulation process.

4.1.3 Source

The source term is integrated by assuming that the specific source at the CV center point represents the mean value over the whole control volume. However, all of the source terms are also a function of the corresponding unknown. For instance, the plasma continuity source, due to neutral ionization, is expressed as $nn_o < \sigma v >_{ie}$. Thus, for implicitness, the plasma density is treated as unknown. After taking the integration, the discretized form, the source term for the plasma continuity equation is expressed as :

$$S_n(i,j) = n(i,j)n_o(i,j) < \sigma v >_{ie}(i,j)vol(i,j) \quad (4.7)$$

Other source terms for momentum, ion energy and electron energy equations are treated identically.

4.2 Continuation Method

4.2.1 Newton's Method with Continuation

Recall that one of the shortcomings of Newton's method is the inability in finding an initial guess which resides well within the radius of convergence. A change in the physical parameters typically causes Newton's method not to converge on any given grids. To overcome the shortcomings of Newton's method, a continuation method or homotopy method, which is based on the approximation of a curve (homotopy paths) is considered. The definition of homotopy paths is described by Leray-Schauder's theorem (without proof) as follows [32].

Theorem 2 *There exists a one-dimensional continuum, Γ , of solutions of the homotopy equation that connects the solution of $f_{initial}(\vec{\Psi}) = 0$, which is known or can be easily obtained, to the solution of $f_{final}(\vec{\Psi}) = 0$ which is sought.*

The connection of $f_{initial}(\Psi)$ and $f_{final}(\Psi)$ is usually indicated by a general parameter λ . This parameter indicates that by changing its value slightly, a possible significant change in the overall result may occur. Intuitively, for example, the change in $D_{\perp}$ would significantly affect the overall flow profile due to the tendency of plasma particles to flow perpendicular to the direction of $D_{\perp}$. In this work, λ consists of transport coefficients ($D_{\perp}$ and χ_i), boundary values ($T_{i,core}$, $T_{e,core}$ and n_{core}) and physical parameters (gas puff rate or impurity fraction).

The application of the continuation method in the present work is realized in the form of a predictor-corrector continuation method [32]. The development of this method was inspired by the classical continuation (embedding) method, in which the transformation from an easily solved to difficult problem is done through a fixed increment of λ (λ_o -known, λ_n -desired). The classical embedding method starts with a solvable problem of $f_o(\vec{\Psi}, \lambda_o) = 0$. The next step is to solve $f_1(\vec{\Psi}, \lambda_1) = 0$, where $\lambda_1 = \lambda_o + \Delta\lambda$, using the solution of $f_o(\vec{\Psi}, \lambda_o) = 0$ as the initial guess in the Newton's method. The obvious drawbacks of this classic method are as follows. A fixed $\Delta\lambda$

sometimes results in nonconvergence, due to the notion that the predicted solution ($\vec{\Psi}_i(\lambda_i = \lambda_{i-1} + \Delta\lambda)$) may be too far from the solution point. In contrast, very small $\Delta\lambda$ can lead to excessive computations. Figure 4.2 shows that based on the predictor step of the classical embedding method, the possibility of the predicted solution (the initial guess for Newton's method) resides outside the radius of convergence is large. As an improvement, the predictor-corrector method modifies the predicted solution to the form of (figure 4.2) :

$$\vec{\Psi}_i = \vec{\Psi}_{i-1} + \frac{\partial \vec{\Psi}}{\partial \lambda}|_{i-1} \Delta\lambda \quad (4.8)$$

and the computation of the tangent vector $\vec{u}_{i-1} = \frac{\partial \vec{\Psi}}{\partial \lambda}|_{i-1}$ is described next.

Let's assume that for a given λ_o , the solution of $f_o(\vec{\Psi}, \lambda_o)$ is known and our goal is to find a solution for $f_n(\vec{\Psi}, \lambda_n)$. Assume also that the one-dimensional continuum, $\Gamma = \Gamma(\lambda_o, \lambda_1, \dots, \lambda_n)$ exists. Then by taking the derivative of $f_o(\vec{\Psi}, \lambda_o)$ with respect to λ_o , we get :

$$\frac{df_o(\vec{\Psi}, \lambda_o)}{d\lambda_o} = \frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \vec{\Psi}} \frac{d\vec{\Psi}}{d\lambda} + \frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \lambda_o} = 0 \quad (4.9)$$

or,

$$\vec{u} = \frac{d\vec{\Psi}}{d\lambda}|_{\lambda_o} = - \frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \lambda_o} / \frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \vec{\Psi}} \quad (4.10)$$

This is also known as Davidenko's equation and the computed values are substituted back into equation 4.8.

The term $\frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \vec{\Psi}}$ is the Jacobian of $f_o(\vec{\Psi}, \lambda_o)$ and it is automatically computed during the Newton's iteration. Referring to figure 4.2, the solution of $f_1(\vec{\Psi}, \lambda_1)$, $f_2(\vec{\Psi}, \lambda_2), \dots, f_n(\vec{\Psi}, \lambda_n)$ exists and is smooth, if and only if $\frac{\partial f_o(\vec{\Psi}, \lambda_o)}{\partial \vec{\Psi}}$ is locally non-singular (Implicit Function Theorem) [32].

The corrector step is performed by employing Newton's method with $\vec{\Psi}_1$ as an initial guess. This method differs from the classical embedding method in that the predicted step is controlled by the tangent of the function. One drawback of this

form of homotopy is when f'_Ψ vanishes. However, based on our experience in using the classical embedding continuation method, this condition is not expected. Thus, the method of continuation provides a possible means for finding solutions of a difficult nonlinear problem $f_n(\vec{\Psi}^*)$ for an easy problem $f_o(\vec{\Psi})$. The continuation method covers a wide range of possible forms of $f_n(\vec{\Psi}^*)$. The form of $f_n(\vec{\Psi}^*)$ can be simplest when $f_n(\vec{\Psi}^*)$ is different from $f_o(\vec{\Psi}_o)$ by a single parameter. In contrast, $f_n(\vec{\Psi}^*)$ can be also in a functional form which is relatively different from $f_o(\vec{\Psi}_o)$. To find $\vec{\Psi}^*$, there is a large class of methods available, and in this work, the selection will be oriented toward a relatively simple method. This is mainly due to the fact that the sensitive parameter relates only to the transport coefficients, Dirichlet core boundaries and puffing/impurities parameters.

The pseudo-code tangent-predictor algorithm is then as follows.

Predictor-Corrector Solution Scheme

- Find tangent vector, $\vec{u}$ at $\lambda = \lambda_i$ and predict solution at $\lambda = \lambda_{i+1}$ according to

$$\vec{\Psi}_*^{k+1} = \vec{\Psi}_*^k + \vec{u}\Delta\lambda$$

This is the predictor step

- Use $\vec{\Psi}_*^{k+1}$ as a guess in Newton scheme to converge to $\vec{\Psi}^{k+1}$. Recall Newton's method is defined as :

$$J(\vec{\Psi}_*^k)\delta\vec{\Psi}_*^k = -f(\vec{\Psi}_*^k) \quad (4.11)$$

and the new solution is computed as :

$$\vec{\Psi}^{k+1} = \vec{\Psi}_*^k + \alpha_N \delta\vec{\Psi}_*^k \quad (4.12)$$

This is the corrector step

- Repeat Process until solution at desired λ is achieved.

Note that the term tangent vector $\vec{u}$ can be misleading, since in reality its product with $\Delta\lambda$ is added into each and every unknown.

Another attractive feature of the continuation method is its turning point detection on the solution path. This is useful when a multiple solutions branch ($f'_{\psi} = 0$) exists. Our predictor-corrector method does not have the capability of fully following the solution path, however, it will be able to obtain solution on another branch. At the present time, it is understood that there are two possibilities of solution states in divertor plasmas. The first is a high-temperature and low-density solution due to a low rate of neutral recycling. The second is a low-temperature and high-density one due to a high rate of neutral recycling [3]. The physical reasoning of the existence of those two solutions can be explained as follows. The low-density condition may exist due to the fact that the neutral mean free path is much longer than the divertor dimension, allowing the neutrals to escape from the divertor region. In the other case, a high-density condition may exist due to the fact that the neutral mean free path is much shorter than the divertor dimension, except near the plate where the temperature is low. A one dimensional study has been performed and through a simple path following technique multiple solutions were obtained by Vu and Prinja [33] among others.

4.3 Multigrid Method

The multigrid idea was developed because of the inefficiencies of conventional iterative solvers to resolve low frequency errors (errors with a long wavelength) on a fine grid. By performing the Fourier analysis, standard/conventional iterative solvers (point Gauss-Seidel or Jacobi) are known to resolve high frequency errors in just a few relaxation sweeps and that the low frequency errors converge very slowly [34]. This difficulty is resolved in the multigrid method, which discretizes the problem on varying coarse and fine grids. The premise of the multigrid method is a systematic algorithm that unites the solution process on several (fine and coarse) grid densities by combining relaxation sweeps with corrections involving the current guess of the solution on both the fine and coarse grids. The coarse grids are primarily used to

supply fine grids with an estimate of the solution containing the low frequency error information, which is typically difficult or computationally expensive to obtain on the fine grids. The fine grids are used to resolve the high frequency errors in the solution, which are then used to improve coarse grid solutions. Thus, the underlying idea is to exchange the information of error and solution between grids.

For nonlinear problems, one common method to use is the Full Approximation Scheme (FAS). This method is an extension of the Coarse Grid Correction (CGC) method for linear problems in which the problem of interest is solved first only on the finest grid, while the coarser grids are used to solve the residual equations [34]. The coarse grid solution to the residual equations is then used as a correction to the residuals on finer grids. FAS extends the CGC method in such a way that the fine grid solution is used to modify the coarse grid, forcing the function to coincide with the fine grid solution (to be explained later). A conceptual algorithm for the multigrid procedure to be used in this research is shown in figure 4.3. The algorithm shows that the method automatically moves between coarse and fine levels (driven by the rate of convergence) until overall convergence is ultimately obtained on the finest (maximum) level. A more detailed algorithm is described in the following.

4.3.1 FAS Multigrid Solver

The FAS algorithm is shown in figure 4.5 and the following description follows the flowchart closely. As indicated earlier the underlying concept of the multigrid method is to expediently remove each Fourier component of the error spectrum on the coarsest possible grid [34]. The direction of grid changing seems to be just the opposite of common mesh sequencing methods in which information from coarse grids is passed upward to provide a starting point for the computation on finer grids. The reason for incorporating coarser grids is that low frequency errors tend to be effectively damped in the coarse grid iteration. In contrast, the high frequency errors are most effectively smoothed out in the iterations on a fine grid.

The development of the FAS method was originated from the Coarse Grid Correction (CGC) for linear systems. Thus, the following description of the FAS method will be initiated by the CGC method. The presentation is done from a practitioner's point of view and follows closely the description by Brandt's [34]. However, detailed description of the mathematical analysis is avoided since it can be referred to in Brandt's classical works [34] [35].

Consider a linear system

$$L_k \Psi_k = f_k \quad (4.13)$$

on a certain grid k and let $\tilde{\Psi}_k$ be an approximation to Ψ_k . Then the residual of the approximation can be written as $r_k = f_k - L_k \tilde{\Psi}_k$ and the error of approximation or correction is expressed as $v_k = \Psi_k - \tilde{\Psi}_k$. Subtracting equation 4.13 from the residual equation we get :

$$L_k \Psi_k - L_k \tilde{\Psi}_k = r_k \quad (4.14)$$

After rearrangement by using the error approximation expression,

$$L_k v_k = r_k \quad (4.15)$$

Since, the CGC is intended to smooth out the low frequency errors of the fine grid on the coarse grid, the residuals, r_k , must be transferred from the fine grid to the coarse grid (Restriction process). In this coarse grid, the intention is not to fully solve the problem, but to map the frequency content known on the fine grid onto the coarse grid such that the errors are smoothed out. In the coarse grid the error of approximation is smoothed out by :

$$L_{k-1} v_{k-1} = R_k^{k-1} r_k \quad (4.16)$$

where R_k^{k-1} is a restriction operator (from grid k to $k-1$) and $k-1 = 2k$ (larger grid

spacing but a smaller number of unknowns). Thus L_{k-1} essentially approximates L_k on the coarse grid. Once equation 4.16 is solved (v_{k-1} falls below a certain criteria), then v_{k-1} is transferred (interpolated) back to the fine grid and used as a correction for the fine grid solution :

$$\tilde{\Psi}_k^{new} = \tilde{\Psi}_k + I_{k-1}^k v_{k-1} \quad (4.17)$$

where I_{k-1}^k is an interpolation operator (from $k-1$ to k) The FAS follows generally the same steps as CGC, except that instead of v_{k-1} in equation 4.16 we use :

$$\hat{\Psi}_{k-1} = I_k^{k-1} \tilde{\Psi}_k + v_{k-1} \quad (4.18)$$

as the coarse grid's unknown function. For FAS, in transferring to a coarse grid, it is desired to approximate the current fine grid solution on the coarse grid (full intended solution represented on the coarse grid). Thus, with respect to the coarse grid correction, the FAS equation can be rewritten as:

$$L_{k-1} \hat{\Psi}_{k-1} = \hat{f}_{k-1} \quad (4.19)$$

where :

$$\hat{f}_{k-1} = L_{k-1}(R_k^{k-1} \tilde{\Psi}_k) + R_k^{k-1}(f_k - L_k \tilde{\Psi}_k) \quad (4.20)$$

Note that equation 4.19 is simply obtained by substituting $v_{k-1} = \hat{\Psi}_{k-1} - R_k^{k-1} \hat{\Psi}_k$ into equation 4.16. The coarse grid forcing function includes the residual and the solution from the fine grid. Now equation 4.19 can be rewritten as :

$$L_{k-1} \hat{\Psi}_{k-1} = L_{k-1}(R_k^{k-1} \tilde{\Psi}_k) + R_k^{k-1}(f_k - L_k \tilde{\Psi}_k) \quad (4.21)$$

Having obtained an approximate solution $\tilde{\Psi}_k$ to equation 4.19, the finer grid solution can be obtained by either directly interpolating $\tilde{\Psi}_k$ to finer grid or by using the correction scheme. The decision is obviously based on whether the finer grid has been visited. If it has not, then it is implied that the finer grid is the current finest

level of the multigrid cycle. In this case the solution can be transferred directly, since to be able to use the correction scheme, the grid must have already been visited. The direct transfer can be performed by :

$$\tilde{\Psi}_{k+1} = I_k^{k+1} \tilde{\Psi}_k \quad (4.22)$$

where I_k^{k+1} is the interpolation operator.

When transferring to a finer level which has already been visited, a coarse grid correction step must be taken. The correction is intended so as to include the most recent low frequency information in the solution from a coarse grid onto the next finer level,

$$\tilde{\Psi}_{k+1} = \tilde{\Psi}_{k+1} + I_{k-1}^k (\tilde{\Psi}_{k-1} - R_k^{k-1} \tilde{\Psi}_k) \quad (4.23)$$

since at this point the low frequency errors contained in the fine grid solution which were difficult to eliminate at grid $k+1$ now have been smoothed out.

For nonlinear problems equation 4.15 cannot be applied directly, since the correction is valid only for linear L_k . Since L_k is a nonlinear operator, the correction scheme can instead be written as :

$$L_k(\tilde{\Psi}_k + v_k) - L_k \tilde{\Psi}_k = r_k \quad (4.24)$$

Note that no linearization is done in equation 4.24. The coarse grid correction equation is obtained by replacing L_k by L_{k-1} , $\tilde{\Psi}_k$ by $R_k^{k-1} \tilde{\Psi}_k$, v_k by v_{k-1} and r_k by $R_k^{k-1} r_{k-1}$ in equation 4.24 such that :

$$L_{k-1}(R_k^{k-1} \tilde{\Psi}_k + v_{k-1}) - L_{k-1} R_k^{k-1} \tilde{\Psi}_k = R_k^{k-1} r_k \quad (4.25)$$

or

$$L_{k-1} \hat{\Psi}_{k-1} = L_{k-1} R_k^{k-1} \tilde{\Psi}_k + R_k^{k-1} r_k \quad (4.26)$$

This is identical to equation 4.21 and it signifies an important advantage of the FAS method over other nonlinear schemes in terms of direct applicability. Unlike other nonlinear methods where global linearization are usually needed, FAS requires only local linearization. By appropriately employing a suitable local relaxation method this can be very advantageous.

The intergrid transfer within the multigrid cycle must be treated carefully. The type of intergrid transfer depends upon whether the destination is a coarser or finer grid. The interpolation process (coarse to fine) must be done with an order of interpolation at least equal to the order of the differential equations ($\hat{n}$) being solved [34, 35]. Except for a few cases, the interpolation effectiveness of higher order is no more than the minimum required order. Thus, minimal order interpolation will be used, as they are less complex and just as effective as higher order interpolations. In this work, as it is also used in the mesh sequencing process of the original NEWEDGE [5], a bilinear-like interpolation which is based on the contribution of fine grid control volume (weighting function) is used (figure 4.4). Since the fine grid is generated cutting each coarse control volume in half in both spatial directions, the weighting functions are defined as :

$$\begin{aligned}w_1 &= A(\Psi(ic, jc)) \\w_2 &= A(\Psi(ic + 1, jc)) \\w_3 &= A(\Psi(ic, jc + 1)) \\w_4 &= A(\Psi(ic + 1, jc + 1))\end{aligned}$$

where $A(\Psi)$ is the area of control volume Ψ . Note that by assuming that the coarse grid size is uniform, the weighting function is the following common matrix weighting function interpolation from $\Psi(ic, jc)$ to $\Psi(if, jf)$.

$$\begin{bmatrix} \frac{3}{16}\Psi(ic, jc + 1) & \frac{1}{16}\Psi(ic + 1, jc + 1) \\ \frac{9}{16}\Psi(ic, jc) & \frac{3}{16}\Psi(ic + 1, jc) \end{bmatrix}$$

Using the computed weighting function the fine grid point (if, jf) , a function of

$(ic, jc), (ic + 1, jc), (ic, jc + 1)$ and $(ic + 1, jc + 1)$ can be computed as :

$$\begin{aligned}\Psi(if, jf) = & (1 - w_1)(1 - w_2)\Psi(ic, jc) + w_2(1 - w_1)\Psi(ic + 1, jc) \\ & + w_3(1 - w_1)\Psi(ic, jc + 1) + w_1w_4\Psi(ic + 1, jc + 1)\end{aligned}\quad (4.27)$$

Other fine grid points are treated identically.

The restriction process for the solution is executed by computing a weighting function which is based on the area of the contributing fine grids. On the other hand the natural choice of the residual restriction is by summing up all residuals from contributing fine grid cells and they are expressed as [34]:

$$\begin{aligned}R_k^{k-1}\Psi_k = & \Psi(if, jf)(1 - w(if, jf)) + \Psi(if - 1, jf)(1 - w(if - 1, jf)) \\ & + \Psi(if - 1, jf - 1)(1 - w(if - 1, jf - 1)) \\ & + \Psi(if, jf - 1)(1 - w(if, jf - 1))\end{aligned}\quad (4.28)$$

where $w(i, j) = 1 - Area(i, j) / \sum A$, and,

$$R_k^{k-1}r_k = r_{if,jf} + r_{if-1,jf} + r_{if-1,jf-1} + r_{if,jf-1}\quad (4.29)$$

This type of restriction process is also called the volume-weighting restriction in which the method preserves the mass conservation content of the fine grid. It also makes full use of the information available on the fine grid when correcting the coarse grid equations.

When multigrid processing takes places on any level, the decision whether to remain at the current level or move to a finer or coarser grid is determined by an acceptable rate of convergence. To check for convergence at the current level, the measure of residuals e_k is compared to a tolerance ϵ_k . The norm of the residual is defined as :

$$e_k = \|r_k\|_2\quad (4.30)$$

and the tolerance is designed such that when $e_k < \epsilon_k$, convergence is obtained. This condition indicates that the problem has converged at the current level and a move to the next finer grid is made. If the current level is at the finest level ($k = l = M$), then the process is stopped. If the tolerance criteria is not met then the decision whether to remain at the current grid or move to a coarser grid must be made. If we sense that convergence at any fine level is slow, then we must switch to a coarse grid. The question is "what is slow?". To assure reasonable convergence rates, the norm of residual e_k , at the current relaxation sweep must be less than some fraction of the previous norm of residual $\hat{e}_k$.

$$\frac{e_k}{\hat{e}_k} < \eta \quad (4.31)$$

Typically η has the range of 0 – 1 and it usually set equal to 0.5 [35].

The determination of tolerance (ϵ_k) is by no means fixed. The value of ϵ_k must be appropriately adjusted according to the direction into which the grid is moving. This is very important when a move to a coarser grid is made. Suppose that N relaxation sweeps have been completed on the fine grid k before moving to coarse level $k - 1$. At this point, the high frequency error on level k would have been reduced by the factor μ^N , where μ indicates the attenuation in the high frequency errors due to a single relaxation sweep on level k . Here, the solution at grid level k is not yet known to within the truncation error $(\Delta x_k)^2$, so it is not desirable to spend a great deal of effort to obtain a fully accurate solution on grid level $k - 1$. The objective to move to coarser grid $k - 1$ is to reduce the errors that were low frequency errors on level k (which are now high frequency errors on level $k - 1$) by a similar factor. The convergence criteria at the coarse grid is set by :

$$\epsilon_{k-1} = \delta |e_k| \quad (4.32)$$

The value of δ is typically set to be 0.25 and it is selected based on the smoothing factor [35].

As previously mentioned, the success of a multigrid cycle depends partly on the chosen relaxation scheme which is mainly determined by effect of the smoothing property of the relaxation scheme to the overall rate of convergence. This will be described in more detail in the next section.

4.3.2 Relaxation Procedure

The validity of the multigrid method is not affected by the choice of the smoothing (relaxation) procedure. However, a poor smoothing property would significantly downgrade efficiency. In this work, a variation of Vanka's Block Gauss-Seidel (BGS) method is selected [36]. The method (BGS) was developed by the simplicity of the traditional Gauss-Seidel method in finding solutions for fluid dynamics continuity, momentum and energy equations (Navier-Stokes). In this work, two types of Gauss-Seidel relaxation processes, namely, point and line will be explored. The point Gauss-Seidel is closely related to the BGS method in which within each control volume (block) a point Gauss-Seidel relaxation is performed. The line Gauss-Seidel performs the relaxation within a collection of control volumes in the radial or poloidal directions. To illustrate the procedure we will use the continuity equation. Other equations follow identical procedures.

At any given grid level, consider a control volume or cell (i, j) . Using a finite volume approach, the continuity equation is discretized as follows [27].

$$a_p(i, j) = a_w n(i - 1, j) + a_e n(i + 1, j) + a_n n(i, j + 1) + a_s n(i, j - 1) + q \quad (4.33)$$

or,

$$A_p n(i, j) = F(i, j) \quad (4.34)$$

where :

$$a_w = \text{MAX}(F_w, 0.0)$$

$$a_e = \text{MAX}(-F_e, 0.0)$$

$$a_n = D_n$$

$$a_s = D_s$$

$$a_p = \text{MAX}(F_e, 0.0) + \text{MAX}(-F_w, 0.0) + a_n + a_s$$

$$q = n(i, j)n_o(i, j) < \sigma v >_{ie} (i, j) \text{vol}(i, j)$$

$$F_e = dy(i, j)u(i, j)$$

$$F_w = dy(i - 1, j)u(i - 1, j)$$

$$D_n = \frac{2D_{ni}dx(i, j)}{dy(i, j) + dy(i, j + 1)}$$

$$D_s = \frac{2D_{ni}dx(i, j - 1)}{dy(i, j) + dy(i, j - 1)}$$

and

$$A_p = a_p + Q$$

$$F(i, j) = a_w n(i - 1, j) + a_e n(i + 1, j) + a_n n(i, j + 1) + a_s n(i, j - 1)$$

$$Q = n_o(i, j) < \sigma v >_{ie} (i, j) \text{vol}(i, j)$$

where dx , dy and vol are x and y length, area and volume of each control volume.

Now, let :

$$G(n(i, j)) = A_p n(i, j) - F(i, j) \quad (4.35)$$

Linearize equation 4.35 by Taylor series expansion, keeping the first two terms of its expansion to get :

$$G(n^k) + \frac{\partial G(n^k)}{\partial n} (n^* - n^k) = 0 \quad (4.36)$$

or,

$$A_p \Delta n(i, j) = -G(n^k) \quad (4.37)$$

where $\Delta n(i, j) = n^* - n^k$. Similar steps are taken for the rest of the equations. Thus the general form of equation 4.34 can be written as

$$A_p \Psi(i, j) = F_\Psi(i, j) \quad (4.38)$$

while the corrections form is expressed as :

$$A_p \Delta \Psi(i, j) = -G_\Psi(i, j) \quad (4.39)$$

Overall the obtained corrections then are applied to the current guess solution, i.e.,

$$\vec{\Psi}_{k+1} = \vec{\Psi}_k + \Delta \vec{\Psi}_k \quad (4.40)$$

where k is the iteration step.

The solution approximation is analogous to the Jacobian construction of Newton's method. This is due to the fact that the method was originally developed [36] based on an identical experience with massive memory requirements of the Jacobian matrix. Thus, the flavor of this error approximation is similar to Newton's Jacobian matrix. Note that the corrections are simultaneously solved (in each control volume) and as a consequence the total matrix size is equal to the number of computational grids required. This indicates that a very fine grid computational process can be performed.

Two relaxation methods, namely point Gauss-Seidel and line Gauss-Seidel are explored in this work. The intention is to find a stable scheme which has a reliable smoothing property such that intended simulation cases can be performed well. It is expected that for gaseous/radiative divertor simulation, due to the possible existence of a flame front-like (shock) solution, the relaxation procedure would require an implicit-like method.

1. Point Gauss Seidel (PGS)

The application of this scheme requires that each and every unknown within each control volume is relaxed simultaneously. Thus equation 4.39, in terms of all unknowns can be written as :

$$A_{p,n} \Delta n(i, j) = -G_n(i, j) \quad (4.41)$$

$$A_{p,n_o} \Delta n_o(i, j) = -G_{n_o}(i, j) \quad (4.42)$$

$$A_{p,T_i} \Delta T_i(i, j) = -G_{T_i}(i, j) \quad (4.43)$$

$$A_{p,T_e} \Delta T_e(i, j) = -G_{T_e}(i, j) \quad (4.44)$$

$$A_{p,u} \Delta u(i, j) = -G_u(i, j)$$

The relaxation is performed such that each time the latest available unknowns are used. This method can be regarded also as a variant of Vanka's method [36]. The total memory storage for this method $M_{store}(PGS)$ is a linear function of computational grid and the number of unknowns and it is expressed as follows.

$$M_{store}(PGS) = nx \times ny \times neq \quad (4.45)$$

Thus, for a grid size of 256×48 and 5 equations, the total memory storage is about 62 kiloword. It is substantially less than the memory storage for Newton's method where the Jacobian requires that every connected unknown derivative must be stored.

2. Line Gauss Seidel (LGS)

For a certain class of problems, the PGS method does not perform as expected. Typically, the next logical step is to use the Line Gauss-Seidel (LGS) method at which implicitness is preserved in the chosen line. This type of problems arises regularly in hypersonic flow problems [37] and the LGS method has been found to perform well. In this work, the chosen direction is the radial direction. The selection is based on the sensitivity of D_{ni} , radial diffusivity, experienced during the continuation process. Moreover, the radial direction floating point operation is substantially less than the one in the poloidal direction. Thus the sequence of the unknowns in LGS is set as : $n(i, j), n(i, j + 1), n(i, j + 2), \dots, n(i, ny), n_o(i, j), n_o(i, j + 1), \dots, n_o(i, ny), \dots, u(i, ny)$ and referring to equation 4.39, the continuity relaxation takes the form of (equation 4.36) :

$$G(n^k) + \frac{\partial G(n^k)}{\partial n_j} \Big|_{jn} = 0 \quad (4.46)$$

where $jn = j - 1, j, j + 1$, or for continuity equation the matrix system is as :

$$\mathbf{A}_I \Delta_n = \mathbf{G} \quad (4.47)$$

where :

$$\mathbf{A}_I = \begin{bmatrix} A_{p,n}(i, j) & a_{n,n}(i, j+1) & 0 & 0 & 0 & 0 & 0 \\ a_{s,n}(i, j) & A_{p,n}(i, j+1) & a_{n,n}(i, j+2) & 0 & 0 & 0 & 0 \\ 0 & a_{s,n}(i, j+1) & A_{p,n}(i, j+2) & a_{n,n}(i, j+3) & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & a_{s,n}(i, ny-1) & A_{p,n}(i, ny) \end{bmatrix}$$

where all the coefficients are as defined by equation 4.33, and

$$\Delta_n = \begin{bmatrix} \Delta n(i, j) \\ \Delta n(i, j+1) \\ \Delta n(i, j+2) \\ \vdots \\ \Delta n(i, ny) \end{bmatrix}, \mathbf{G} = \begin{bmatrix} -G_n(i, j) \\ -G_n(i, j+1) \\ -G_n(i, j+2) \\ \vdots \\ -G_n(i, ny) \end{bmatrix}$$

The total memory storage for the LGS method is different from the PGS method only in the additional working storage to solve the tridiagonal matrix structure of equation 4.47.

Both of the aforesaid methods will be tested for different simulation conditions. Their results are discussed in chapter 5.

Figure 4.1: Computational Control Volume

CONTINUATION DIAGRAM

Figure 4.2: Continuation Diagram

Figure 4.3: Conceptual Multigrid Method

Figure 4.4: Coarse and Fine Grids Structure

Figure 4.5: FAS Multigrid Scheme

Chapter 5

Simulation Results for the ITER Divertor

Numerical simulations are performed for four different cases of the ITER configuration. Case 1 represents the basic model, in which the governing equations are the continuity, FFCD neutral, ion and electron energy, as well as the momentum equations, with fixed density and temperatures at the boundary with the core. We refer to this as a reference case. Case 2 represents the simulation radiation loss through impurities. The nature of the atomic interaction between impurities and the plasma particles may result in a more 'structured' solution than in case 1. This is indicated by the existence of a shock-like temperature profile near the divertor plates. Case 3 involves the injection of Deuterium into the private flux region. It is expected that the solution will have a similar structure to that of the impurity simulation. The injected neutral gas and impurities may force the temperature solution to collapse, due to energy loss through various atomic processes. For each case, the performance of the tangent-predictor and the multigrid method will be discussed. Both case 2 and 3 are intended to investigate the robustness of the numerical schemes for gaseous-radiative divertors. Finally, in case 4 the stability of the solutions which were obtained with puffing as well as impurity radiation is investigated. A time dependent term is added to the coarse grid equation, such that the stability of solutions obtained from the

steady state mode can be analyzed. The stability analysis is by no means complete, yet it gives a sense of direction.

5.1 Reference Case

5.1.1 Continuation Process

A complete successful cycle of the FAS multigrid method will not be possible unless a converged solution on the coarsest grid is available. Thus, the continuation process in parameter space is first used to obtain the coarsest grid solution with the desired parameter set. The continuation is carried out on a 32×6 grid and the initial and desired transport parameters to be used are presented in table 5.1. The desired set is selected based on the parameter space that ITER is expected to operate in [1]. This set is solely intended to show the performance of the continuation technique on the system parameters. Later, the same technique will also be applied to puffing rate and impurity fraction).

Table 5.1: Continuation simulation condition

Parameters	Initial	Desired
$D_{\perp}, m^2/s$	1.0	1.333
$\chi_i, m^2/s$	1.0	1.333
$\chi_e, m^2/s$	4.0	4.0
Core Temperature, eV (ion and electron)	100	300
Core Density, $10^{19}/m^3$	1.8	3.0

Note that a continuation process was not necessary for the χ_e .

In the course of the tangent-predictor (TP) continuation method application, as a comparison, a classical embedding (CE) technique, is also performed and its results are contrasted with the TP technique. From the simulation results (table 5.2), it is

clear that the TP technique consistently decreases the corrector (Newton's iterations) steps significantly. This is due to a better initial guess that was obtained from the predictor step in which $\Delta\lambda$ is corrected by the tangent vector $\vec{u}$. In this work, the choice of $\Delta\lambda$ ($\lambda = D_{\perp}, \chi_i$, etc) for the CE method as well as for the TP method is based on the experience obtained when the manual $\Delta\lambda$ was implemented [38]. The TP method is carried out one λ at a time, and its sequence is indicated by the parameter numbers in table 5.2.

Table 5.2 shows also that the TP method reduces the CPU time from the CE method by about 30 %. We conclude from these results that the predictor step of the TP method brings the guessed solution well within the radius of convergence for Newton's method of the corrector step, and thus represents an effective modification of Newton's method. Here, a damped Newton iteration was used identical to the one used in the original NEWEDGE.

The continuation simulation is performed until a desired error criterion is achieved ($\epsilon = \text{MAX}(\|n\|_2, \|n_o\|_2, \|T_i\|_2, \|T_e\|_2, \|u\|_2)$). From table 5.2, it is shown that $\epsilon = 10^{-9}$ is used as the stopping criterion. The value of ϵ naturally can be reduced as much as one desires and it is selected based on the fact that beyond $\epsilon = 10^{-9}$ the overall solution does not change significantly. Table 5.3 shows that during $D_{\perp}$ simulation, the peak electron temperature at both inner and outer divertor plates for $\epsilon = 10^{-9}$ (compare with $\epsilon = 10^{-15}$) only changes after 8-9 significant digits, indicating that the use of $\epsilon = 10^{-15}$ is not necessary. The total number of iterations is also substantially different and the CPU time was reduced from 254.3 seconds ($\epsilon = 10^{-15}$) to about 136.5 seconds ($\epsilon = 10^{-9}$). A reduction of about 50 %. Based on the observations, usually, when the residual reaches a range of 10^{-7} to 10^{-8} , the overall solution starts to converge rapidly. Another indication is that the factorization term α_N , the damping factor (see equation 3.6), reaches 1.0, i.e., full Newton.

Table 5.2: Corrector step numerical performance comparison between classical embedding (CE) and tangent-predictor (TP) for transport parameters simulation with convergence criteria of $\epsilon \leq 10^{-9}$, where, $\epsilon = \text{MAX}(\|n\|_2, \|n_o\|_2, \|T_i\|_2, \|T_e\|_2, \|u\|_2)$

Parameter Number	Δ_λ	CE Iterations	TP Iterations
1	$\Delta D_{\perp,1} = 0.1$	5	4
	$\Delta D_{\perp,2} = 0.1$	5	4
	$\Delta D_{\perp,3} = 0.1$	5	3
	$\Delta D_{\perp,4} = 0.033$	3	2
	Total	18	13
2	$\Delta \chi_{i,1} = 0.1$	4	3
	$\Delta \chi_{i,2} = 0.1$	4	3
	$\Delta \chi_{i,3} = 0.1$	3	2
	$\Delta \chi_{i,4} = 0.033$	3	2
	Total	14	10
3	$\Delta T_{core,1} = 50.0$	7	3
	$\Delta T_{core,2} = 50.0$	6	3
	$\Delta T_{core,3} = 50.0$	5	2
	$\Delta T_{core,4} = 50.0$	2	2
	Total	21	10
4	$\Delta N_{core,1} = 0.2$	5	3
	$\Delta N_{core,2} = 0.25$	4	2
	$\Delta N_{core,3} = 0.25$	4	2
	$\Delta N_{core,4} = 0.25$	2	2
	$\Delta N_{core,5} = 0.25$	2	2
	Total	17	11
	Total time, s	453.2	305.6

5.1.2 Multigrid Process

Prior to the discussion of the multigrid method performance, it is important to note that the clear advantage of the multigrid method over Newton's method on fine grids is memory storage. Multigrid memory storage is linearly dependent on the number of computational grids. This is not the case for Newton's method. Knoll [5] indicates that depending on the order (i , poloidal or j , radial) the simulation is performed, the memory storage can increase in an exponential-like fashion. Figure 5.1 clearly shows the advantage in memory storage of the multigrid over Newton's method.

Figure 5.1: Comparison of memory storage requirement for banded Gaussian (i-fastest running index) and multigrid, Grid sequence : $\Gamma_0 = 32 \times 6$, $\Gamma_1 = 64 \times 12$, $\Gamma_2 = 128 \times 24$, $\Gamma_3 = 256 \times 48$ and $\Gamma_4 = 512 \times 96$ and $n_{equation} = 5$

The first operation on the multigrid cycle is to interpolate the coarsest grid converged solutions and residuals obtained from the continuation process into the next fine grid of $\Gamma_1 = 64 \times 12$ (level $k = 1$). At this point the multigrid cycle starts. In this work, the whole sequence of grids Γ_k , where $k = 1 \rightarrow 4$, is used. As indicated previously, two relaxation methods will be employed to find the most effective smoother. The effectiveness of Line Gauss-Seidel (LGS) over Point Gauss-Seidel (PGS) is marked

by the straight mesh sequencing in the LGS process. This is explained as follows. Table 5.4 shows that at level $k = 1$, for the our standard case, a revisit to coarse grid for PGS needs to be done. This is due to the fact that the solution structure at Γ_o is significantly different from Γ_1 . At this level the convergence rate is slowing down to approximately 10^{-6} .

The difference in solution is indicated by figure 5.2 where at the outer divertor plate there is a distinct shift from Γ_o to Γ_1 , while within the sequence of $\Gamma_{1 \rightarrow 4}$, the shift is less pronounced. As Γ increases, the solution merges closer. The weakness of the PGS method, although it is performed in a block manner, is a classical example of the need of implicitness in nonlinear problems.

Figure 5.2: Outer electron plate temperature for Γ_k , $k = 1 - 4$

The mesh sequencing is an excellent check to the sensitivity of the solution. The highly nonlinear coupling between the governing equations and the system configuration complexities result in a situation where there is no analytical solution which one can compare against. Thus, the stability of the solution, as the grid size increases, is an assurance in obtaining a solution within the constraints of the numerical discretization schemes. The results from figure 5.2 indicate also that grid Γ_1 is the coarsest

grid size in which the mesh spacing is close or may be within the range of the neutral particle mean-free-path (mfp). The compatibility of mesh spacing and particle mfp is particularly important near the plates, where the solution gradient is obviously steep. The mean-free-path near the plate, depending on the condition, is in the order of 1-2 cm and for a large machine like ITER, this may well translate into an ultra fine grid for which the multigrid can serve well. Figure 5.2 also indicates that computation at Γ_4 is not necessary, since the solution of Γ_4 is identical to Γ_3 .

Better performance of the LGS method over the PGS method is expected because of the implicitness of the former. However, the CPU time of the LGS method is about 7-8 % higher than for the PGS method. This is due to the time required to temporarily store and solve the tridiagonal system. If the simulation is stopped at Γ_3 , the CPU time of the LGS method is relatively the same as for the PGS method, not an advantage from a CPU time point of view. This may seem to downgrade the LGS performance, but for more complex (puffing or impurity) problems, as will be discussed next, the LGS is superior than the PGS method.

Figures 5.3, 5.4 and 5.5 are contour plots of T_i , T_e , n and Mach numbers respectively. The general nature of the solution is consistent with the physical expectations. Due to neutral recycling at both divertor plates (100%), the plasma density rises near both divertor plates and correspondingly the ion and electron temperatures drop. At the inner divertor legs, where no neutral pumping is done, the plasma density is higher than at the outer leg. At this region all neutrals are essentially ionized. The concomitant effect is that the ion and electron temperatures at the inner legs are lower than the ones at the outer divertor legs. Because of the sheath boundary condition that is imposed at both divertor plates, ions and electrons enter the sheath at the speed of sound (figure 5.4) (Mach number = 1). The whole domain electron temperature and plasma density profiles are shown in figure 5.5.

The replacement of the single energy neutral diffusion model by the FFCD model shows that in general the diffusion model overestimates plasma density. Apparently, the deeper penetration of the FFCD model neutrals yields less localized recycling

Figure 5.3: Inner and outer divertor legs ion T_i and electron temperatures T_e (eV). From top left, clock wise : inner T_i , outer T_i , outer T_e and inner T_e

Figure 5.4: Inner and outer divertor legs plasma density (n) and mach number (M) profiles. From top left, clock wise : inner n , outer n , inner M and outer M

Figure 5.5: Plate to plate electron temperature and plasma density profiles

than in the diffusion model and results in a drop of the plasma density near the plate. This is clearly demonstrated in figure 5.6, where the plasma density profiles along the separatrix are slightly lower (with and without molecules) than for the diffusion model. The plasma density profile with molecules merely indicates that there is an additional source term in the collided density equation.

Figure 5.6: Outer leg plasma density profile for diffusion single energy model, FFCD with molecules and FFCD without molecules

The neutral density profiles (figure 5.7) show that the solution for the neutral diffusion decays more sharply than neutrals in the FFCD model. The poloidal neutral density profiles for atoms and molecules show that first flight densities are dominant near the plate but are strongly attenuated over distance into the plasma, yielding a distributed source of charge exchange for the collided density (figure 5.8).

The impact of the FFCD model on the numerical performance is shown in figure 5.9. As indicated above, the plasma density profile of the FFCD model near the plate is not as steep as for the diffusion model, leading to a slightly better convergence performance of the code.

While the focus of the discussion is mainly on the outer leg region, where the neutral pumping is expected to take place, the inner leg results show similar charac-

teristics. Because of lack of pumping, the densities generally tend to be higher at the inner leg. At the present time, a detailed atomic data for molecules is still lacking, thus, in the next sections, the neutral model will include only the FFCD atoms.

The electron temperature and plasma density profiles will be used more often in the following sections as the base for comparing reactor conditions when neutral gas puffing or impurity simulations are applied. The choice of both parameters is due to the fact that the computation of peak heat flux at the plates depends upon their values. Based on the satisfactory numerical and physical performances in this ideal case, a more realistic scenario will be ventured upon numerically. The next scenario is the impurity simulation.

5.2 Simulation Results with Impurity Radiation

The impurity simulation is performed by using the impurity fraction f_{imp} as the continuation parameter, with a range of f_{imp} from 0 – 8%. The parameter f_{imp} indicates the fraction of the impurity density with respect to the plasma density. To show the impact of impurities to the overall solution, three values of f_{imp} are selected for comparison ($f_{imp} \rightarrow 0.5, 3, 8\%$). Table 5.5 shows that at the early stages, the number of iterations during the continuation process increases until f_{imp} is about 3%. Afterward, the iterations are essentially leveling off. Later, from the multigrid results it is understood that this is due to the fact that beyond $f_{imp} = 3\%$, the solution 'collapses'. The 'collapse' of the solution is indicated by the fact that at high f_{imp} the electron temperature at the whole SOL region is very low.

Within each Δf_{imp} , the iterations are relatively fast, indicating that the guessed solutions are predicted properly. For high f_{imp} , the guessed solution will not significantly affect the overall performance, consistent with the previous argument that any perturbations will not affect the overall profile considerably. The total iterations from 0 – 8% are relatively high (504), but it takes only about 10 minutes CPU time to perform the simulation. At this point, no comparison with the CE method is done,

since from the previous analysis, it has been shown that the TP method outperforms the CE method in terms of CPU time savings and total number of Newton iterations.

At each selected f_{imp} value, the coarsest grid solutions and residuals are interpolated into the multigrid cycle. Within the multigrid cycle, two relaxations are again employed (PGS and LGS). Immediately as seen from table 5.6, when the PGS method needs to visit a coarse grid, the method is essentially stalled. At this level, the convergence rate is slowing down at approximately 10^{-6} . Referring to equation 4.31, typically the speed (slowness) of convergence is determined when η reaches 0.5. Recall that η determines the fraction of the current residual (e_k) with respect to the previous residual ($\hat{e}_k$). In this simulation, η is extended to 0.9, allowing the current norm of residual to change only 10% from the previous value. The intention is to experiment with the convergence behavior of the existing relaxation scheme. Since Γ_o is the coarsest grid available, and with the addition of excessive iterations and extremely slow change in the convergence rate at this level of η (the change in convergence rate is only about 10%), the iterations for the PGS method must be terminated. The effect of the interpolation operator (area law) can be argued to be the major reason for PGS failure, but observing the performance at level Γ_1 , the argument is incorrect. A value of $\eta = 0.9$ will be used for the PGS method in all simulations, while η will remain at $\eta = 0.5$ for the LGS scheme. The extension of η for the PGS method is intended to investigate whether within a reasonable range of η the PGS method remains useable. However, based on the impurity simulation results, the PGS method does not show the characteristics to become a useful solver.

Apparently, the 'flame front profile' that the impurity simulation produces (see figures 5.10 and 5.11) necessitates the use of the LGS relaxation method. For relatively high f_{imp} , due to the steep gradient of the overall solutions in the radial direction, the implicitness in radial direction is important. As indicated above, to determine the slowness of the LGS relaxation, η is set to be 0.5. The numerical performance indicates that the LGS method performs remarkably well within this criterion. This is indicated by the straightupwardness of the mesh sequencing process to the finest

grid available. As the f_{imp} increases, as was seen during the continuation process, the number of multigrid iterations is leveling off. The iterations are basically done to smooth out interpolation errors from the previous coarser grid.

The total CPU time for the selected f_{imp} is reasonably high. However, as shown earlier, the computation at Γ_4 is unnecessary. Here, the computation at Γ_4 is performed with the intention of showing the flexibility of the multigrid method. Provided that finer grids are available, the multigrid method can be extended to finer ones. If the CPU time at Γ_4 is subtracted, then the total CPU time is equal to 324.2, 839.2 and 934.6 for each selected f_{imp} respectively. The jump of CPU time from $f_{imp} = 0.5\%$ to $f_{imp} = 3\%$ demonstrates the development of the flame front. At this level of f_{imp} more iterations are needed to resolve the shock-like characteristics of the solution. The LGS method, although laborious in CPU times and iterations, is able to resolve the shock characteristics of the solution. Later on, the electron temperature profile is presented to show the distinction in the solution profile for f_{imp} below 3%.

Figures 5.10 and 5.11 show the collapsing electron temperatures solutions at both inner and outer divertor plates as f_{imp} increases, leading to a situation where the peak radiated power has shifted away from the plates. These figures also reinforce the argument that the characteristic of the solution (shock) is the primary reason why the number of iterations increases considerably for $0.5\% \leq f_{imp} \leq 3\%$. The plate to plate electron temperature profile from figure 5.12 also shows that, except for near the core boundary, for $f_{imp} = 8\%$ the electron temperatures have basically collapsed. In this case, the electron temperature for the whole SOL region is essentially less than 5 eV.

As for plasma density, figures 5.13 and 5.15 show that at $f_{imp} = 0.5\%$ there is an increase of plasma density near both plates. However, as f_{imp} reaches 5 – 8%, plasma density decreases. This is due to the fact that at this point the temperatures are so low that they lead to a condition where there is no more energy to radiate away. Figures 5.14 and 5.16 show that there is an increase in the mach number such that supersonic flow occurs near the plates. Due to the imposed sheath boundary

at the divertor plates, the particles are impinging the divertor plates at the speed of sound. In real application, where the core boundary conditions are not constant, the existence of a highly reverse flow near the separatrix, which may bring the impurities to the main core, is a primary concern.

The effect of impurities on the divertor plates is clearly demonstrated in figures 5.17, 5.18, 5.19 and 5.20. The peak electron temperature at the outer divertor plates decreases from approximately 17 eV for the no impurity case to as low as 2 eV for $f_{imp} = 8\%$. Correspondingly, the heat flux is reduced from about 38 MW/m^2 to well below 5 MW/m^2 . A similar situation also occurs at the inner divertor plate. The peak heat flux at the outer divertor plate is higher than at the inner divertor plate because of the unsymmetric poloidal equilibrium that gives an outward bulge results in more heat flow towards the outside. Based on the overall results, with an appropriate treatment of the impurities, the peak heat flux has been reduced to within the thermomechanical wall material limitations.

An interesting result is the radiated power due to impurities. In the electron energy equation this is expressed as $f_{imp}n^2L(T_e)$. As f_{imp} increases the position of the peak radiated power moves away from the plate as the collapse stabilizes in region of higher temperature. In the extreme, when $f_{imp} = 8\%$, the peak is essentially at the core boundary (figures 5.21 and 5.22). This, however, must be an unstable situation for the tokamaks as a whole because of excessive radiations is likely to occur within the confined region and lead to a disruptive termination of the discharge. The shift of peak radiated power away from the plates is a desired condition for divertor operation. Table 5.7 shows that as the fraction impurities increases, the total impurity radiation loss increases to almost 99% from the total incoming energy. The incoming energy is computed from the total energy across the separatrix.

As a summary, the numerical schemes have shown that the flame front characteristics of the solution can be handled in a systematic and versatile manner, although the impurity radiation model used here is an idealized one. Other important factors, such as multiple species and particles momentum interactions, can be significant fac-

tors in determining the true two dimensional nature radiation profile. However, as the structure of the impurity density and momentum equations [24] is similar to the basic edge plasma equations considered in this work, the numerical methods developed and implemented here should be readily adaptable to the general case.

5.3 Deuterium Injection

The configuration Deuterium puffing is shown in figure 5.23. At the private flux region, where neutral gas is injected, the boundary condition is modified to include an external source Γ_o (rate of injected neutrals, $\#/s$). In this work, two neutral gas rates are to be investigated ($\Gamma_o \rightarrow 1 \times 10^{21}$ and 3×10^{21}). At the coarsest grid, where the continuation process is implemented, a continuation parameter f_{puff} is used in which $\Gamma_o = f_{puff} \Gamma_p$ (where $\Gamma_p = 3 \times 10^{21}$ and $0 \leq f_{puff} \leq 1$).

In this work, the Δf_{puff} is set to be equal to 0.16667, i.e.,

$$\Gamma_o \rightarrow (0 - 3 \times 10^{21}), \Delta f_{puff} = 0.1667$$

This choice of the Δf_{puff} value gives a somewhat optimum path along Γ_o .

The continuation results show that as f_{puff} increases, the number of Newton's iterations for the corrector step are levelling off (table 5.8) until f_{puff} reaches 1.0. Again, as was seen during the impurity simulation, this is due to the fact that the guessed solution is well within the radius of convergence of Newton's method. The total CPU time and the total number of iterations are 491.03 seconds and 280 iterations respectively. When f_{puff} reaches near 3, the total number of iterations suddenly increases to 75. This is contrary to the nature of the predictor step, the function of which is to bring the solution well within the radius of convergence of Newton's method. Later, it is understood that, when $f_{puff} = 3.0$, the physical solution reaches its limit. The multigrid results in general show the same characteristics as in the impurity simulation. However, at a puff rate that equals 1×10^{21} , the PGS method still performs relatively well. At this rate it is obvious that a true flame front solution

has not been established. As the puff rate goes higher, the PGS method fails. At this stage a switch to the LGS method is required.

Table 5.9 shows that as f_{puff} increases total CPU time also increases. The total time for each f_{puff} is relatively high, but if the CPU time for Γ_4 is neglected than the total CPU time becomes reasonable. Without Γ_4 , the total CPU time for the two selected puffing fractions are 679.6(PGS), 719(LGS), 0(PGS) and 1030.8(LGS) seconds respectively. A similar characteristic, in terms of CPU time as was found in the base case and impurity simulations, illustrating the competitiveness of the PGS and LGS methods. When the PGS method works, its CPU time is slightly better than for the LGS method. But for high f_{puff} , the superiority of the LGS method is obvious.

The physical solutions show that (figures 5.24 and 5.25) as f_{puff} increases the peak plasma density is shifted toward the private flux region. This is due to the fact that neutrals are introduced through the private flux region. The peak plasma density at the outer divertor plate is again consistently higher than at the inner divertor plate. The electron temperatures are also higher at the outer divertor leg than at the inner divertor leg. In this simulation the observation of the divertor plates performance is focused only at the outer divertor. The reason is that the heat flux at the outer divertor is higher than at the inner divertor. It is obvious that from figures 5.26 and 5.27 that the incoming heat flux and the electron temperatures at the divertor plate is reduced substantially. At $f_{puff} = 3 \times 10^{21}$, the peak heat flux, which is about $6 - 7 \text{ MW/m}^2$, is essentially within the thermomechanical limitation of the divertor material. The power balance (table 5.10) shows that unlike the impurity simulation, the total energy at the plates can not be reduced as effectively as in the impurity simulation. During the puffing process, due to higher number of plasma particles, the energy per particle is low. However, the number of particles is high, leading to a condition where the heat flux is still relatively high than in the impurity radiation. At maximum f_{ouff} , table 5.10 shows also that 73% of the incoming energy is converted to the $H\alpha$ radiation. With the above gas puffing scenario, our simulations indicate that

beyond 3×10^{21} particles/s, there appear to be no solutions. This will be the subject of the next section, where numerical stability considerations will be addressed. As indicated at the beginning of this chapter, this phenomenon has also been observed by others. However, as of to date, based on the available information, there has been no thorough investigation on this phenomena.

5.4 Numerical Stability

As stated above, in our gas puffing simulations, it is found that for Γ_o above 3×10^{21} , no converged solution on any given grid was found. At this level of puffing the residuals essentially oscillate between 10^{-1} to 10^{-4} . As this indicates an absence of equilibrium solutions, it was decided that the stability of solutions for lower values of Γ_o must be investigated. This was done by introducing time dependence and perturbing the obtained equilibrium solutions.

The first step is carried out by perturbing the converged solution for Γ_o equals 2×10^{21} and 3×10^{21} respectively. The converged solutions of electron temperature and plasma density are perturbed by about 10%. At the coarsest grid, the perturbed solution is used as an initial guess for the corrector step. Within the multigrid cycle, the solutions of grid Γ_2 and Γ_3 are also perturbed. The perturbed solutions are assumed to be the converged solutions from the previous coarse grid. The determining value of the status of the solutions is the peak electron temperature at the outer diver-tor plate. Obviously, when there is no change in the solutions after the perturbation, the solution is considered to be stable.

Within the continuation process, as in the previously unperturbed solutions, the same values are found at $\Gamma_o = 2 \times 10^{21}$. The difference is only at the 7th and 8th significant digits. For $\Gamma_o = 3 \times 10^{21}$, the perturbation is done in a more systematic manner. At this point, the plasma density is perturbed in two ways, i.e., multiplying the converged solution by 110% and 90% respectively. An identical process is performed on the electron temperature. The first set consists of a higher plasma

density and a lower electron temperature (S_1) and the second set consists of a lower plasma density and a higher electron temperature (S_2). For the set S_2 the solution apparently comes back to the original solution, but not for the case of S_1 . When $f_{pu\text{ff}} = 2 \times 10^{21}$ the direction of the perturbation does not affect the performance, i.e., both return the perturbed solution exactly to the initial state. The outer divertor peak electron temperature for $f_{pu\text{ff}} = 2 \times 10^{21}$ is found to be exactly 3.45 eV for both prior to and after the perturbation, indicating that the solution at this stage is stable. This is not the case for the set S_1 . The residuals for the S_1 case show an identical behavior as when $f_{pu\text{ff}}$ goes above 3×10^{21} , i.e., the residuals oscillate, indicating an absence of equilibrium solutions.

Within the multigrid cycle, an identical situation occurs. For $\Gamma_o = 2 \times 10^{21}$, the solutions at levels Γ_2 and Γ_3 are basically unaffected by the perturbation. The outer divertor peak electron temperature essentially remains exactly 3.76 eV for both prior to and after the perturbation. This is not the case for the high Γ_o , in which the S_2 set brings the solutions back to the original values but S_1 is seen to oscillate indefinitely.

Both methods (continuation and multigrid) show that there is a possibility that beyond $\Gamma_o = 3 \times 10^{21}$ the solution ceases to exist. The oscillating behavior of the residuals indicates that time may have a significant affect on the solution. This leads to the next stability analysis, where a time dependent term is added to each equation. Due to the structure of the code, the transient analysis is performed only on the coarsest grid.

With the addition of the transient term, equation 2.1 now is expressed as :

$$\frac{\partial \vec{T}}{\partial t} + \frac{\partial}{\partial x}(\vec{C}_x - \vec{D}_x \frac{\partial \vec{\Psi}}{\partial x}) + \frac{\partial}{\partial y}(\vec{C}_y - \vec{D}_y \frac{\partial \vec{\Psi}}{\partial y}) = \vec{S} \quad (5.1)$$

where $\frac{\partial \vec{T}}{\partial t}$ is defined as :

$$\vec{T} = \begin{bmatrix} n \\ \frac{3}{2}nT_i \\ \frac{3}{2}nT_e \\ mn u_{\parallel} \end{bmatrix} \quad (5.2)$$

A transient term of $\frac{\partial n_o}{\partial t}$ is also added to the neutral equations.

The next step is to assume that the solutions at $\Gamma_o = 3 \times 10^{21}$ are not stable, i.e., a transient simulation will be applied, with the aforementioned Γ_o solutions to be used at initial solutions (t_o). The results indicate that the exact same solutions are obtained leading to the conclusion that the solutions are stable. An identical process is also performed on lower f_{puff} values, and these solutions are stable as well. The difference usually occurs at the 8th or 9th decimal points of the electron temperature, a negligible effect on the overall solution. However, when the solution of $f_{puff} = 3 \times 10^{21}$ is used as an initial guess (t_o), no solution can be found. This is a second indication that a solution beyond $f_{puff} = 3 \times 10^{21}$ does not exist.

While further work, possibly involving a detailed stability analysis, will be necessary to obtain a full understanding of the disappearance of solutions at high puff rate, we have noted that radiation plays an important role. In figure 5.28 it is seen that if at $\Gamma_o = 3 \times 10^{21}$, which is the critical value for the existence of solutions, the radiation losses due to the $H\alpha$ are eliminated, the solution space can be extended to larger puff rates. In fact we have not found another hard boundary beyond which solutions again cease to exist, in the absence of radiation. However, radiation cannot be the complete story because similar behavior was not seen when impurity radiation was included, up to almost 100% radiation of the incident power flux. We believe that particle balance must play a significant role as solutions are obviously dependent on the rate of which particle are exhausted. More work is necessary in this subject.

Table 5.3: Peak electron temperature at inner and outer divertor plate as a function of ϵ (for $D_{\perp} = 1.00 - 1.333 \text{ m}^2/\text{s}$)

Divertor Plate	$\epsilon = 1.0^{-9}$	$\epsilon = 1.0^{-15}$
Inner	10.3244652697844	10.3244652697833
Outer	13.0253435294325	13.0253435294381
Total Iterations, time (s)	18, 136.5	31,254.3

Table 5.4: Comparison of convergence history between PGS and LGS relaxations, $\epsilon = 10^{-9}$, (iterations and time, sec)-reference case

Level	PGS	LGS
$\Gamma_o = 32 \times 6$	from continuation	from continuation
$\Gamma_1 = 64 \times 12$	18, 47.8 (slow)	22, 56.5
$\Gamma_o = 32 \times 6$	21, 28.5	-
$\Gamma_1 = 64 \times 12$	24, 44.9	-
$\Gamma_2 = 128 \times 24$	27, 81.3	31, 98.6
$\Gamma_3 = 256 \times 48$	28, 148.2	24, 191.2
$\Gamma_4 = 512 \times 96$	29, 279.4	26, 306.8
Total time	630.1	653.1

Figure 5.7: Outer leg neutral density profile for diffusion single energy model, FFCD with molecules and FFCD without molecules

Figure 5.8: Component of neutral density profile near outer divertor plate

Figure 5.9: Convergence behavior of diffusion model and FFCD model

Table 5.5: Corrector step (Newton's iterations) numerical performance for impurity simulation ($\epsilon \leq 10^{-9}$). Superscript * indicates selected values for comparison.

$\Delta\lambda$	TP
$\Delta f_{imp} = 0.5$	Iterations
$f_{imp,1}^* = 0.5$	19
$f_{imp,2} = 1.0$	25
$f_{imp,3} = 1.5$	27
$f_{imp,4} = 2.0$	32
$f_{imp,5} = 2.5$	33
$f_{imp,6}^* = 3.0$	35
$f_{imp,7} = 3.5$	36
$f_{imp,8} = 4.0$	35
$f_{imp,9} = 4.5$	37
$f_{imp,10} = 5.0$	35
$f_{imp,11} = 5.5$	34
$f_{imp,12} = 6.0$	32
$f_{imp,13} = 6.5$	31
$f_{imp,14} = 7.0$	31
$f_{imp,15} = 7.5$	32
$f_{imp,16}^* = 8.0$	30
Total iterations	504
Total time, s	619.13

Table 5.6: Comparison of convergence history between PGS and LGS relaxations for impurity simulation with $\epsilon = 10^{-9}$, (iterations and time, sec). Solution at Γ_o is obtained from the continuation process

Level	$f_{imp} = 0.5\%$		$f_{imp} = 3\%$		$f_{imp} = 8\%$	
	PGS	LGS	PGS	LGS	PGS	LGS
Γ_1	37, 98.3 (slow)	43, 126.5	64, 197.3	74, 216.5	72, 227.8	82, 256.5
Γ_o	245, 460.3 (stalled)	-	221, 376.5 (stalled)	-	243, 407.2 (stalled)	-
Γ_1	-	-	-	-	-	-
Γ_2	-	88, 293.1	-	113, 327.3	-	123, 367.8
Γ_3	-	127, 304.6	-	154, 495.2	-	160, 510.3
Γ_4	-	154, 462.3	-	161, 700.2	-	169, 778.2
Total time	-	1186.5	-	1739.2	-	1912.8

Figure 5.10: Outer divertor electron temperatures for $f_{imp} = 0.5, 3, 8\%$

Figure 5.11: Inner divertor electron temperatures for $f_{imp} = 0.5, 3, 8\%$

Figure 5.12: Plate to plate electron temperatures for $f_{imp} = 8\%$

Figure 5.13: Outer divertor plasma densities for $f_{imp} = 0.5, 3, 8\%$

Figure 5.14: Outer divertor mach number for $f_{imp} = 0.5, 3, 8\%$

Figure 5.15: Inner divertor plasma densities for $f_{imp} = 0.5, 3, 8\%$

Figure 5.16: Inner divertor mach number for $f_{imp} = 0.5, 3, 8\%$

Figure 5.17: Outer divertor electron temperatures

Figure 5.18: Outer divertor heat flux

Figure 5.19: Inner divertor electron temperatures

Figure 5.20: Inner divertor heat flux

Table 5.7: Power balance for impurity simulation (MW)

Level	Impurity fraction		
	0.5%	3%	8%
Incoming	145.23(100%)	146.26(100%)	149.61(100%)
Plates	48.98(34%)	4.52(3%)	0.56(0.4%)
Impurity	70.43(48%)	118.32(80%)	146.78(98%)
H2- α	25.82(18%)	23.42(17%)	2.27(1.6%)

Table 5.8: Corrector step (Newton's iterations) numerical performance for gas puffing simulation ($\epsilon \leq 10^{-9}$). Superscript ⁺ indicates selected values for comparison

$\Delta\lambda$	TP
$\Delta f_{puff} = 0.1667$	Iterations
$f_{puff,1} = 0.1667$	25
$f_{puff,2^*} = 0.3333$	34
$f_{puff,3} = 0.5$	41
$f_{puff,4} = 0.6667$	52
$f_{puff,5} = 0.8333$	53
$f_{puff,6^*} = 1.0$	75
Total iterations	280
Total time, s	491.03

Figure 5.21: Outer divertor leg radiation loss

Figure 5.22: Plate to plate radiation loss, $f_{imp} = 8\%$

Table 5.9: Comparison of convergence history between PGS and LGS relaxations for gas puffing with $\epsilon = 10^{-9}$, (iterations and time, sec). Solution at Γ_o is obtained from the continuation process

Level	$f_{puff} = 1.0 \times 10^{21}$		$f_{puff} = 3.0 \times 10^{21}$	
	PGS	LGS	PGS	LGS
Γ_i	28, 68.8 (slow)	33, 86.4	44, 127.7 (slow)	53, 146.5
Γ_o	33, 87.3	35, 95.3	48, 146.5 (stalled)	58, 163.9
Γ_1	32, 84.1	-	-	-
Γ_2	48, 189.3	49, 193.1	-	63, 225.2
Γ_3	54, 250.1	57, 344.2	-	84, 495.2
Γ_4	55, 291.4	64, 362.5	-	101, 590.5
Total time	971.0	1081.5	-	1621.3

Figure 5.23: Neutral gas puffing configuration

Table 5.10: Power balance for gas puffing simulation (MW)

Level	Gas puffing ^{rate} fraction, $\times 10^{-21}$		
	1	2	3
Incoming	125.16(100%)	125.92(100%)	127.76(100%)
Plates	75.2(60%)	64.71(51%)	34.18(27%)
H. - α	49.96(40%)	61.21(49%)	93.58(73%)

Figure 5.24: Electron temperature as a function of f_{puff}

Table 5.11: Particle balance for gas puffing simulation (particles/s)

Level	Gas puffing fraction		
	1%	2%	3%
Incoming	5.34e21	5.33	5.31e21
Pumping	6.34e21	7.33e21	8.31e21
Puffing	1.00e21	2.00e21	3.00e21

Figure 5.25: Plasma density as a function of f_{puff}

Figure 5.26: Outer divertor plate temperature

Figure 5.27: Outer divertor heat flux

Figure 5.28: Outer plate peak electron temperature (with and without ionization term)

Chapter 6

Summary, Conclusions and Future Work

6.1 Summary and Conclusions

In this work, it has been shown that, for the given sets of parameters (transport coefficients), the Tangent-Predictor (TP) continuation method, which was used in the coarsest grid, works remarkably well. The problems in finding an initial guess that resides well within Newton's method radius of convergence are alleviated by correcting the initial guess (usually based on a known converged solution) by the predictor step of the TP method. The TP method works well also in neutral gas puffing and impurity simulations. The neutral gas puffing simulation is performed by systematically increasing the fraction of puffing rate according to the TP method until it reaches a desired condition. Similarly, the impurity simulation characterized by using the fraction of impurity density as the continuation parameter, is carried out in line with the TP method. Both methods show, as expected, a better performance than the classical embedding (CE) method. The convergence criteria ϵ is set to be 10^{-9} based on the fact that lower value of ϵ does not alter the solution significantly. Correspondingly, the number of Newton's iterations in the corrector step of the TP method decrease substantially, an *extra point* in terms of code speed. The success of

the TP method enlarges the possibility of including other sets of parameters (operations and physics). With the availability of the converged coarsest grid solution, the next forward step to the multigrid cycle becomes possible.

The multigrid method shows that the memory storage problems that plagued the application of Newton's method on fine grids, are of no concern. The mesh sequencing process, if necessary, can be extended to ultra fine grids (larger than 512×96). With the dynamic development of edge plasma atomic physics often requiring dense computational grids, the multigrid method can serve as a useful tool. Two relaxation processes are used as a smoother within the multigrid cycle, namely the Point Gauss-Seidel (PGS) and the Line Gauss-Seidel (LGS) techniques. The LGS method is implemented with the intention to include implicitness in the smoothing process. The results show that the PGS method works remarkably well when there is no gas puffing or impurity radiation. However, when high puffing rates and high fraction of impurity are applied, the PGS method fails to yield converged solutions. The switch to the LGS method clearly shows that for edge plasma problems with flame front, this method is superior than the LGS method, a clear indication that implicitness is a critical issue. The LGS shows also that within the multigrid cycle no revisit to coarse grid is needed, leading to a mesh sequencing process in which the LGS method is essentially identical to the upward process of the full multigrid method. Within the framework of the governing equations used in this research, by observing the electron temperature profile at the divertor plate, it is obvious that a grid size of 256×48 is adequate.

The physical solutions show that when gas puffing rate is high enough, the electron temperature near the divertor plates is essentially collapsed. At this stage, the peak heat flux at the divertor plates is well within the thermomechanical limit of the divertor material, a desired condition for divertor operation. An identical situation exists when high impurity fraction is applied. The radiation loss due to line radiation is so dominant that the electron temperatures at the whole SOL region are collapsed. At high impurity fractions (5 – 8%), the number of iterations within the multigrid

cycle are basically constant. This is due to the fact that above 5%, there is almost no change in the overall solution (all collapsed). The peak heat flux at the divertor plates is essentially below 1 MW/m^2 , an ideal condition for tokamak reactor.

An important result that needs to be noted here is the performance of the FFCD model. The FFCD model is relatively simple and is based on the overall results the model has shown to predict different divertor plasma parameters. The FFCD model, treats exactly the implementation of the deep penetration of energetic neutrals emerging from the divertor plate. The resulting ionization profiles are relatively smooth as a consequence of the less localized recycling, leading to an improved convergence rate of the numerical algorithm. Peak plasma density is lower and the temperature correspondingly higher than those predicted by the standard diffusion model. It is believed that the FFCD model is more accurate.

The gas puffing simulation results indicated that for a puff rate of approximately above 3×10^{21} converged solutions on any grid cease to exist. However, when $H\alpha$ radiation is eliminated, the solution space is recovered and it can be extended to larger puff rates. At this time, we do not believe that $H\alpha$ radiation is the only primary cause of the solution disappearance. As more studies are needed, other factors such as particle balance or others may have a significant role.

With both the TP continuation and multigrid methods, we have demonstrated the robustness of these two methods. A mutually beneficial hybridization between the TP method and multigrid methods is clearly an alternative for edge plasma simulation. While the fundamental transport model considered in this work has ignored important physics such as drifts and currents, we have nevertheless demonstrated the versatility and robustness of our numerical scheme to handle such new physics. The application of gaseous-radiative divertor model in this work is just a beginning and up to this point numerically, the future is exciting.

6.2 Future Work

The application of the TP method clearly opens up the possibility of testing any future sets of parameters. The dynamics of atomic physics is progressive and challenging. A steady state ITER analysis can be performed routinely with little difficulty. Thus, in the future, the TP method is assured to facilitate simulation on a vast range of system parameters in a robust manner. The extension of impurity simulation to account for two-dimensional variation of the impurity density is an obvious next step. This extension conceptually should not pose any problem to the numerical performance since an identical impurity fraction can be used to control the radiation loss in the electron energy equation.

In the context of the FFCD model, perhaps the most advanced and useful implementation of the first flight concept would be in the generation of first flights by Monte Carlo simulation. The advantage of this approach is that realistic wall geometry can be modeled accompanying the detailed surface and atomic data bases. In this way, complete and accurate energy-angular distributions and species type from all solid boundaries in contact with the edge plasma and their transport to the first interaction can be incorporated virtually exactly. However, the numerical robustness in terms of CPU time savings remains a sticking point that needs to be thoroughly investigated.

From a numerical point of view, with the inclusion of impurity simulation, the realm of numerical experiments expands significantly. With respect to the multigrid method there are two possible expansions which can be implemented. The first expansion is implementing the adaptive multigrid method. This expansion is very useful in tracking down the region of the highest radiation. Typically this region will be a few centimeters away from the divertor plates where the computational points may need to be very dense. To be computationally (CPU) effective, the calculations should be contained within this region. The implementation of adaptive multigrid method essentially lifts the domain of numerical complexity to a higher level. The adaptive

method appears rather complicated yet in relation with the gaseous-radiative divertor it can be extremely useful. The second expansion is to include a continuation method within the multigrid cycle. Again, the degree of complexity is high because this type of method has not been implemented widely. The safest starting point will be to implement the multigrid continuation on the basic equations. The application of this method is guaranteed to be very significant not only to the edge plasma community but to the multigrid community as well.

Within the multigrid cycle itself, the expansion of the relaxation method can be an additional benefit. The first obvious step is to apply the LGS method in the poloidal direction. The next step is to implement the Red-Black PGS method. ~~This method~~ This method has been found to be useful in some complex fluid dynamics problems. The Red Black PGS is also an extremely efficient smoother for parallel machines. As physical complexity increases, a robust relaxation may be needed to smooth out the multigrid error efficiently.

Finally, in the context of solution stability and the existence of multiple solutions, the arclength path following continuation method must be implemented. Unlike the TP method, an arclength parameter must be established as the continuation parameter. This method guarantees convergence even if the Jacobian matrix is ill-conditioned. The application of the arclength method is commonly and widely used for the chaotic problems. With this in hand, any folding curves or bifurcation points can be traced and detected accurately.

Appendix A

Coding Structure of NEWEDGE-MG

NEWEDGE-MG is written in such a way that future additions of physical models or extension of numerical scheme can be inserted relatively easily. Each discretized governing equation is written modularly, so that it is easily callable from both the Newton with continuation and multigrid routines. The coding structure of NEWEDGE-MG is shown in figure A.1.

Figure A.1: Coding Structure of NEWEDGE-MG

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