Chapter 6

General conclusions and future work

6.1 General conclusions and summary

This thesis has presented a general investigation into spectral series emission and population modelling valid for both astrophysical and laboratory fusion plasmas. Starting with an overview of basic escape factor techniques, their usefulness in modelling opacity effects on population structure and emergent flux was shown within the context of four sets of observations. A branching line ratio study of the solar atmosphere demonstrated the use of escape probabilities as an optical depth diagnostic. Observations of the L_β/H_α ratio from the divertor region of the ASDEX upgrade showed the use of absorption factors in calculating optically thick population densities. Series limit observations of solar prominences and the JET divertor highlighted the possibility of developing a spectral feature code as an electron density, temperature and plasma recombination state diagnostic.

A thorough treatment of low series member opacity was then developed in association with the conversion of the code of Behringer into ADAS 214. The use of the new code in the CDS line identification work was presented and an extension of the model to include a background radiation field given. The modified adf04 files produced by this code are immediately applicable in existing ADAS collisional-radiative routines, and can be used to investigate the effects of moderate opacity on excited state populations. The need to model series limit spectra led to the proofs of analytic continuity contained in chapter 3. This allows opacity adjustments to the flux and populations to be dealt with smoothly across the ionisation threshold. The treatment of the series limit taken in this thesis is contrasted with the usual technique of assuming that a statistical microfield 'dissolves' bound excited states into the continuum.

This led to the population work of chapter 4 where a high quantum shell collisional-radiative model and code were developed. The model forms part of a larger plan to model the populations of heavy species, with the code developed in this chapter providing a natural module which will be added to a low level code of similar type to ADAS 208. An outline of the heavy species model was given, with a description of the approach to be taken in the assembly of each collisional-radiative module. As part of this plan, new Gaunt factors were developed. A scheme to automatically detect the critical n-shells between bundling regimes was also shown. The high quantum shell code of this chapter evaluates the $(\gamma_p \pi_p J_p)n$ and $(\gamma_p \pi_p J_p)nl$ block primitives of the new scheme. A test module for the $(\gamma_p \pi_p J_p)nlj$ component was developed and can be extended to evaluate a complete nlj block primitive. The code of chapter 4 is immediately applicable to the hydrogen series limit spectral feature work of chapter 5.

The assembly of such spectral features was then described, bringing together the continuity, opacity and population work of the previous chapters as well as including expected contribution of impurity species to the background continuum. A description of a code designed as a diagnostic tool for the JET divertor is then given. It was shown that the code can fit both high and low density observations and return local plasma parameters.

6.2 Areas for future work

The studies in this thesis indicate some areas in which the usefulness of existing ADAS procedures handling opacity can be improved. The principal of these is to introduce some special capacity in ADAS 214 for a radiation field consistent with the population structure, more details are given in section 6.2.1. There are two major conceptual issues from this thesis which are expected to influence substantially our research in the immediate future. These planned developments are outlined in sections 6.2.2 and 6.2.3.

6.2.1 Extensions to ADAS 214

At the moment ADAS 214 starts with a modified Boltzmann population distribution, evaluates the resultant radiation field and uses this to calculate absorption factors and hence a thick population structure. If these populations are used as the starting point of further iterations, a population structure which is consistent with the plasma radiation field may be achieved, the system being iterated until the population converged.

6.2.2 Future work for the series limit code

The future series limit work divides into two approaches. Firstly one can construct spectral feature fitting procedures which use plasma information from other diagnostics or plasma codes to constrain certain fitting parameters. An optimised fit of the observed series limit is then done as in the existing ADAS fitting codes. This technique can be immediately pursued and a further member of the ADAS series 6 will be provided.

The second approach is more long term. The fitting code can be made part of a global optimisation procedure. Thus, instead of performing a fit based upon external bounding data from other codes and diagnostics, the fitting code is one part of an integrated fit to the complete set of tokamak parameters. This has particular application to fusion, where the series limit code can be integrated with existing plasma transport codes. In this approach the whole set of codes forms the fitting procedure, and consistency amongst all fitted parameters must be achieved for a valid fit. This presents a significant task, both in the assembly of the set of codes and in the computational optimising of the fit.

Both approaches require development of series limit procedures which are robust, efficient and tailored to the specific experimental setup of the plasma under investigation. Initially there are two types of experimental spectra which will be modelled.

Hydrogen series limit code

With minor modifications the divertor series limit code of chapter 5 can be integrated into the JET divertor diagnostic software. Constraints must be put on the initial fitting parameters, based upon information from other plasma diagnostics. In particular, more detailed knowledge of the core impurity contribution to the spectrum can be measured using the KS4 spectrometer. The code of chapter 5 will be called as part of a least squared fitting procedure, in the same manner as the existing ADAS fitting codes. A useful capability of these codes are that they allow impurity lines as well as the generated spectral feature to be incorporated in the fit (the presence of impurity lines in the JET data can be seen from figure 1.15). It is hoped that such a fitting code will resolve the discrepancy found when the FWHM analysis is used to diagnose electron densities from various series limit lines where agreement was found using the 11-2 and 8-3 lines but not using the 7-3 line (Meigs et al., 2000). This work is planned for the immediate future.

Helium series limit code

The principles of continuity and feature generation can be extended to model helium series limits. Here of course both singlet and triplet series limits will be produced. There have been two recent observations of the helium Lyman series limit. The first was in a high density laboratory plasma and analysed using a collisional-radiative model (Namba et al., 2000) which included an escape probability to account for opacity. This allowed the observed plasmas to be classified into ionising and recombining type. The Lyman series limit was also observed in the DIII-D tokamak (Whyte et al., 2000) and the recombination spectrum used to diagnose the plasma electron temperature and effective ionic charge during plasma disruption.

While the Lyman series is of interest, the main opportunity for future research lies in modelling the triplet series. For higher quantum shells L-S coupling breaks down, and the excited electrons can be thought of as a mixture of singlet and triplet states. Thus electron on the triplet side effectively spend some time in a singlet state and are no longer mainly confined to decaying down to the $1s2s\,^3S$ shell. Thus one would expect that the resulting triplet spectrum would consist of discrete lower series lines and that as one progresses up the series a partial quenching of the spectrum would be observed at the point where the spin system breakdown allows triplet electrons to decay down to the ground on the singlet side. Such a quenching has been observed (Ohno et al., 1998), though it was interpreted as evidence of molecular activated recombination.

Collisional redistribution is an essential ingredient for such quenching to take place. The collisional-radiative modelling of the highly excited states of helium is an area requiring attention, and a technique which allows the nature of the spin system breakdown to be investigated would be useful. Improvements in the collisional-radiative model would then reap further benefits in all helium based diagnostics. It should also be noted that the new scheme proposed for the heavy species work does not use the conventional L-S coupling for the excited states and so will be able to track the behaviour of these excited states, and the expected series quenching. The density sensitivity of the spin system breakdown could also be used as a diagnostic tool.

In a recent experiment at JET some preliminary observations were taken to evaluate whether any helium triplet series could be observed (Meigs, 2001). In the region 3640 Å → 3520 Å members of the triplet series (to $1s\,2p\,^3P$) were observed, and quenching effects detected. Thus it appears that further work into series limit modelling for helium triplet series is justified.

6.2.3 Population extension for heavy species

The extension of the population work of chapter 4 to deal consistently with heavy species populations provides a variety of future applications. The primary motivation for this work at the present time is the need to be able to detect heavy species at typical ITER temperatures and densities. It has been proposed that heavy species be embedded at different depths in certain of the carbon fiber composite wall tiles of ITER as erosion markers. As the tiles are eroded the heavy species layer is ejected into the plasma core and its spectral signature detected. It will also be necessary for ITER to take advantage of the good thermal resistance of heavy species in the tokamak design. Consider the spectrum from a species such as tungsten. One observes a complex grass-like spectrum arising from a combination of the many ionisation stages of the species and the complex set of energy levels present. The grass-like spectrum does however have a recognisable 'spectral envelope' arising from imperfectly resolved 'transition arrays'. This envelope shows a strong temperature dependence. The marching of transition arrays as one progresses iso-nuclearly and iso-electronically has been shown theoretically (O'Mullane & Summers, 1999). This will allow even adjacent heavy species to be resolved. The higher levels become hydrogenic in behaviour and their series limit spectra merge with the general continuum-like appearance of the spectral envelopes.

Pixel sums over specified wavelength intervals will be performed on the observed envelopes using 'computational filters'. This will be used to extract a set of numbers ('signature numbers') to be used as the parameters to be matched in a high throughput fitting procedure. Both neural networks and genetic algorithms will be investigated as potential pattern recognition methods. It will be possible to generate training data to test the fitting procedures. At present experimental spectra for the heavy species at expected ITER conditions cannot be generated, and as the transition array are markedy temperature sensitive, lower temperature data will not be sufficient. Thus computational modelling will be relied upon to generate synthetic signature numbers and provide the necessary training datasets. To test the robustness of the fitting procedures the synthetic envelopes will be combined with actual noise from an experimental device such as JET. This will produce test datasets of 'noisy' signature numbers to be fitted by the code.

The work required for the completion of the heavy species collisional-radiative model is significant, but achievable. The new coupling scheme has been outlined in chapter 4. The $(J_p)nl$ and $(J_p)n$ resolved block primitives can be evaluated at present. The single n-shell test code for the $(J_p)nlj$ resolution will be extended to encorporate an entire block primitive. This will then be used to test condensation schemes, the effects of the redistributive rates and methods of population solution. An $(J_p)nlj$ block primitive code will then be written.

The initial baseline data for the low level blocks will be generated using ADAS 801, and will be produced in adf04 format. The data will be complete for the species under investigation, but of fairly low quality. The low level data will then be supplemented with higher quality data from codes such as HULLAC and R-matrix. The low level rates will be assembled in the ADAS 208 approach. The influence of the higher populations can then be projected onto these low lying results and a population solution obtained.

The modularisation of the code outlined here allows advantage to be taken of modern high performance parallel computers. Each block primitive can be calculated independently on a different processing node. The block primitives can then be assembled into the blocks and the final superblock matrix. Such parallel techniques are likely to be required for the assembly and solution of the large matrices needed for heavy species modelling.

The collisional-radiative code will be combined with an ionisation balance calculation to predict a synthetic feature. The feature will then be isolated into components and fitted to the observed filtered envelope segments. The final model will be linked to a plasma transport code and used in a global optimisation routine wherein theoretical spectral features, elemental concentrations, densities and spatial distributions are simultaneously fitted to observed plasma parameters.