NEPTUNE Workshop 6 September 2022

1 Topic, Location

Topic Physical data

Moderator, Assistant Wayne Arter, Matthew Barton

Time 2pm-3.30pm

Location Abbey Rm, Guildhall

2 Notes

WA explained that he had worked for a number of years in neutronics, which was one of a number of fields besides plasma radiation, where the solution of rate equations was critical. The neutronics rate equations are referred to as the Bateman equations. They are a large system of sparse ordinary differential equations where each nuclide (atomic nucleus of a certain weight and charge) evolves in time at a rate depending on the neutron flux proportional to the instantaneous amounts of other nuclides (and if unstable of course, decays at a rate proportional to how much of itself there is). WA's studies had concentrated on UQ and he showed a loop whereby

1. Rate coefficients (proportionality constants) are found by physics experiments or quantum mechanical calculation as functions of energy and added to a database
2. Data is extracted from the database and weighted with a given spectrum of energy
3. The Bateman equations are solved to give the inventory, ie. numbers of different nuclides, at one or more specified times.
4. Based on sensitivity studies and/or comparison with experiment, improved rate coefficients are sought and the process repeats.

Martin O'Mullane (MOM) explained that there were key differences in that sufficently hot plasma experiments inevitably involved a wider range of effects that needed disentangling. There was also difficulty in the specification of the radiation field in that it might be inadequate to specify in terms of a single temperature (non-Maxwellian). Rates could not be regarded as fixed if the temperature, and to a lesser extent the density, of the background plasma were varying. Further, the rate equations for atomic processes had more nonlinear terms and notably, many more coefficients than the Bateman equations, to the extent that 'sparseness' could not be assumed. Their fuller matrices would lead to asymptotically much more expensive calculations scaling as the cube of the size of the rate equation matrix.

MOM confirmed the accuracy of the division into two classes of data requirements described in WA's annex on radiation effects to the Equations document [1, Annex A], namely (1) for the overall plasma dynamics and (2) much more detailed information required to interpret diagnostics related to the spectrum of plasma emission, eg. the strength of spectral lines.

Most atomic processes have rates so fast that they are effectively instantaneous on the timescale of collective plasma dynamics, the exception being the so-called 'forbidden' transitions involving metastable atomic states which frequently have millisecond timescales. Of course, there are also transitions which may be ignored because they have long timescales compared to discharge lifetime.

(If neutral particles are present in sufficient numbers, which is usually the case in the tokamak edge, then a range of processes such as charge exchange and recombination are able to modify the plasma dynamics on relevant timescales. Verhaegh et al [2] is a recent reference, suggesting the importance of molecular processes in the SOL. In some regions, there may be present sufficient neutrals that they may be treated using a fluid approximation, with interaction terms that resemble those of ionised species.)

Thus mathematically, the effect of atomic processes in a fluid model, is to couple at each point in position space, rate equations to the advection-diffusion equations representing evolution of the fluid moments (mass, monmentum and energy). The rate equations are probably best treated as being of differential-algebraic type. It is helpful to order the atomic analogues of nuclides (in the neutronics case) by element, atomic number, number of bound electrons, shell occupancy by the electrons, orbitals etc. WA suggested that there might be a role for eigenanalysis of rate matrix to help identify which species could be treated as reacting instantaneously (and thereby algebraically), and possibly reduce the number of variables to be time evolved to those representing a comparatively small number of eigenvectors.

Stefan Mijin indicated that he felt his approach to modelling both kinetic and fluid effects of electron transport as implemented in the SOL-KiT software [3] could be extended relatively quickly to deal with many if not all of the above issues. He recommended the work of Greenland [4, 5] as an elegant treatment of rate equations for radiation modelling.

References

[1] W. Arter. Equations for EXCALIBUR/NEPTUNE Proxyapps. Technical Report CD/EXCALIBUR-FMS/0021-1.00-M1.2.1, UKAEA, 2020. `https://github.com/ExCALIBUR-NEPTUNE/Documents/blob/main/reports/ukaea_reports/CD-EXCALIBUR-FMS0021-1.00-M1.2.1.pdf`.

[2] K. Verhaegh, B. Lipschultz, J.R. Harrison, B.P. Duval, A. Fil, M. Wensing, C. Bowman, D.S. Gahle, A. Kukushkin, D. Moulton, et al. The role of plasma-molecule interactions on power and particle balance during detachment on the TCV tokamak. *Nuclear Fusion*, 61(10):106014, 2021.

[3] S. Mijin, F. Militello, S. Newton, J. Omotani, and R.J. Kingham. Kinetic effects in parallel electron energy transport channels in the scrape-off layer. *Plasma Physics and Controlled Fusion*, 62(12):125009, 2020.

[4] P.T. Greenland and D. Reiter. Collisional radiative models with loss and recycling. *Journal of Applied Physics*, 83(12):7496–7503, 1998.

[5] P.T. Greenland. Collisional-radiative models with molecules. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, 457(2012):1821–1839, 2001.