Impurity accumulation and performance of ITER and DEMO plasmas in the presence of transport barriers

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Abstract. In this work, the impurity accumulations and their performance in the presence of both ITB and ETB in ITER and DEMO plasmas are investigated using a BALDUR integrated predictive modelling code. In these simulations, a combination of a neoclassical transport model NCLASS and an anomalous transport model Mixed Bohm/gyro-Bohm is used. The boundary condition is described at the top of the pedestal, which is calculated theoretically based on a combination of magnetic and flow shear stabilization pedestal width scaling and an infinite-n ballooning pressure gradient model. The toroidal flow is calculated based on the NTV (neoclassical toroidal viscosity) toroidal velocity model. The time evolution of plasma temperature and density profiles of ITER and DEMO (Korean K-DEMO and Japanese DEMO models A, B and C) plasmas are simulated in H-mode scenario with and without ITB formation. It is found that Japanese DEMO model C yields highest plasma temperature; while Korean DEMO yields the best plasma performance among those designs considered. Impurity accumulation is found to be highest in Japanese DEMO model B.

1. Introduction
Generally, the fusion reactions in tokamak experiments can be improved with the increase of plasma density, temperature and confinement time. It was discovered that when the plasma made a transition to a high confinement mode (H-mode), resulting from formation of an edge transport barrier (ETB), the plasma performance is significantly increased [1, 2]. The performance of the plasma can be further enhanced with the formation of an internal transport barrier (ITB) in the plasma core [3]. The formation of transport barriers is very important that the burning plasma experiment like ITER project [4] is designed to perform in H-mode operational regime. Furthermore, in the next step of fusion experiments, the DEMO experiments must operate based on advance scenario. In other words, both ITB and ETB must be simultaneously formed and sustained, so the plasmas are able to operate in a steady state fashion.

Density control is one of the essential parts for burning plasma in a fusion reactor. Impurity particles are composed of two different sources: intrinsic helium which is a product of deuterium-tritium reaction and impurities that come from plasma-wall interaction process such as beryllium, carbon, tungsten etc. Impurity accumulation can severely detriment fusion performance because these particles dilute the plasma and radiate energy away from the plasma core [5]. Experimentally, it was found that formation of ITB lead to impurity accumulation in the plasma core. For example, in JT-60U reverse shear experiments, strong peak impurity (argon and carbon) density profile was observed [6].
The helium density was not observed to be strongly peaked because it has low Z value [7]. Hence, the helium diffusivity and convection velocity found by JT-60U team illustrated that there was sufficient exhaust even in the plasma with ITB formation [8].

In this paper, a 1.5-dimensional BALDUR integrated predictive modelling code is used to simulate the time evolution profiles of electron and ion temperatures and electron, hydrogenic and impurity densities for ITER- and DEMO-like plasmas. ITB formation is simulated through a semi-empirical transport model called Mixed Bohm/gyro-Bohm. The model assumes that ITB formation occurs when anomalous transport is quenched due to flow shear and magnetic shear stabilization [9]. The flow shear is calculated from the radial electric field through the force balance equation, where toroidal rotation term is needed. In this work, a theoretically based toroidal velocity model is calculated based on NTV concept [10]. ETB formation is modelled based on the works in Ref. [11], where ETB is calculated using a pedestal model. The pedestal temperature is determined using a pedestal width model with pressure gradient limits ballooning mode instability. The simulation results will examine plasma performance, i.e. electron and ion temperature and impurities density.

The paper is organized as follows: the simulation setup as well as the important models used are introduced in section 2; simulations results of ITER and DEMOs and discussion are given in section 3; and the conclusion is presented in section 4.

2. BALDUR and Simulations Setup
All simulations in this work are carried out using an 1.5D BALDUR integrated predictive modelling code[12]. BALDUR is a time-dependent transport modelling code, which can compute tokamak plasma quantities such as electron and ion temperatures, electron, hydrogenic and impurities densities, safety factor $q$ and toroidal flow [13, 14]. The code self-consistently computes those physical quantities by combining several physical processes together in form of modules. Important modules used by BALDUR are transport, plasma heating, particle flux, boundary conditions and sawtooth oscillations modules. This section discusses the three main modules used in the simulations: neoclassical transport module, toroidal velocity module and pedestal module. In short, BALDUR calculates the plasma profiles by solving the transport equations. The transport is composed of neoclassical transport module, computed by NCLASS, and anomalous transport, where the diffusivities are calculated using Mixed Bohm-Gyro-Bohm model (section 2.1). The toroidal velocity is an ingredient needed to compute the anomalous transport; it is calculated based on neoclassical toroidal viscosity (NTV) physics (section 2.2). The boundary of the transport equations are set at the top of pedestal, where its value is calculated based on a pedestal model (section 2.3).

2.1. Mixed Bohm/Gyro-Bohm model
In this work, an anomalous transport at the core of the plasma is modelled using a semi-empirical transport model called mixed Bohm/gyro-Bohm (Mixed B/gB) [9]. This version of Mixed B/gB includes ITB formation modelling based on the well-known assumption that ITB can form when the anomalous transport is suppressed by the $\omega_{\text{Bx}}$ flow shear and magnetic shear [9]. ITB effect is implemented using a cut-off Heaviside function in the Bohm term. The model computes electron diffusivity $\chi_e$, ion diffusivity $\chi_i$, hydrogenic diffusivity $D_H$ and impurity diffusivity $D_Z$ as follows:

$$\chi_e = 1.0 \chi_{gb} + 2.0 \chi_B,$$

$$\chi_i = 0.5 \chi_{gb} + 4.0 \chi_B,$$

$$D_H = D_Z = \left(0.3 + 0.7 \rho\right) \frac{\chi_e \chi_i}{\chi_e + \chi_i},$$

where

$$\chi_{gb} = 5 \times 10^{-6} \sqrt{T_e \left| \frac{\nabla T_e}{B^2} \right|}.$$  

(4)
\[ \chi_B = \chi_{B0} \times \Theta \left( -0.14 + s - \frac{1.47 \omega_{E-B}}{\gamma_{ITG}} \right), \quad (5) \]

\[ \chi_{B0} = 4 \times 10^5 R \left( \frac{n_e T_e}{n_i B_\phi} \right)^2 \left( \frac{T_e (0.8 \rho_{max}) - T_s (\rho_{max})}{T_s (\rho_{max})} \right), \quad (6) \]

where \( \chi_{B0} \) is the gyro-Bohm contribution, \( \chi_B \) is the Bohm contribution, \( \rho \) is normalized minor radius, \( T_e \) is the local electron temperature in keV, \( B_\phi \) is the toroidal magnetic field, \( s \) is the magnetic shear, \( \omega_{E-B} \) is the shearing rate, \( \gamma_{ITG} \) is the linear growth rate, \( R \) is the major radius, and \( n_e \) is the local electron density. The linear growth rate \( \gamma_{ITG} \) can be calculated as \( \nu_0 / qR \), where \( \nu_0 \) is the electron thermal velocity.

The \( \omega_{E-B} \) shearing rate can be calculated as [15, 16]:

\[ \omega_{E-B} = \frac{B_\theta^2}{B_\phi} \frac{\partial (E_r / B_\phi)}{\partial \psi}, \quad (7) \]

where \( B_\theta \) is the poloidal magnetic field, \( \Psi \) is the poloidal flux, and \( E_r \) is the radial electric field, which can be calculated as follows:

\[ E_r = \frac{1}{Ze n_i} \frac{\partial p_i}{\partial r} - v_\theta B_\phi + v_\phi B_\theta \]

where \( p_i \) is plasma pressure, \( v_\theta \) and \( v_\phi \) are the poloidal and toroidal velocities, respectively, \( n_i \) is the ion density, and \( Z \) is the ion charge number. The poloidal flow is estimated using NCLASS module, while the toroidal flow is calculated as discussed in section 2.2.

2.2. Toroidal velocity model

According to equations (7) and (8), the toroidal velocity is one of the elements needed for the suppression of anomalous transport by the flow shear, leading to ITB formation. The model used in this work is based on NTV physics, where the offset toroidal rotation is caused by the neoclassical toroidal viscosity dissipation. This dissipation is a result of symmetry breaking generated by a non-axisymmetric field [17]. Additionally, the rotation is theoretically described to be intrinsic, hence its existence is crucial for enhancement operation of tokamak experiments. The development and implementation of the model into BALDUR code can be seen in Ref. [10], where a local and strong ITB is to be expected in ITER. In short, the model is in the form:

\[ v_\phi \propto \frac{dT_i}{dr}, \quad (9) \]

implying that the rotation is driven by local ion temperature gradient.

2.3. Pedestal model

Throughout this work, the boundary condition for the transport equations is set to be at the top of the pedestal [18]. This is the location where the edge transport barrier (ETB) is observed. So all simulations are set to be in \( H \)-mode operation regime. The pedestal region is the edge area of the plasma with steepest gradient compared to other regions. The pedestal temperature \( T_{ped} \) is calculated as follows:

\[ T_{ped} = \frac{1}{2k n_{ped}} \Delta \left| \frac{\partial p}{\partial r} \right|, \quad (10) \]

where \( n_{ped} (m^{-3}) \) is pedestal density, \( k \) is the Boltzmann’s constant, and \( \Delta \) is the pedestal width. Details of the models can be seen in Ref. [11]. In essence, the pedestal pressure gradient and pedestal width are limited by the ballooning mode instability and the magnetic and flow shear stabilization [19, 20].
Note that the pedestal density is empirically assumed to be a fraction (0.71) of electron line average density [21].

3. Results and Discussions

3.1. ITER simulations

In this work, standard type I ELMy H-mode ITER simulations are investigated using BALDUR. The design parameters used in the simulations are: major radius $R$ of 6.2 m, minor radius $a$ of 2.0 m, plasma current $I_p$ of 15.0 MA, toroidal field of 5.3 T, elongation $\kappa$ of 1.7, triangularity $\delta$ of 0.33, RF (radio frequency) heating of 7.0 MW, NBI (neutral beam injection) heating of 33.0 MW and line average density $n_l$ of 1.0x10^{20} m^{-3} [22]. Figure 1 illustrates simulation results of ITER-like plasma. The top left panel shows central ion temperature $T_i$ (top) and central electron temperature $T_e$ (bottom). It can be seen that initially the central temperatures are slowly increasing until around 100 seconds where the plasma has reach quasi-stationary state. This is because the plasma current has been set to slowly increase to the designated value. At quasi-stationary state, the temperatures are fluctuated around 10% of their average values. This is due to sawtooth instability, which occurs at the center of plasma. Quantitatively, the ion temperature fluctuates around 40 keV and electron temperature around 35 keV.

![Figure 1](image1.png)

Figure 1. Time evolution of temperatures at plasma center (top left), transport diffusivities (top right) and plasma density and temperature profiles during quasi-stationary state (bottom) for ITER.

The bottom panels of figure 1 illustrate profiles of ion temperature, electron temperature, deuterium density ($n_D$), tritium density ($n_T$), beryllium density ($n_{BE}$), and helium density ($n_{HE}$) as a function of normalized minor radius $r/a$ at arbitrary time during quasi-stationary state (2,900 seconds). Note that units of densities are 1x10^{19} m^{-3} for deuterium and tritium and 1x10^{18} m^{-3} for beryllium and helium. Obviously, the plasma temperatures are highest at plasma center and decrease toward the edge. It appears that a wide ITB are formed from $r/a = 0.2$ to 0.6. This agrees with the profiles of ion diffusivity $\chi_i$ and electron diffusivity $\chi_e$ as shown in the top right panel of figure 1. Moreover, deuterium and tritium densities have roughly the similar profiles, which is quite flat, just above 4x10^{19} m^{-3}, with strong gradient near the edge. Interestingly, beryllium is found to be able to penetrate into
the plasma core, though its profile is rather flat. Whereas, helium is found to accumulate in the plasma core so it is also affected by ITB formation.

3.2. DEMO simulations

Two different DEMO projects are investigated in this work: Korean DEMO (K-DEMO) and Japanese DEMO. The design parameters of K-DEMO used in simulations are $R = 6.8$ m, $a = 2.1$ m, $I_p = 12$ MA, toroidal field of 7.4 T, $\kappa = 2.0$, and $\delta = 0.625$ [23]. For Japanese DEMO, three different models are investigated; model A, model B and model C. The design parameters used in simulations can be seen in table 1 [24]. In addition to the parameter used in table 1, it is calculated that tokamak built by model C will have the most weight of 23,900 ton, while the tokamak built by model C will have the lowest weight of 15,700 tons. Example of DEMO simulations are shown in figures 2 and 3, which are the simulation results from K-DEMO and Japanese DEMO model C, respectively.

| parameter               | model A | model B | model C |
|-------------------------|---------|---------|---------|
| Major radius (m)        | 5.1     | 5.5     | 6.5     |
| Minor radius (m)        | 2.1     | 2.1     | 2.1     |
| Aspect ratio            | 2.5     | 2.6     | 3.1     |
| Elongation              | 2.05    | 2.0     | 1.9     |
| Triangularity           | 0.1     | 0.4     | 0.4     |
| Magnetic field (T)      | 5.6     | 6.0     | 6.8     |
| Plasma current (MA)     | 17.4    | 16.7    | 15.0    |
| Current drive power (MW)| 63      | 59      | 54      |

Table 1. Parameters used for simulations of Japanese DEMOs [24].

The top left panel of figure 2 shows that the plasma has reached quasi-stationary state at around 400 seconds. The ion temperature fluctuates around 45 keV and electron temperature around 40 keV. Furthermore, in K-DEMO a wide ITB formation can be found from $r/a = 0.1$ to 0.5 as illustrated by
the drop in diffusivities (top right panel of figure 2). It also appears that deuterium, tritium, and beryllium densities profiles are relatively flat, with a sharp gradient at plasma edge for deuterium and tritium. Similarly, helium is also accumulated inside the ITB.

![Figure 3: Time evolution of temperatures at plasma center (top left), transport diffusivities (top right) and plasma density and temperature profiles during quasi-stationary state (bottom) for Japanese DEMO model C.](image)

Figure 3 illustrates simulation results of Japanese DEMO model C. Evidently, the plasma has reached a quasi-stationary state after 300 seconds. The ion temperature fluctuates around 50 keV and electron temperature around 40 keV. Furthermore, in Japanese DEMO model C, a wide ITB formation can be found from r/a = 0.1 to 0.5 as illustrated by the drop in diffusivities (top right panel of figure 3). It also appears that deuterium, tritium, and beryllium densities profiles are relatively flat, with a sharp gradient at plasma edge for deuterium and tritium. Helium peaking profile is found inside the ITB.

### 3.3. Performance comparison

Table 2 summarizes the performance of each tokamak simulated in this work. Note that $W_{\text{TOT}}$ represents plasma total power yielded, $P_{\alpha}$ is alpha power, $P_{\text{aux}}$ is auxiliary heating power and Fusion Q is the ratio of the output power to the input power, which is used to represent plasma performance. It can be calculated as:

$$Q = \frac{5 \times P_{\alpha}}{P_{\text{aux}}}. \quad (11)$$

Overall, Japanese DEMO model C yields the highest temperatures at plasma center, while ITER yields the lowest. The same machine also yields highest fusion power ($W_{\text{TOT}}$), which includes both power from alpha and neutron particles, but Japanese DEMO model B yields the most alpha heating power. On the other hand, Japanese DEMO model A yields lowest fusion power and ITER yields the least alpha heating power. Nevertheless, considering for fusion performance is best through the fusion Q. Apparently, K-DEMO yields highest value of Q. This is because it uses less heating input of 40 MW, comparing to 54 MW used in Japanese DEMO model C. On the other hand, Japanese DEMO model A is the worst in term of fusion performance comparison. For impurity accumulation, it is found from
simulations that beryllium concentration at plasma center is highest in Japanese DEMO model B and lowest in ITER. Helium accumulation is highest in Japanese DEMO model B and lowest in K-DEMO.

Table 2. Comparison of simulation results from ITER and DEMOs (average values during quasi-stationary state).

| Parameters     | ITER  | K-DEMO | J-DEMO A | J-DEMO B | J-DEMO C |
|----------------|-------|--------|----------|----------|----------|
| $T_{i,0}$(keV) | 37.99 | 43.42  | 38.66    | 44.43    | 51.00    |
| $T_{e,0}$(keV) | 34.15 | 37.27  | 34.45    | 37.86    | 41.35    |
| $W_{TOT}$ (MW) | 426   | 441    | 404      | 461      | 534      |
| $P_{AUX}$ (MW) | 40    | 40     | 63       | 59       | 54       |
| $P_p$(MW)      | 133   | 153    | 151      | 187      | 176      |
| $Q$            | 16.63 | 19.13  | 11.98    | 15.85    | 16.30    |
| $n_{BE,0}$ ($10^{18}$ m$^{-3}$) | 3.03 | 3.12   | 3.90     | 4.01     | 3.37     |
| $n_{HE,0}$ ($10^{18}$ m$^{-3}$) | 4.13 | 3.59   | 4.25     | 5.16     | 5.02     |

4. Conclusion

Simulations of ITER, Korean DEMO and Japanese DEMO (models A, B and C) in the presence of both ITB and ETB are carried out using BALDUR integrated predictive modelling code. The core transport is predicted using NCLASS and Mixed B/gB models with the toroidal velocity predicted using NTV offset rotation model and the boundary condition predicted using the magnetic and flow shear stabilization width scaling and an infinite-n ballooning pressure gradient limiting model. The ITB formation is found in all simulations, resulting an increase of fusion reactions and, consequently, helium accumulation and a decrease of beryllium accumulation in the core. In general, the plasma starts with slowly ramp-up phase until quasi-stationary state is achieved, where plasma temperatures fluctuate around 10% due to the sawtooth oscillation. It is found that among the designs considered, the best plasma performance, based on Q value, is observed in K-DEMO even though Japanese DEMO model C yields higher plasma temperatures and total fusion power. On the contrary, Japanese DEMO model A yields lowest plasma performance among the designs studied. For future work, this set of codes can be used to also simulate the performance of other DEMO designs such as European DEMO, Indian DEMO and Chinese DEMO. Based on all results, the performance optimization of the future DEMO can be predicted.

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