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ABSTRACT.

This paper studies the effect of bundling groups of contiguous carbon and tungsten ionization stages on the calculated impurity screening. EDGE2D/EIRENE was used to calculate the charge state distribution in the SOL and the edge of the plasma core, which resulted from the puffing of either atomic carbon or tungsten at the JET outer mid-plane. The input parameters were constant for a number of code calculations where the only parameter changed was the number and/or charge states bundled in either carbon or tungsten. In this manner, the effect of bundling on the carbon or tungsten screening or fuelling efficiency was determined. For carbon and tungsten there was only a weak dependence upon the actual bundling scheme used.

INTRODUCTION

JET is changing from carbon plasma facing components to a tungsten divertor and a beryllium main chamber [1]. The SOL code EDGE2D has been used to describe many carbon phenomena in JET [2] and so, is also being upgraded to handle tungsten as well as tungsten/beryllium combinations. For example, JET methane injection experiments have helped to understand the carbon screening, contamination, and migration in JET. Self consistent models of carbon behaviour were developed using EDGE2D/NIMBUS and reasonably described many JET plasmas [3, 4]. This paper extends EDGE2D to describe tungsten screening which further required that EDGE2D be used in conjunction with the EIRENE neutrals code [5]. Future EDGE2D studies will describe W sputtering, migration, and W/Be interactions.

The large number of W charge states is a difficult computationally, and bundling [6-8] of the W charge states into groups of charge states has been attempted. Thus instead of solving all 74 ionizations stages of tungsten with their own separate conservation equations, the conservation equations of a smaller number of bundled charge states are solved, requiring fewer equations. This paper describes the consequences of bundling upon the calculated SOL behaviour and in particular the impurity screening, and attempts to determine the validity, if any, of EDGE2D for impurities with bundled charge states.

Since JET has a large experimental and computational data set of carbon screening, this paper follows the approach of Ref. 4 by first calculating the effects of bundling carbon on the carbon screening. The calculated carbon screening was reduced up to 10% of the unbundled carbon calculations. This reduction is considered to be insignificant.

For tungsten, the maximum number of states with stable calculation was 14, so that unlike carbon, a complete unbundled case could not be calculated. The reduced calculation stability is probably associated with the larger number of equations. Instead, a reference for the 12 lowest ionization stages was calculated using a case of individual charge states below 12 and all states above 12 in a single bundle. This reference was then compared to other cases where the 12 lowest stages were bundled into different combinations. The prediction of the charge state density of the 13-74 superstate was also reduced up to 10% by the bundling of the 12 lowest states. In some cases, the calculated screening was not reduced at all.

The results indicate that gross groupings will yield acceptable screening results for C or W. However, the highest (13-74) W bundle is not confined to the core, and extends significantly into the SOL. Thus uncertainty exists about the general applicability of the W results. Taking the extra uncertainty of bundling upon the calculation of impurity screening by EDGE2D to be the deviations form the unbundled cases, then the extra uncertainty is about 10% which is insignificant.

2. CHARGE STATE BUNDLING

EDGE2D is a fluid code which typically treats 1 ion fluid for deuterium, and all the ionization stages of up to two light impurities (e.g. carbon and helium). Inclusion of heavier impurities, in particular all 75 ionization stages of tungsten were not originally considered. The main issues are the calculation size limits, the stability of the calculation, and error propagation. The method used to reduce the number of equations to a manageable level is called bundling, by establishing a partition of the ionization stages into superstages [6, 7]. In this scheme, the number of equations is reduced to the number of partitions of ionization stages. The choice of which and how many states to compose the bundles is an open question which is the topic of this paper. "Natural partition" bundling schemes [6, 9] group together stages with similar ionization potentials. For tungsten, natural partition required 35 bundled stages which are too many for EDGE2D calculations. In this study, the EDGE2D code was not stable when more than 14 ionization stages were included for tungsten, and the calculations with 14 W stages were about 3 times longer to complete than calculations with only 3 W stages.

The EDGE2D modelling uses the charge, charge squared and the ionization potential from the individual ionization stages. For the bundled stages, these quantities are no longer constants for each ionization stage, but are functions of the local plasma electron temperature and density. The parameters of the bundled stage are developed by assuming coronal equilibrium inside the bundle [6]. Departure from coronal equilibrium is probably minimal in the plasma core but might be 20% in the SOL [4], so that some errors in the EDGE2D calculations areanticipated by using bundled ionization stages.

Part of the difficulty with modelling the SOL behaviour of any impurity is that highly ionized charge states exist in the SOL. Charge states appear when the electron temperature is greater than a fraction of the ionization potential. The fraction is about 1/3 for W and 1/5 for C [10]. The SOL electron temperatures are so large that even C^{6+} is produced in the JET SOL and W charge states of up to about 12 are produced (fig.1). Further, for the case studied here, the electron temperature increases by about 1keV in about 1cm in the edge transport barrier region (immediately inside of the separatrix). The barrier electron temperature gradient causes a source of highly charged W ions to exist close to the separatrix. These more highly ionized charge states can diffuse from the core and have a low recombination rate in the SOL. Thus an edge code such as EDGE2D must be able to describe the motion of highly ionized charge states. The calculations in this paper (e.g. fig.1) describe an ELM-free JET plasma with 8MW flowing into the SOL, a separatrix density of 1 10^{19} /m^3 and transport coefficients (1m^2/s in the core and SOL and 0.5 m^2/s in the barrier region) similar to those for H-Modes[11].

The existence of highly ionized carbon was experimentally observed (figure 2) in DITE and TEXTOR [12] where the difference in spectra between the two machines was assumed to be due to different observation location (being near the carbon source for DITE and distant for TEXTOR). A similar carbon charge state distribution at the EDGE2D grid edge was observed in JET EDGE2D calculations when carbon was introduced at either the outer mid-plane or the vessel top and observed at the outer mid-plane. In agreement with Ref 11, the charge state, the 1st and 2nd carbon ionization stages are localized to the vicinity of the injection while the higher stages (4-6) are more global. The agreement between the DITE and TEXTOR observations and the JET calculations indicates that the fundamental atomic physics must dominate the far SOL region and overcome the differences of limiter operation on DITE and TEXTOR as opposed to divertor operation on JET.

For tungsten, the charge states from 2-7 exhibit high localization, and the stages from 8-11 exhibit moderate localization, while the stages above 12 exhibit little localization (figure 3). The charge states above 12 also exist throughout the SOL. Thus, the impurity poloidal localization in the SOL is one factor to consider when deciding upon the bundling groupings. The poloidal localization of some charge states motivated attempts to bundle separately those charge states which are highly localized, from those which are more uniform in the SOL.

3. BUNDLING EFFECTS

In order to test the bundling concept, effects of bundling on the EDGE2D calculated carbon screening were calculated. The unbundled carbon screening was compared to the screening from the groupings of charge states in table 1. In each case, the first ionization stage is the one directly coupled to the Monte-Carlo neutrals code and has been kept as an individual ionization stage. Also the fully ionized carbon was chosen to be an individual ionization stage in order to compare the C^{6+} core densities for the differently bundled calculations (Table 1).

The bundling reduces the calculated core C^{6+} density (Fig.4) by up to 10%. In figure 4, the charge states 2 to 5 were bundled together and compared to the summation of the unbundled states 2+3+4+5. Since the 6th is populated by ionization from the lower states, then the errors accumulate and maximize in the density of the highest stages. The calculated carbon screening weakly changes with different groupings of charge states in the bundles. The screening differences are small and would usually be ascribed to the impurity cross-field diffusion coefficient [3] in the analysis of an actual experiment. Typically, the impurity diffusion coefficient is unconstrained in experiments.

The inability to compare the bundled with all 74 individual charge state W calculations, or even one where all the SOL charge states are treated individually, means that the reference is less accurate than the carbon reference. The approach taken here is to bundle states 1 to 12 individually and then bundle together stages 13-74. Now the effects of bundling the lowest 12 stages (in other calculations) could be referenced to this case and the effect of bundling in tungsten could be assessed.

The charge state spatial distribution of one example of bundle groupings is shown by the solid lines in figure 5. Charge states 2-7 are bundled together and represent the charge states concentrated in the outer SOL which are highly localized. The charge states 8-12 form the next bundle and these

are states which peak in the near SOL region. The charge states 13-74 form the core charge states. Figure 5 indicates that the 1st ionization stage is the same for the two calculations. For comparison, the charge state densities for the 3 bundles are re-composed (dashed lines in figure 5) from the individual charge states. In this manner, the solid line for 2-7 is the calculation of the 2-7 bundle while the dashed line is the sum of the individual charge state 2+3+4+5+6+7, essentially recomposing what the bundle should have been. In this case, although the 2-7 bundle is about 5% less than the re-composed density, and the 8-12 bundle is about 10% less than expected, the core bundle (13-74) is within a few %. The reason that the bundling reduces the density of say the 2-7 charge states even though the ionization into the singly ionized charge state is the same (fig. 5) is that the parallel motion of the bundled state to the divertor is different than the parallel motion of the individual states to the divertor. So, the bundled density is different than the sum of the individual densities since the impurity losses to the divertor are different.

For the bundling cases (Table 2) of the lowest 12 W ionization stages, the gross bundling (2-74 or F=.08) was about as accurate as any while reducing the number of impurity equations to a minimum.

SUMMARY

The screening (or fuelling efficiency) for the bundled cases is shown in figure 5 where the charge states are characterized by the fractional reduction of charge states (F = 1 indicates 8 unbundled or no reduction in the number of SOL impurity equations, while the minimum F indicates a reduction to 1 equation for the SOL charge states). Overall, the present work indicates that tungsten is better screened than carbon and beryllium (figure 6), and that the uncertainties in bundling tungsten or carbon will be about 10% which is insignificant.

ACKNOWLEDGEMENT

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C^+	C^{++}	C^{3+}	C^{4+}	C^{5+}	C^{6+}	F	Sc (%)
						1.0	4.5
						.75	4.3
						.5	4.6
						.5	4.5
						.5	4.5
						.25	3.9

Table 1. The solid areas indicate the individual charge states or bundles used in separate carbon screening calculations with EDGE2D. F describes the fractional reduction of the number of impurity equations, where F=1 means there is no reduction. The screening is a fuelling efficiency parameter and was discussed extensively in Ref [3].

W^+	W^{++}	W^{3+}	W^{4+}	W^{5+}	W^{6+}	W^{7+}	W^{8+}	W^{9+}	W^{10+}	W^{11+}	W^{12+}	W^{13-74+}	F	Sc (%)
													1.0	2.4
													.50	
													.42	2.5
													.28	2.8
													.18	
													.08	2.3

Table 2. The solid areas indicate the individual charge states or bundles used in separate tungsten screening calculations with EDGE2D as for table 1 with carbon.
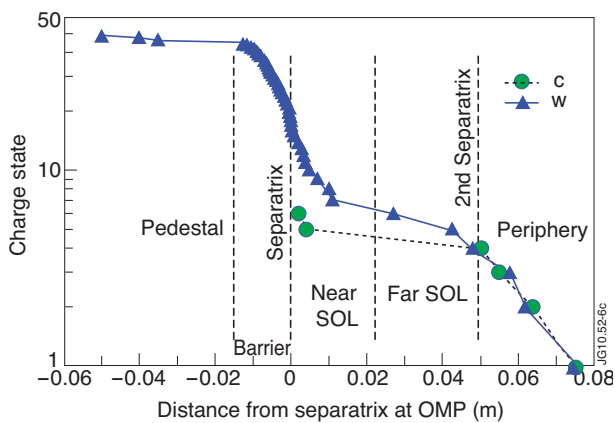

Figure 1: The ionization state charge number plotted against the radius where it willapproximately begin to be observed or the plasma studied. The EDGE2D grid edge is the location of the second separatrix. The boundary between the near and far SOL is determined primarily by the thermal force acting near the divertor entrance. The electron temperature at the top of the barrier was 1.2keV.
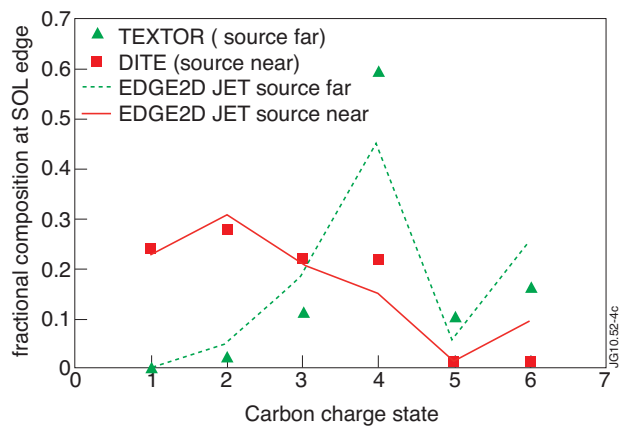
Figure 2: Fraction of each charge state to the total carbon at the edge of the SOL for DITE and TEXTOR measurements [12] while the lines at the EDGE2D calculations for JET when the carbon injection is either near or away from the observation location.
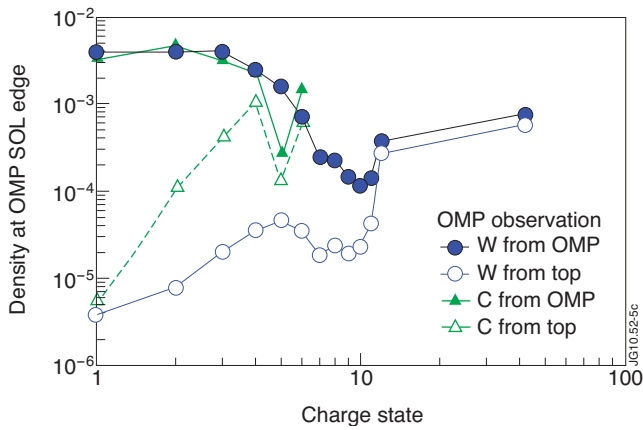
Figure 3: C and W density calculated by EDGE2D at JET SOL edge plotted against charge state number for injection near and away from observation location.
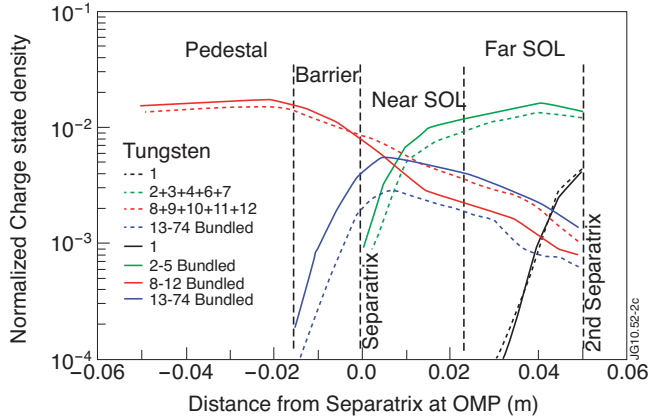

Figure 4: Spatial distribution of the C charge states observed at the JET outer mid-plane for C injected at the outer mid-plane. The solid lines are from an EDGE2D calculation where C was bundled as 1: 2-5; 6 while the dashed lines are for unbundled C where the 2+3+4+5 charge states were added together to re-construct the 2-5 bundle.
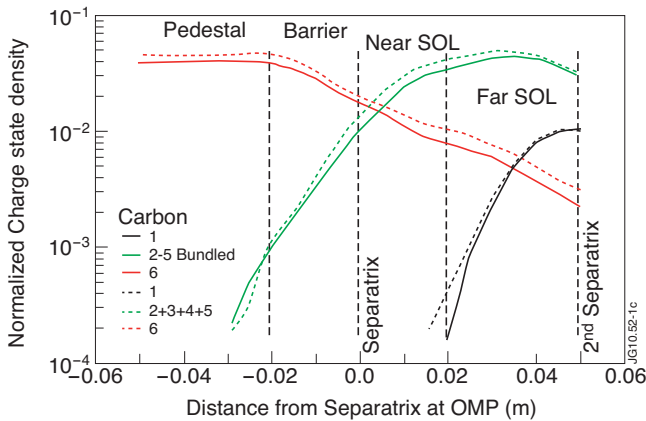

Figure 5: Spatial distribution of the W charge states observed at the JET outer mid-plane for W injected at the outer mid-plane. The solid lines are from an EDGE2D calculation where the W was bundled as 1: 2-7: 8-12: 13-74 while the dashed lines are for the W bundled with the 12 lowest states as individual states and 13-74 bundled together. The 12 lowest were then added to re-construct the 2-7 and 8-12 densities.
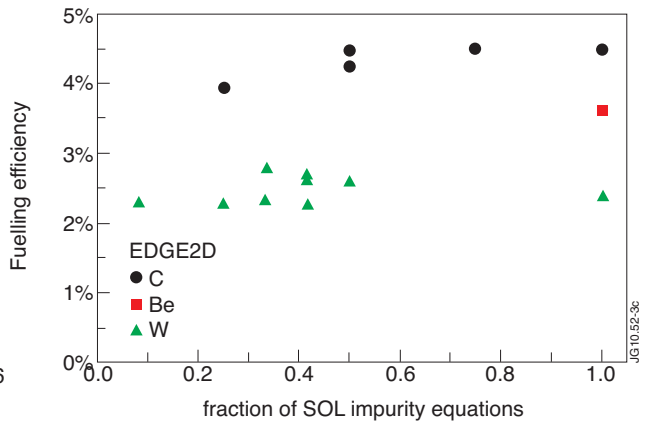

Figure 6: The impurity screening or fuelling efficiency from EDGE2D calculations plotted against the fractional reduction in the number of SOL impurity equations. Unity implies that there is no reduction, while smaller numbers indicate that greater numbers of charge states were grouped together (see tables 1 and 2).