Simulations of the edge plasma: the role of atomic, molecular and surface physics

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Abstract. Atomic, molecular and surface physics plays an important role in simulations of the edge plasma in present day tokamaks, and in the predictive simulations of new devices. The edge plasma — in this context, the Scrape-Off Layer (SOL), the Private Flux Region (PFR) and core region close to the separatrix (or Last Closed Flux Surface, LCFS) — provides the boundary conditions for the main plasma, and is the region where much of the power and all of the particle exhaust occurs. It is also the region where the plasma interacts with solid surfaces, puffed gases and gas arising from recycling. The results of plasma edge simulations can depend strongly on the availability and quality of the atomic, molecular and surface data (the peak plasma temperature at the divertor was found to vary by a factor of five dependent on the choice of atomic physics data in a recent sensitivity analysis). The current material choice for ITER with Plasma Facing Components (PFCs) consisting of C, Be and W also presents challenges, both in the availability of the necessary data for W, and in the plethora of charge states for W. Another challenge presented by the material choice is the likely presence of mixed materials formed by the migration of material from one surface to another. These introduce effects like alloying and preferential sputtering as well as new (much longer) time-scales in the problem.

Efforts to incorporate a bundled charge state model within one of the present edge simulation codes, SOLPS, will be described, as well as efforts to address some of the questions raised by mixed materials. Some issues related to data consistency and traceability within the context of the European effort on Integrated Tokamak Modelling will also be addressed.

Keywords: SOLPS, Plasma Edge Simulations, Atomic-Molecular-Surface Processes in a Plasma
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INTRODUCTION

Atomic, molecular and surface data often play a key, but sometimes neglected, role in simulations of fusion plasma behaviour. For the core plasma, usually only atomic (and nuclear) data are needed, but for simulations of the edge, atomic, molecular and surface data are important. The role played by the data is described below by highlighting their use in one of the standard fusion device edge simulation packages, SOLPS, described below. Following this, the wider use of Atomic, Molecular, Nuclear and Surface (AMNS) data is described in the context of the European Fusion Development Agreement Task

Force on Integrated Tokamak Modelling (EFDA-TF-ITM). A new interface to AMNS data is proposed, and the paper finishes with a discussion.

ITER: THE PATH TO ENERGY PRODUCTION FROM MAGNETICALLY CONFINED PLASMAS

The main reason for the strong interest in fusion research is the goal of large scale energy production without the CO_2 production associated with the burning of fossil fuels, and without the production of long-lived radioactive waste associated with fission power plants. Amongst the various routes to fusion being followed, the tokamak is probably the furthest along. The tokamak relies on a combination of an externally applied magnetic field in combination with a magnetic field generated by a current flowing in the plasma to confine particles in a toroidal configuration.

The next device, ITER, is currently being built in France by a consortium of seven parties. The materials mix for its first phase of operation is a first wall made of Be, targets made from C and some high heat flux components made of W (though it is likely that the C targets will be replaced by W before the start of the DT phase because of concerns of T co-deposition with C).

This mix of materials means that comprehensive simulations of the edge plasma need to take into account:

- D & T, the fuel, and the associated molecules, D_2, DT and T_2
- H which will be used in the commissioning phase
- He, the waste product produced by the D-T fusion reaction
- C, together with all the hydrocarbons ($C_xD_yT_z$)
- Be
- W (which, with its large number of charge states, is a challenge)
- Ne, Ar and/or Kr (which might be used as radiators to reduce power fluxes to the targets)
- O, F, Fe, Ni, Cu, ... (unwanted contaminants)

and any mixed materials that might form.

SOLPS: SCRAPE-OFF LAYER PLASMA SIMULATIONS

Amongst the codes that have been used to simulate the edge plasma in existing tokamaks, and for predictive simulations for ITER, is SOLPS[1]. The SOLPS package[2, 3, 4] is a suite of codes, the two main constituent of which is formed by the combination of two codes, B2[5, 6], or, in a later version, B2.5[7, 8, 9, 10] (2d fluid codes simulating plasma transport in the edge region of a tokamak) and EIRENE[11, 12] (a 3d Monte-Carlo code simulating the transport of neutrals in the edge region). (In some simulations, though, a simpler fluid neutral model that is part of B2 is used in place of EIRENE.)

B2 solves a set of time dependent transport equations for

- the density of the various charge states
- parallel momentum for the various charge states
- electron temperature
- combined ion temperature

and an elliptic equation giving the electric potential. For each of the transport equations, atomic, molecular and surface processes provide source terms arising from ionization, recombination, radiation and charge exchange. Surface processes describe the interaction of the plasma with material surfaces and provide for recycling of hydrogen isotopes and helium, as well as the production of impurities by physical and chemical sputtering processes.

AMS DATA IN SOLPS

The two main components of SOLPS use different sources for their Atomic, Molecular and Surface (AMS) data.

The plasma code, B2, derives its atomic data from one of STRAHL[13], ADPAK[14] or ADAS[15] and a pre-processor (b2ar) prepares interpolation tables (as a function of electron density and temperature) used by the main program. Except that the standard version of the code uses a simple fit for charge-exchange rate coefficients (which works well for H, less well for everything else, but can be disabled so that, for example the ADAS rates can be used), and uses a standard database (WEISHEIT[16]) for hydrogen (which substitution can now be disabled). For surface data, tables from TRIM[17] are used to provide sputtering yields and energy, as well as reflection coefficients. The standard Roth formula[18, 19] can be used for chemical sputtering, or, alternatively, a fixed yield can be specified. A simple model for mixed materials has also been implemented[20, 21].

EIRENE uses recombination, dissociation, ionization, elastic and charge-exchange cross sections (if available) or rate coefficients, for a number of molecular species (hydrocarbons, hydrogen, helium, silane, N_2, ...) as well as line shape databases for radiation transfer (opacity) modelling. Databases have been developed for some of them (www.hydkin.de), and an automated interface for EIRENE to this database is currently being tested. Already in place (since approx 20 years) are interfaces to HYDHEL (see also IAEA database), METHANE and AMJUEL (www.eirene.de) databases. Both these databases rely upon polynomial representations and are made redundant gradually, by using physically based fits, see www.eirene.de, A&M data section.

Recently, a bundled charge state option has been implemented in SOLPS[22] which uses a recently released change to ADAS[23] that groups or bundles charge states together. Implementing this change into SOLPS required substantial changes because the atomic charge state of a “species” changed from being a fixed number to a function of electron density and temperature, as did the squared atomic charge, and the ionization potential. As a side effect, the restart file needed to be augmented by the saving of the electron density because of the new dependency introduced: the electron density was

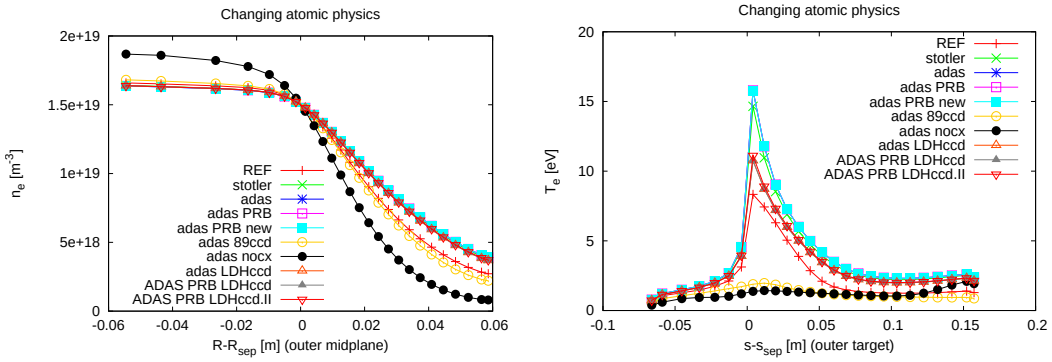

FIGURE 1. Effect of changing the atomic physics on SOLPS solutions of the electron temperature at the outer midplane (left) and outer target (right).

derived from the ion densities and their atomic charges, but this latter quantity now can depend on the electron density. (The implications of this change to EIRENE have not yet been implemented.)

In doing a benchmark between edge codes, one difference in the codes was tracked down to a difference in the atomic physics used[24]. In examining the situation further, it was found that changing the atomic physics assumptions had a much larger effect on the plasma than changing some of the physics choices, figure 1. The simulations using the ADAS '89 charge exchange data are much closer to the simulations with no charge exchange, than to all the other simulations.

AMNS DATA NEEDED BY THE ITM

A variety of Atomic, Molecular, Nuclear and Surface (AMNS) data is needed by the European Fusion Development Agreement (EFDA) Task Force for Integrated Tokamak Modelling (ITM), whose aim is to:

- Co-ordinate the development of a coherent set of validated simulation tools
- Benchmark these tools on existing tokamak experiments
- Provide a comprehensive simulation package for ITER and DEMO plasmas

Within the ITM, two of the Integrated Modelling Projects (IMPs) have particular needs:

IMP3 (responsible for transport) needs atomic, molecular, nuclear and surface data for ionization, recombination, charge-exchange, nuclear reactions, cooling rates with a high priority for H, D, T, He & C for 2008 and a lower priority for Be, O, N, Ne, Ar, Mo, Ni, Li, Si, B & W.

IMP5 (responsible for sources) needs cross sections for electron impact ionization, ion impact ionization and charge exchange for Neutral Beam Injection and nuclear data for fusion reactions and other nuclear reactions between fast ions and impurities for diagnostics.

The use of AMNS data within the ITM should fulfill the following requirements:

- Version control of data imported to the ITM-TF data base is mandatory
- The provenance of the data must be accurate and stored in the ITM database
- For "production" runs with ITM-TF codes using AMNS data it is important that the data have been given a stamp of approval by an expert, with particular emphasis on internal consistency and completeness of the reaction sets to be selected (see e.g. the MAR story in [25])
- The AMNS data must be communicated to ITM-TF codes via a standardized interface (this should also ensure coherence between different ITM-TF codes needing the same type of data)

The first two requirements, together with strict versioning of codes, should mean that a previously performed run can be repeated years later and still obtain the same answer.

In order to implement the above requirements, a new standard interface is proposed for the use by physics codes of AMNS data.

A PROPOSED STANDARDIZED INTERFACE FOR THE USE OF AMNS DATA FOR THE ITM

The aim of the proposed standard interface to AMNS data is to separate the use of the data by a physics code from the details of how the data is provided.

The only communication between the two should be by nine calls, which break into the following:

- initialization (2)
- finalization (2)
- querying parameters (2)
- setting parameters (2)
- getting data (1)

For the first four, there is one call that applies to the entire AMNS system, and one call that applies to a particular table. In all cases a "handle" is used to identify which instance is being addressed. An optional argument can be specified for each call to get the error status — if not provided, an error will cause the code to stop.

Initialization

```
subroutine ITM_AMNS_SETUP(handle, version, error_status)
  optional version, error_status
  type(amns_handle_type), intent(out) :: handle
  type(amns_version_type), intent(in) :: version
  type(amns_error_type), intent(out) :: error_status
```

- Initializes the whole package

```
subroutine ITM_AMNS_SETUP_TABLE( &
    handle,reaction_type,reactant, &
    handle_rx,error_status)
  optional error_status
  type(amns_handle_type), intent(in) :: handle
  type(amns_reaction_type), intent(in) :: reaction_type
  type(amns_reactants_type), intent(in) :: reactant
  type(amns_handle_rx_type), intent(out) :: handle_rx
  type(amns_error_type), intent(out) :: error_status
```

- Initializes the AMNS package for a particular reaction
- reaction specified by:
  - `reaction_type`
  - `reactant`

Finalization

```
subroutine ITM_AMNS_FINISH(handle, error_status)
  optional error_status
  type(amns_handle_type), intent(inout) :: handle
  type(amns_error_type), intent(out) :: error_status
```

- Terminates the use of the AMNS package:
  - frees up allocated memory

```
subroutine ITM_AMNS_FINISH_TABLE(handle_rx, error_status)
  optional error_status
  type(amns_handle_rx_type), intent(inout) :: handle_rx
  type(amns_error_type), intent(out) :: error_status
```

- Terminates the use of the table associated with a particular reaction:
  - frees up allocated memory

Querying parameters

```
subroutine ITM_AMNS_QUERY(handle,query,answer,error_status)
  optional error_status
  type(amns_handle_type), intent(in) :: handle
  type(amns_query_type), intent(in) :: query
  type(amns_answer_type), intent(out) :: answer
  type(amns_error_type), intent(out) :: error_status
```

- provides a mechanism for querying the AMNS package:
  version queries for the version of the data

```
subroutine ITM_AMNS_QUERY_TABLE( &
    handle_rx,query,answer, &
    error_status)
  optional error_status
  type(amns_handle_rx_type), intent(in) :: handle_rx
  type(amns_query_type), intent(in) :: query
  type(amns_answer_type), intent(out) :: answer
  type(amns_error_type), intent(out) :: error_status
```

- provides a mechanism for querying for information about a particular reaction:
  source data source
  no_of_reactants number of involved reactants
  index reaction index (used at the moment for choosing spectroscopic line)

Setting parameters

```
subroutine ITM_AMNS_SET(handle,set,error_status)
  optional error_status
  type(amns_handle_type), intent(in) :: handle
  type(amns_set_type), intent(in) :: set
  type(amns_error_type), intent(out) :: error_status
```

- used for setting global parameters:
  - none implemented yet
  - could implement a global debugging flag

```
subroutine ITM_AMNS_SET_TABLE(handle_rx,set,error_status)
  optional error_status
  type(amns_handle_rx_type), intent(in) :: handle_rx
  type(amns_set_type), intent(in) :: set
  type(amns_error_type), intent(out) :: error_status
```

- used for setting parameters associated with a particular table:
  nowarn Don't complain about extrapolation

Getting data

```
subroutine ITM_AMNS_RX_1(handle_rx,out,arg1,arg2,arg3,&
    error_status)
  optional arg2,arg3,error_status
  type(amns_handle_rx_type), intent(inout) :: handle_rx
  real (kind=R8), intent(out) :: out(:)
  real (kind=R8), intent(in) :: arg1(:),arg2(:),arg3(:)
  type(amns_error_type), intent(out) :: error_status
```

- Used for getting the rate on a grid "out" of the same dimensions as "arg1", "arg2", ...

- There is a generic interface `ITM_AMNS_RX` and particular routines `ITM_AMNS_RX_1`, `ITM_AMNS_RX_2` and `ITM_AMNS_RX_3`:
  - handles 1d, 2d and 3d tables
  - (increasing this is easy!)
- "out" can depend on 1, 2 or 3 physics parameters:
  - for 1, only "arg1" should be specified
  - for 2, "arg1" & "arg2" should be specified
  - for 3, "arg1", "arg3" & "arg3" should be specified
  - (increasing this to 4d is easy, beyond would require additional work)

Using the package

Below, an example of using the package is shown schematically, with initialization of the package, a query of the version number, an initialization of a reaction, a query about the source of the data, the setting of a parameter (switching off warnings related to extrapolation), the actual request for data, and then finalization of the table and the package.

```
  call ITM_AMNS_SETUP(amns)
  query%string='version'
  call ITM_AMNS_QUERY(amns,query,answer)
...
  call ITM_AMNS_SETUP_TABLE(amns, lr_rx, species_lr, amns_lr)
  query%string='source'
  call ITM_AMNS_QUERY_TABLE(amns_lr,query,answer)
...
  set%string='nowarn'
  call ITM_AMNS_SET_TABLE(amns_lr,set)
...
  call ITM_AMNS_RX(amns_lr,rate(:,:,0),ne,te)
...
  call ITM_AMNS_FINISH_TABLE(amns_lr))
  call ITM_AMNS_FINISH(amns)
```

A prototype implementation has been realized, and some results are shown in figure 2. The implementation uses linear/bilinear/trilinear interpolation in tables.

SUMMARY

This paper has summarized the uses of Atomic, Molecular, (Nuclear) and Surface (AMNS) data in fusion simulations, with particular emphasis on edge codes. The sensitivity of the results to some AMNS choices has been indicated. A new approach for accessing AMNS data was also described.

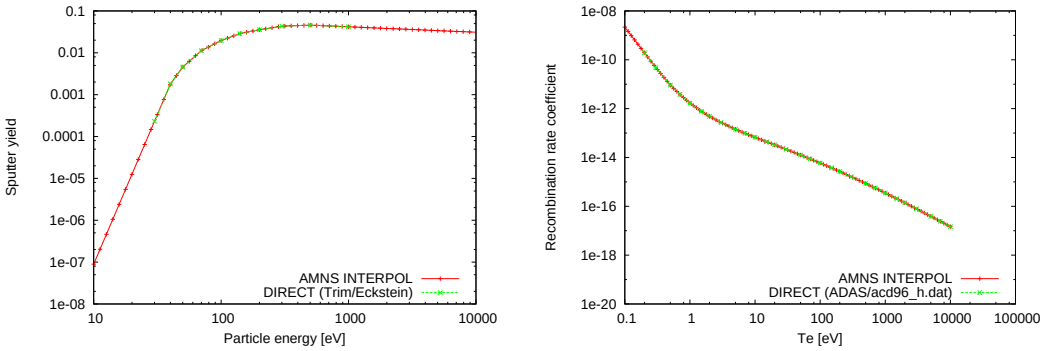

FIGURE 2. Prototype implementation of the AMNS interface comparing (left) sputter and (right) recombination data from the package with the original TRIM and ADAS data, respectively.

An additional point is that we need not only data for individual reactions evaluated carefully, but also the sets of reactions selected properly to avoid artificial bias in the processes we model.

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