Benchmark the ETS/impurity code against SANCO

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Outline

- SANCO code description
- ETS/impurity code description
- Settings and boundary conditions for both codes.
- Summary of the results
- Conclusions

SANCO description

- SANCO solves a set of continuity equations for all ionisation stages of up to two impurity species :

$$\frac{1}{V'}\frac{\partial}{\partial t}(n_i^z V') + \frac{1}{V'}\frac{\partial}{\partial \rho}V'\left[-D_i^z \cdot \nabla n_i^z + V_i^z \cdot n_i^z\right] = S_i^z - Q_i^z - \frac{n_i^z}{\tau_{//}} \cdot \xi \cdot (1-R)$$

  where, S_i^Z *and* Q_i^Z are ionisation and recombination sources and sinks for impurity species specified by the ADAS database with indices *i* and the charge Z;

- In SANCO the boundary conditions can be specified has as a function of flux:

$$V_0 n_{neut}^i(a) = \Gamma_{ext} + R_Z \sum_{z=1}^{Z} n_i^z(a) V_{esc}$$ where $divV_0 \cdot n_{neut} = -\alpha_{ion} \cdot n_{neut}$

and *a* can be the wall or the last closed flux surface

- Or as a function of density:

$$n_i(a) = \sum_{z=1}^{Z} n_i^z(a)$$ where n_i^z is determined by the Coronal distribution

- SANCO has a fixed 30 core radial grid points

ETS/impurity

For the test with SANCO I use in the ETS/impurity, that have not change in magnetic filed in the time and $\left\langle \left|\nabla\rho\right|^2 \right\rangle = 1$, the set of continuity equations for all ionization stages have form:

$$\frac{\partial}{\partial t}\left(n_i V^{'}\right)+\frac{\partial}{\partial\rho}\left[V^{'}\left(-D_i\frac{\partial n_i}{\partial\rho}+n_i V_i^{pinch}\right)\right]=V^{'}\left(S_{i,\exp}-S_{i,imp}.n_i\right)$$

$$S_{i,\exp}=n_e\left(n_{i-1}\alpha_{i-1}+n_{i+1}\beta_{i+1}\right)$$

$$S_{i,imp}=n_e\left(\alpha_i+\beta_i\right)$$

The following boundary condition for the test with SANCO are used:

at the axis: *r=0* $\quad \left.\frac{\partial n_i}{\partial r}\right|_{r=o}=0, v(1)=1, u(1)=0, w(1)=0$

at the plasma edge: $r = r_{bnd}$

$$\left.n_i\right|_{r=r_{bnd}}=n_{i,bnd}; v(2)=0, u(2)=1, w(2)=n_{i,bnd}$$

• In order to solve the impurity transport equations by solvers Solver 3 implemented into ETS. The ETS/impurity code is called twice in the same time step. On the first call the equations are solved starting from the lowest ionization to the highest ionization stage. On the second call, the equations are solved starting form the highest ionization to the lowest ionization stage.

The Solver 3 is a block tri-diagonal solver based on central finite difference approximation in space and backwards Euler method in time .

The ETS/Impurity calculated uniform grid points (NRHO = 100)

Settings and boundary conditions for both codes

- Plasma parameters are setup as a parabolic function:

$$f(\rho) = f(0)(1-\rho^2) + f(1)$$

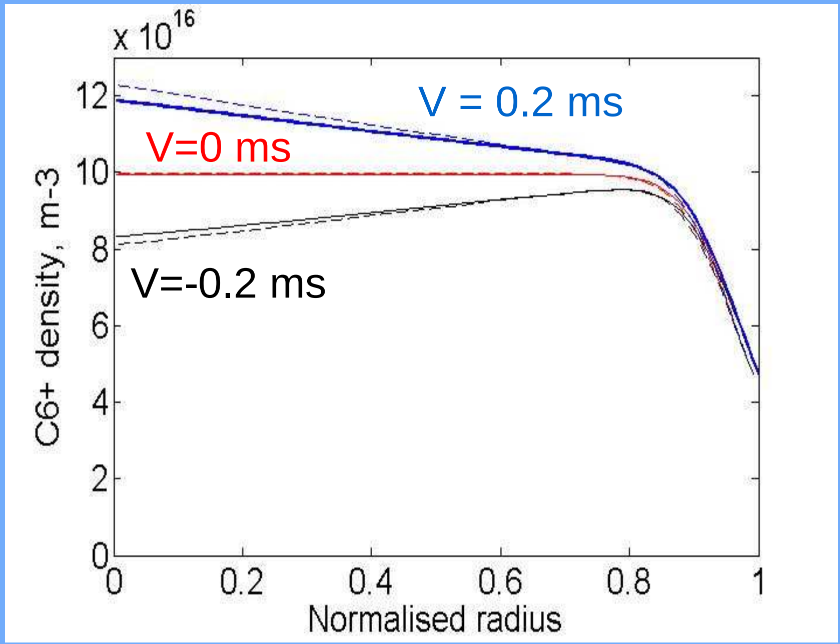
Where n(0)=8.e19 m^{-3}, n(1)=5.e18 m^{-3},   T(0)=1.0 keV, T(1)=100 eV, T=Ti=Te

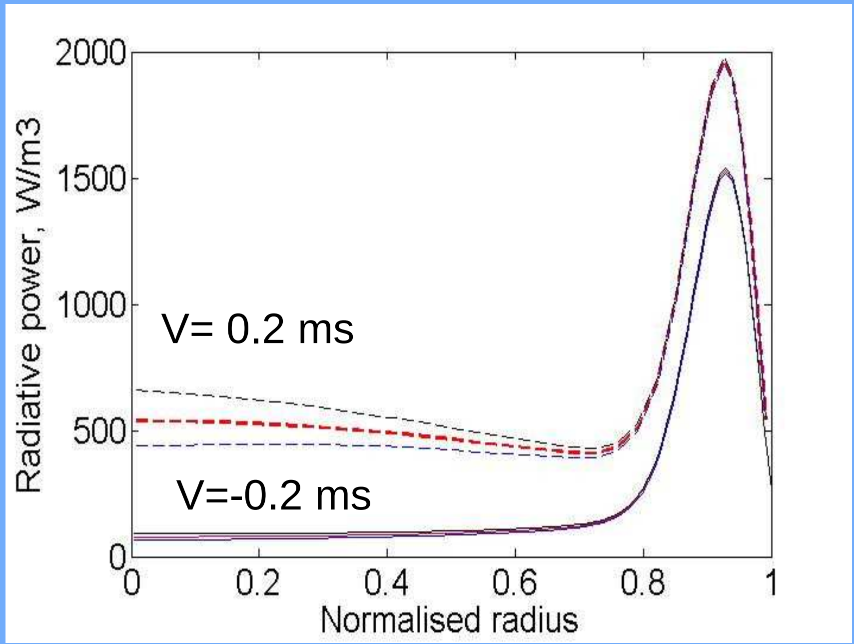
- Equilibrium was used the JET shot 71827 at 52 s
- Run times was until the codes reached steady state
- Time between steps was 1.0e-3 s
- Transport: D=1.0 m^2/s, V=0 ms, V=0.2 ms and V=-0.2 ms
- ETS/impurity used the boundary densities calculated by SANCO using the two different boundary conditions with:
  - The first: R=1, V_{esc}=50 m/s, V_0= 2eV
  - The second: ni(a) = 1.0e17 m^{-3}

ETS-SANCO benchmarking: summary table

transport	Boundary conditions	impurity	SANCO
D=1 m2/s, V=0	$n_0(\rho=1)$=5.13e12 m-3, n_{imp}=1.1e17 m-3, R_{rec}=1	C	pares, seq. 235
D=1 m2/s, V=0	$n_0(\rho=1)$=1.05e12 m-3, n_{imp}=1.74e16 m-3, R_{rec}=1	Ar	pares, seq. 239
D=1 m2/s, V=0	no neutrals, n_{imp}=1. e17, R_{rec}=0	C	pares, seq. 242
D=1 m2/s, V~0.2 m/s	no neutrals, n_{imp}=1.e17, R_{rec}=0	C	pares, seq. 243
D=1 m2/s, V~-0.2 m/s	no neutrals, n_{imp}=0.999812e17, R_{rec}=0	C	pares, seq. 244

C6+ density and radiative power with various convective velocities: ETS/impurity (solid), SANCO (dashed)

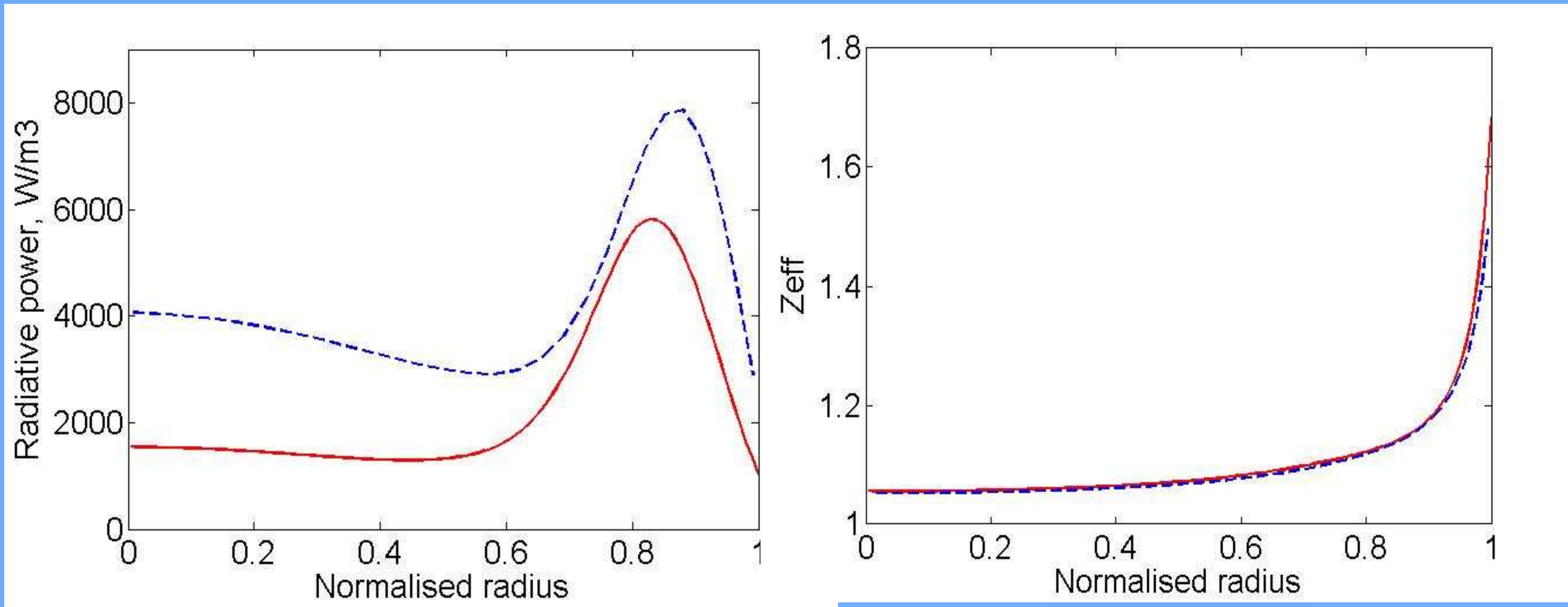




- There is no significant difference in the C+6 radial density at steady state, the main difference is the radiation.

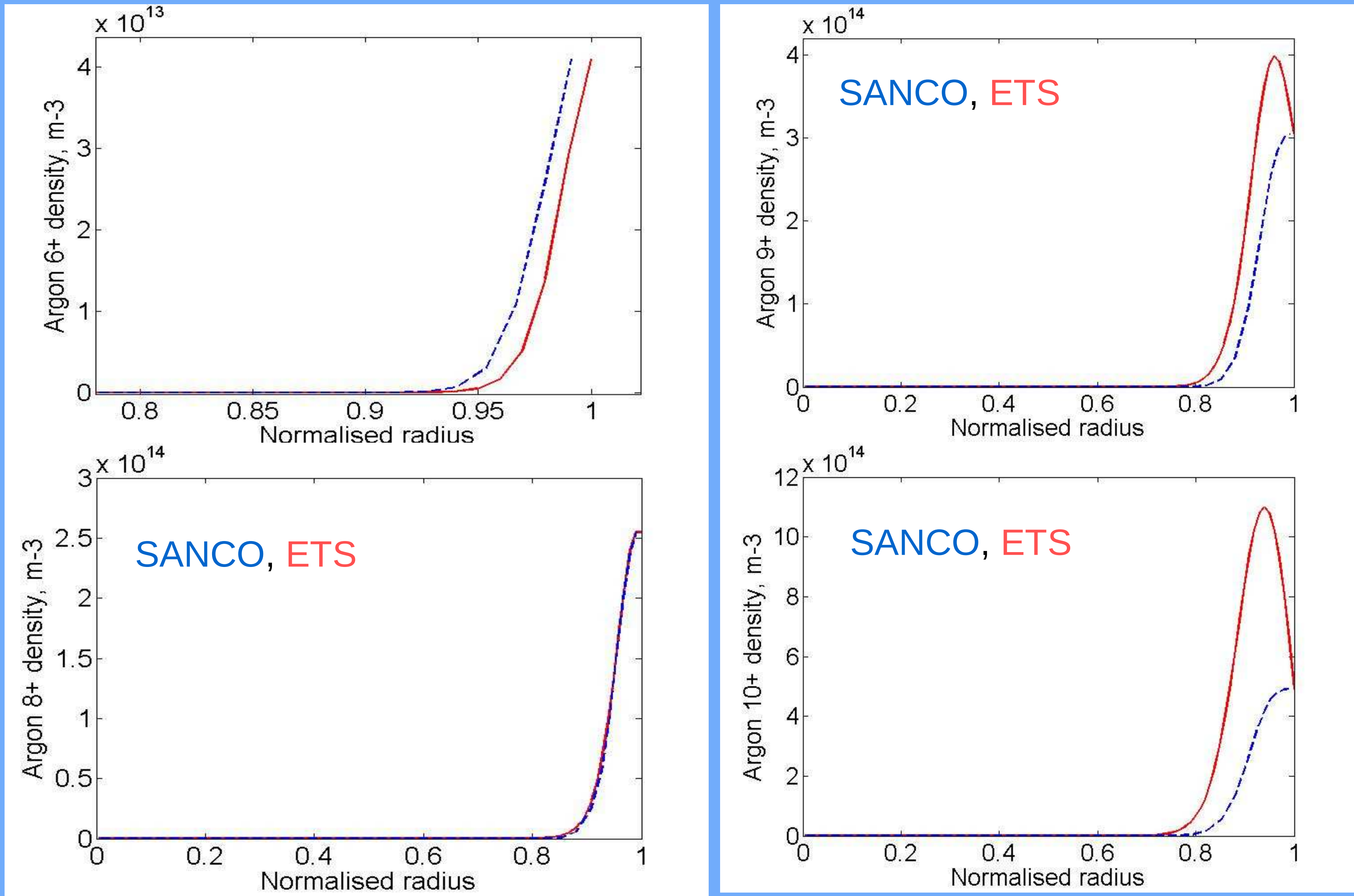
$$SANCO \Rightarrow P(\rho,t) = \overbrace{\underbrace{n_e \sum_{k=0}^{Z} (PLT)_k n_k}_{electron\ impact\ exitaction}}^{ETS/impurity} + \underbrace{n_e \sum_{k=0}^{Z-1} (PRB)_{k+1} n_{k+1}}_{recombination\ \&\ Bremsstrahlung}$$

Argon: radiative power and Zeff (SANCO (blue), ETS (red))

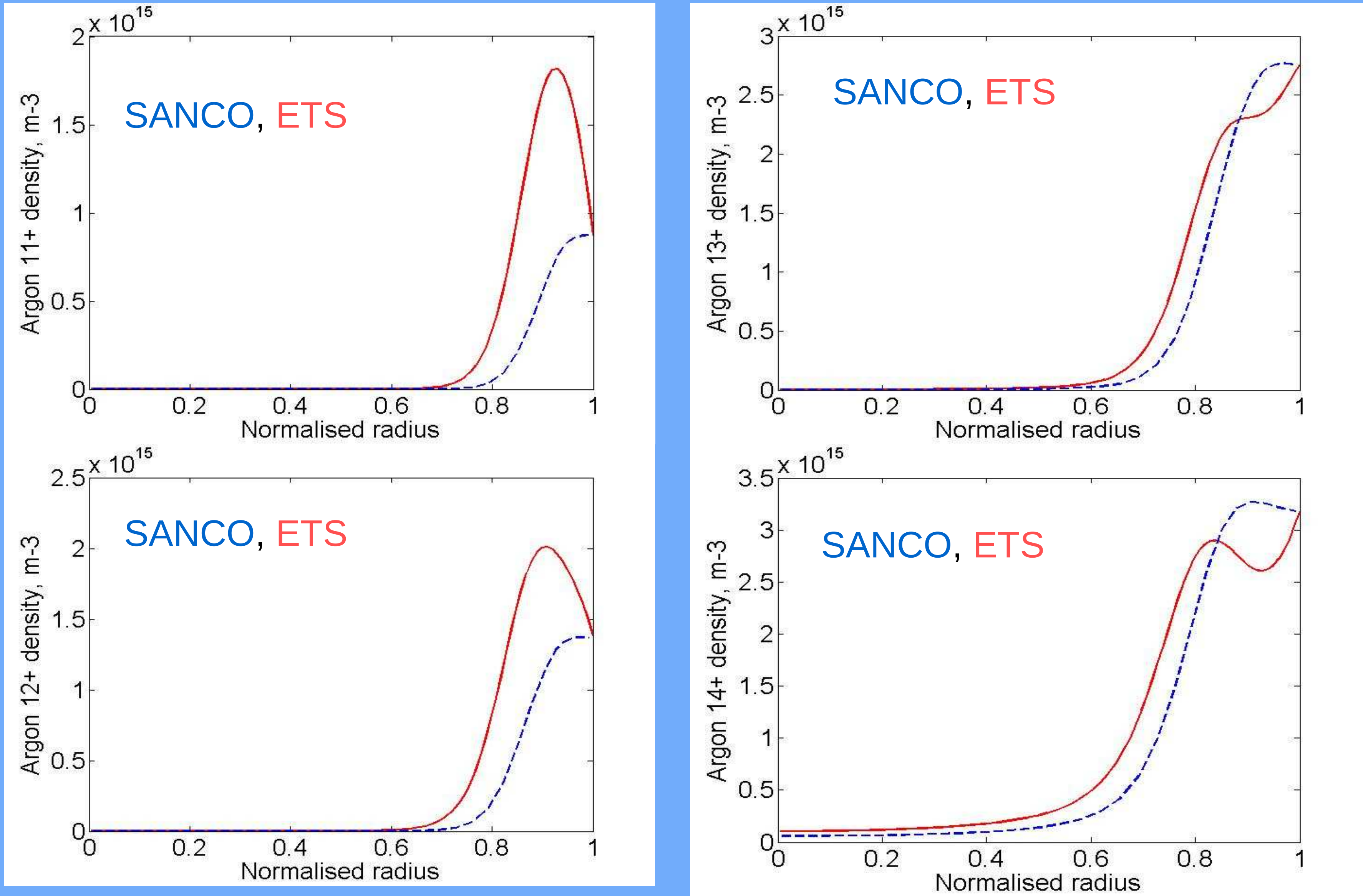


- Again the radiation is different between the two codes.
- Although the Zeff is similar there are some differences in density of some charge states due to the difference of ionisation and recombination coefficients SANCO uses ADAS and ETS/impurity R. Zagorski .

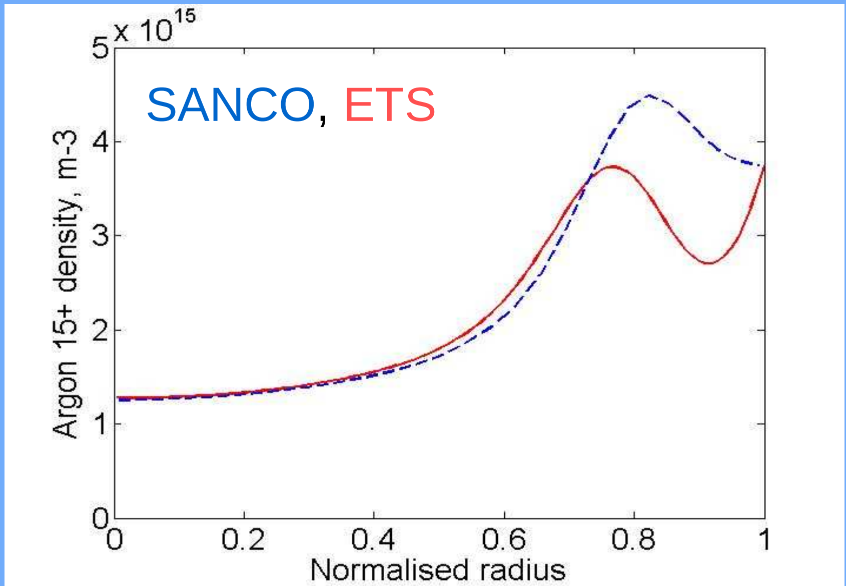
Argon: prescribed flux from +1 to +10

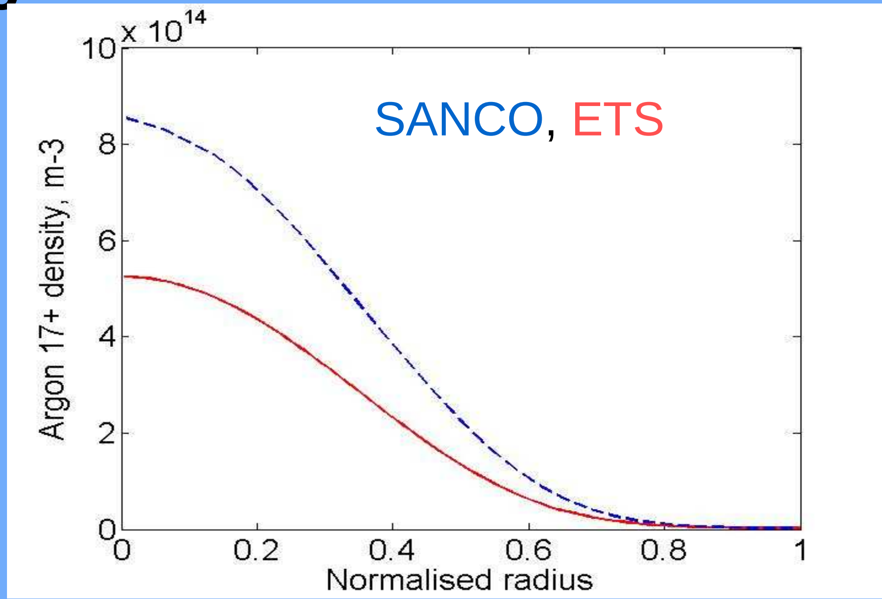


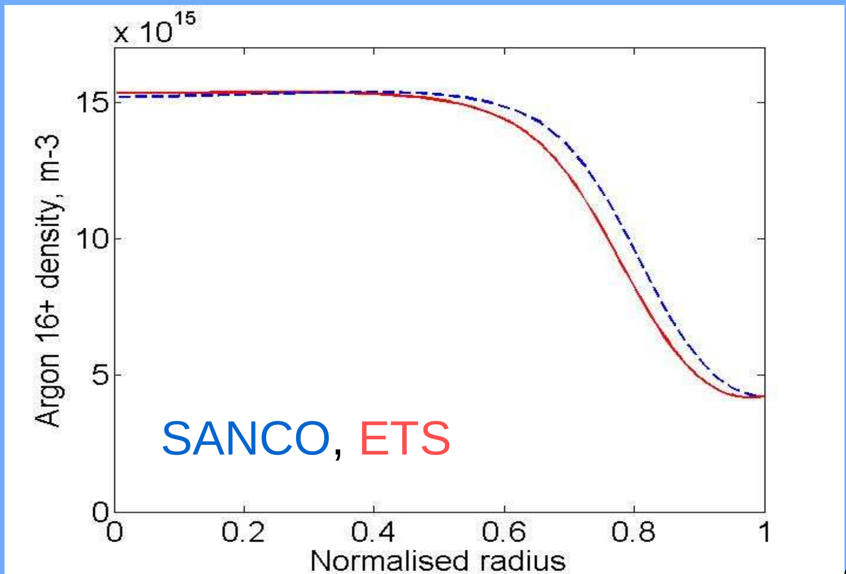
Argon densities with charge states from 11+ to 14+

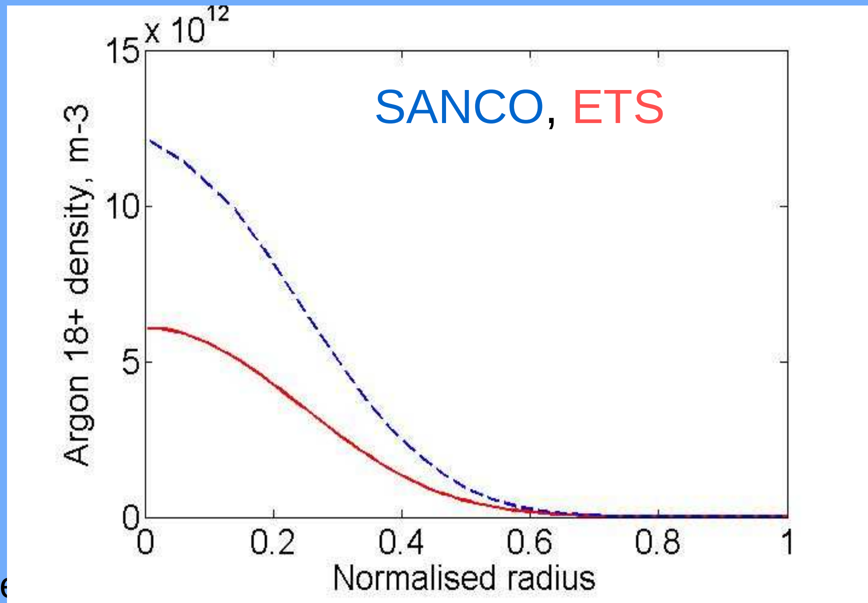


Argon densities with charge states from 15+ to 18+



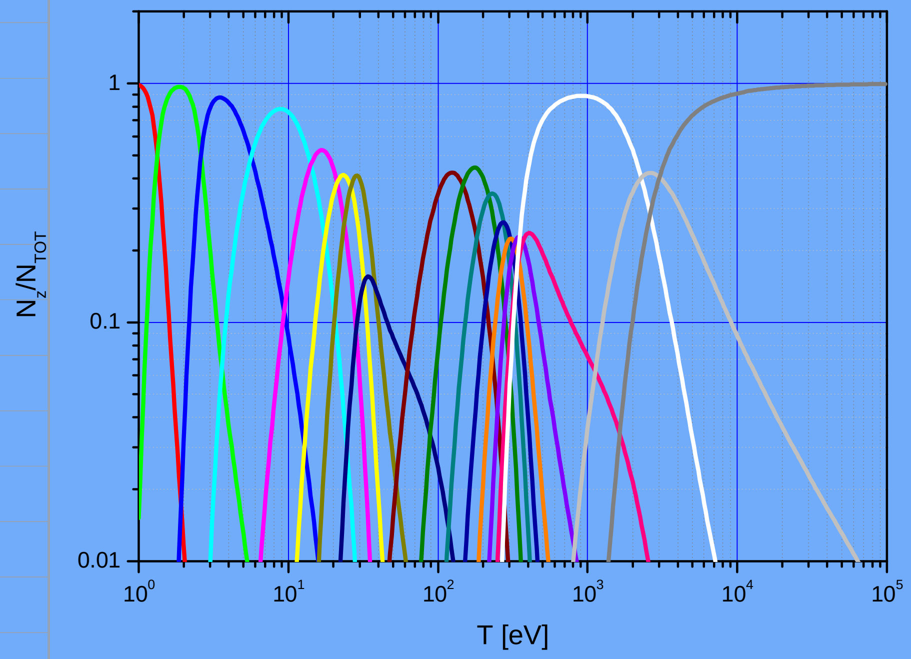






The density on the boundary condition for $N_i^{total}=1.74.10^{16}m^{-3}$ from code SANCO and ETS/Impurity atomic data for 100eV

Argon	***Sanco***	***ETS_Zagórski***
Ar^{+}	$1,55981.\ 10^{12}$	0,44875
Ar^{2+}	$3,33847.\ 10^{12}$	$0,62344.10^{4}$
Ar^{3+}	$7,60142.\ 10^{12}$	$0,88166.10^{7}$
Ar^{4+}	$1,40314.\ 10^{13}$	$0,18392.10^{10}$
Ar^{5+}	$2,39639.\ 10^{13}$	$0,1907.10^{12}$
Ar^{6+}	$4,08639.\ 10^{13}$	$0,14592.10^{14}$
Ar^{7+}	$8,36083.\ 10^{13}$	$0,4265.10^{15}$
Ar^{8+}	$2,55024.\ 10^{14}$	$0,954.10^{16}$
Ar^{9+}	$3,04781.\ 10^{14}$	$0,6027.10^{16}$
Ar^{10+}	$4,92047.\ 10^{14}$	$0,13504.10^{16}$
Ar^{11+}	$8,72677.\ 10^{14}$	$0,4019.10^{14}$
Ar^{12+}	$1,38690.\ 10^{15}$	$0,36192.10^{12}$
Ar^{13+}	$2,75487.\ 10^{15}$	$1,58636.10^{9}$
Ar^{14+}	$3,17999.\ 10^{15}$	$1,736.10^{6}$
Ar^{15+}	$3,74696.\ 10^{15}$	$0,9095.10^{3}$
Ar^{16+}	$4,24036.\ 10^{15}$	0,356
Ar^{17+}	$2,59836.\ 10^{12}$	$0,31355.10^{-13}$
Ar^{18+}	$1,74815.\ 10^{9}$	0



Conclusions

1. Two set of data for coronal equilibrium - R. Zagorski (ETS/impurity code), ADAS (96).(SANCO includes not only ionisation but also recombination)
2. Boundary conditions for impurity density are not always matched in simulations with two codes (no SANCO output for the boundary grid point)
3. Some difference in impurity density at the periphery can be explained by (1) & (2). Forced boundary conditions for Argon, inconsistent with the ETS coronal distribution in the neighbouring grid points → off-axis maximum in Argon profile
4. Difference in core impurity density for Ar, weakly affected by boundary conditions, still need to be investigated (different atomic data?)
5. Differences in power radiation is lower in the ETS/impurity code because it does not include the Bremsstrahlung radiation while in SANCO it is included

6. Next step: ETS/impurity update with Bremsstrahlung & ADAS data