Role of atomic data in the ITC impurity transport code : the example of Ni

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1. Principle : $n_Z(z, r, t)$ calculation from hypothesis on transport
   → Role of ionisation / recombination rate coefficients

2. Method : match calculated emission with measurements
   → Role of emission coefficients

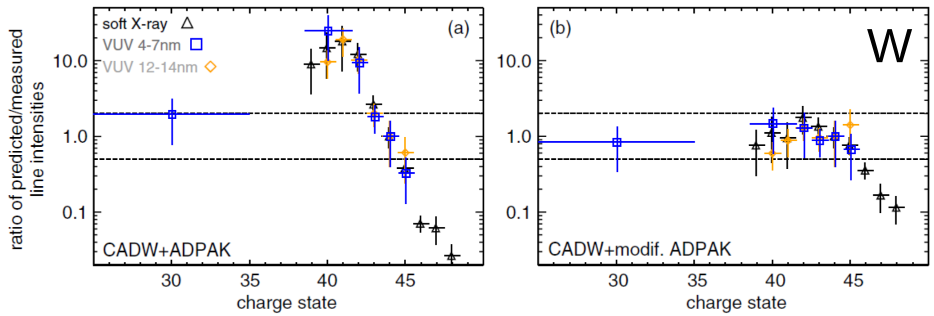
3. Consequences on determination of experimental transport

Introduction

• Impurity transport codes (ITC, UTC, STRAHL,...) use many types of rate coefficients : ionisation, recombination,
spectral line emission (UV, soft-X, CX),
continuum

• Importance of data quality not easy to assess :
measurements integrated over inhomogeneous plasma,
rather lengthy minimisation process, many parameters

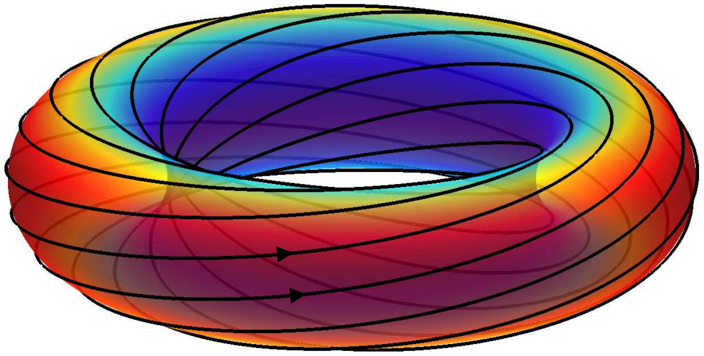
• It has been shown earlier that atomic data matter : e.g. Th. Pütterich PPCF 2008, but not much information available about effect on transport

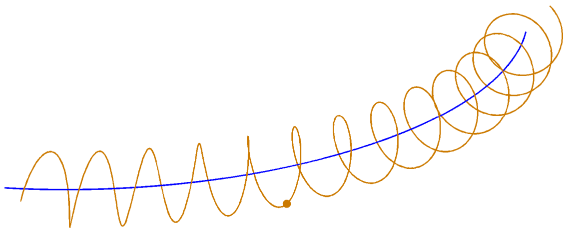


• Investigation made with ITC (CEA) : historical DB (Mattioli) / ADAS

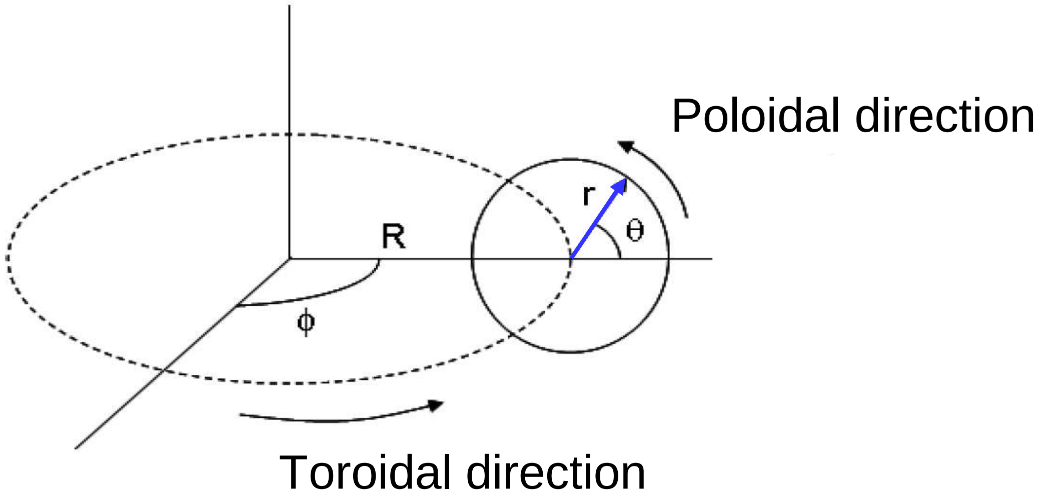
(Tokamak configuration)

Magnetic field lines define closed, toric surfaces



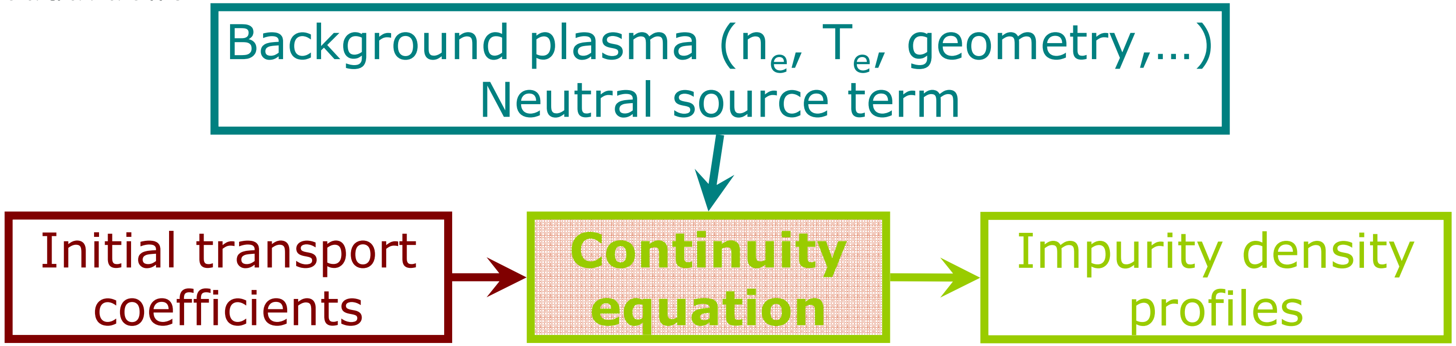


Transport along field lines is very fast ⇒ assume toroidal, poloidal symmetry



Physics is assumed to depend only on the minor radius r

1. Principle : $n_Z(z, r, t)$ calculation from hyp. transport



- Resolution of continuity equation for each ionisation stage

$$\frac{\partial n_Z}{\partial t} + \nabla\Gamma_Z = \alpha n_e n_Z + S n_e n_Z + S_{Z_0}$$

Recombination and ionisation — **Neutral source**

- Transport model : **diffusion** - **convection**

$$\Gamma_Z(r) = -D_Z(r)\nabla_r n_Z(r) + V_Z(r) n_Z(r)$$

$$D_Z = \begin{pmatrix} D_Z & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & D_Z \end{pmatrix} \qquad V_Z = \begin{pmatrix} V_Z & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & V_Z \end{pmatrix}$$

$$\alpha = \begin{pmatrix} 0 & \alpha_1 & 0 & & & 0 \\ 0 & -\alpha_1 & \alpha_2 & 0 & & 0 \\ 0 & 0 & -\alpha_2 & \ddots & 0 & 0 \\ & & 0 & \ddots & \ddots & \vdots \\ & & & 0 & -\alpha_{Z-1} & \alpha_Z \\ 0 & 0 & 0 & \dots & 0 & -\alpha_Z \end{pmatrix}$$

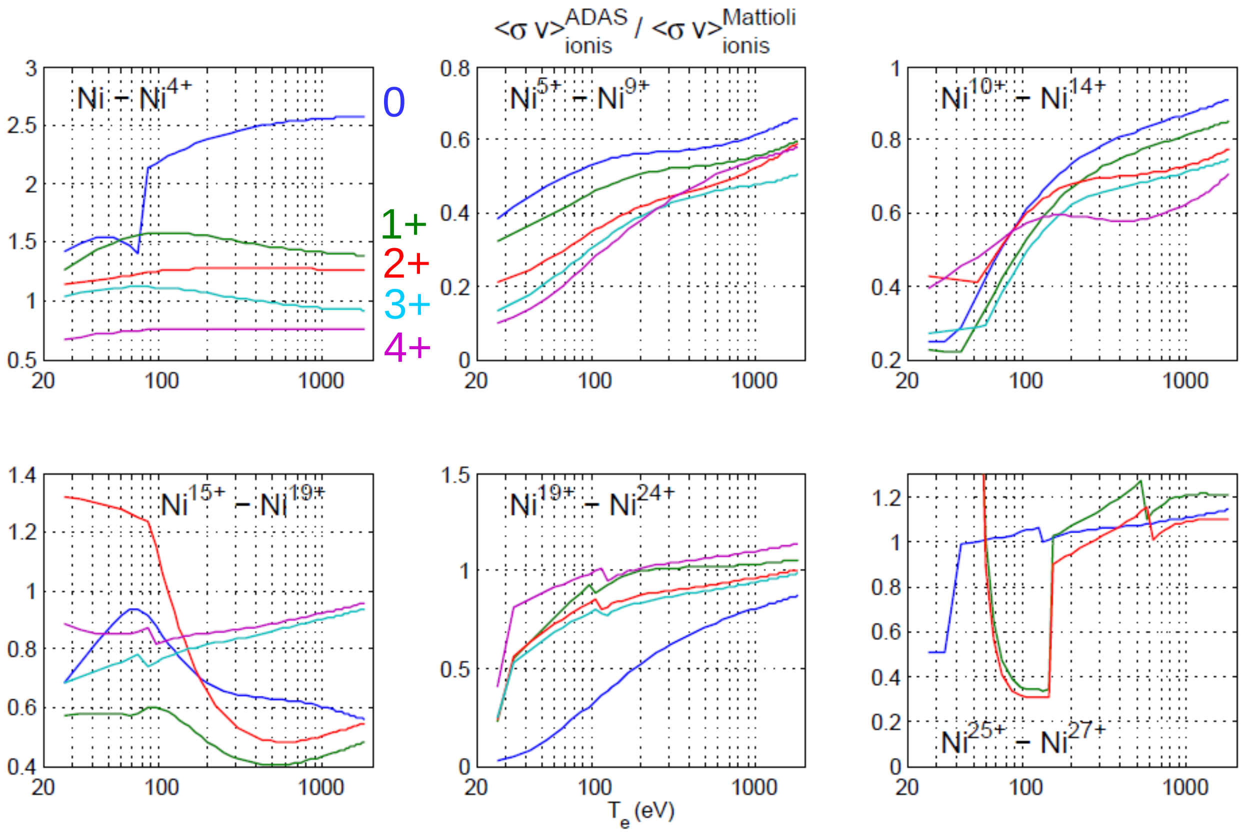
Recomb.

$$S = \begin{pmatrix} -S_0 & 0 & 0 & & & 0 \\ S_0 & -S_1 & 0 & & & 0 \\ 0 & S_1 & -S_2 & 0 & & 0 \\ & 0 & \ddots & \ddots & 0 & \vdots \\ & & 0 & \ddots & -S_{Z-1} & 0 \\ 0 & 0 & 0 & \dots & S_{Z-1} & 0 \end{pmatrix}$$

Ionis.

1.1. Ionisation rate coefficients

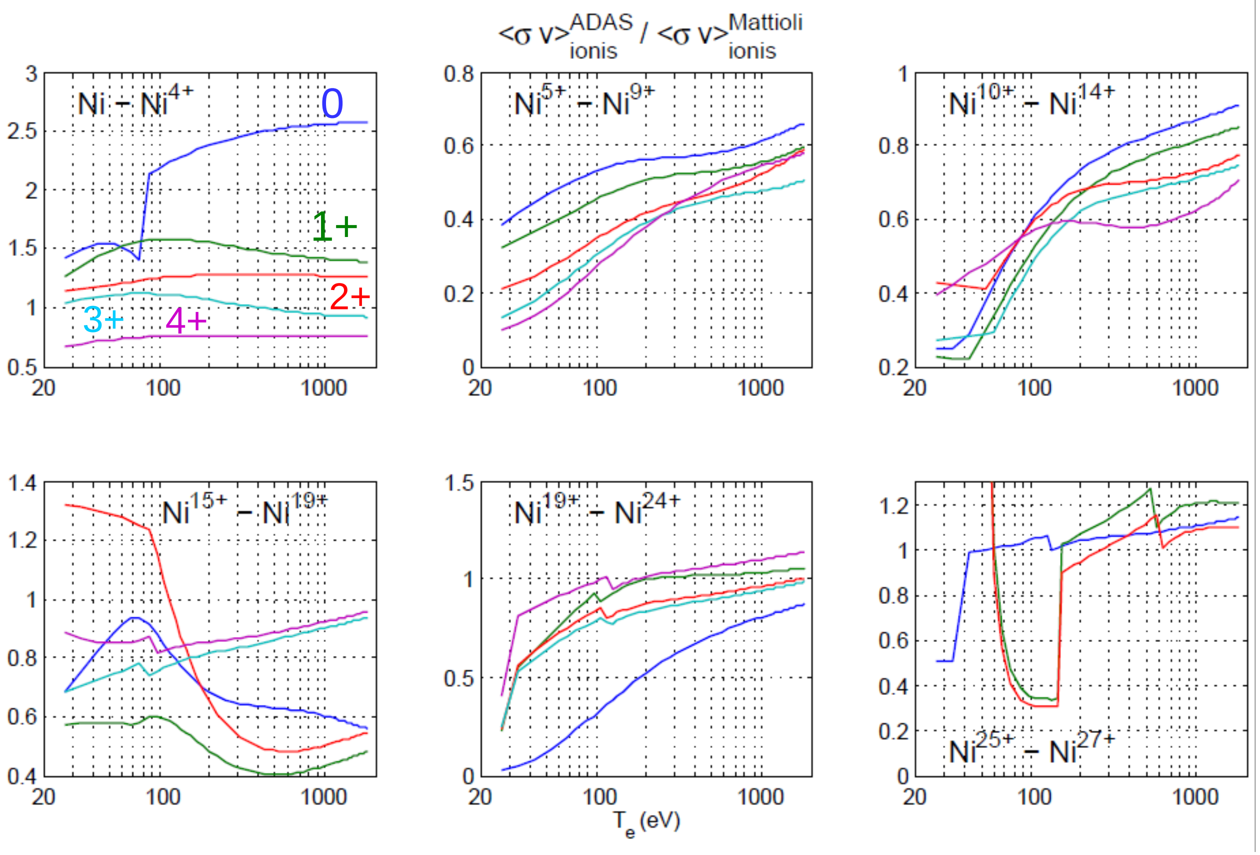
- **ADAS (solid) :** ADAS 408 on ADF03 atompars/atompars#ms_ni.dat
- **Mattioli (dashed) :** M.S. Pindzola et al., Physica Scripta T37, (1991) 35
  (includes inner shell excit. + autoionis.)



- T_e dependences very similar
- Differences not much more than factor 5, gets smaller for higher ionisation stages

1.1. Ionisation rate coefficients

Ratios ADAS / Mattioli



Ratios ~ 1 for ions of greater importance (higher charge) irfm cea cadarache

1.2. Recombination rate coefficients

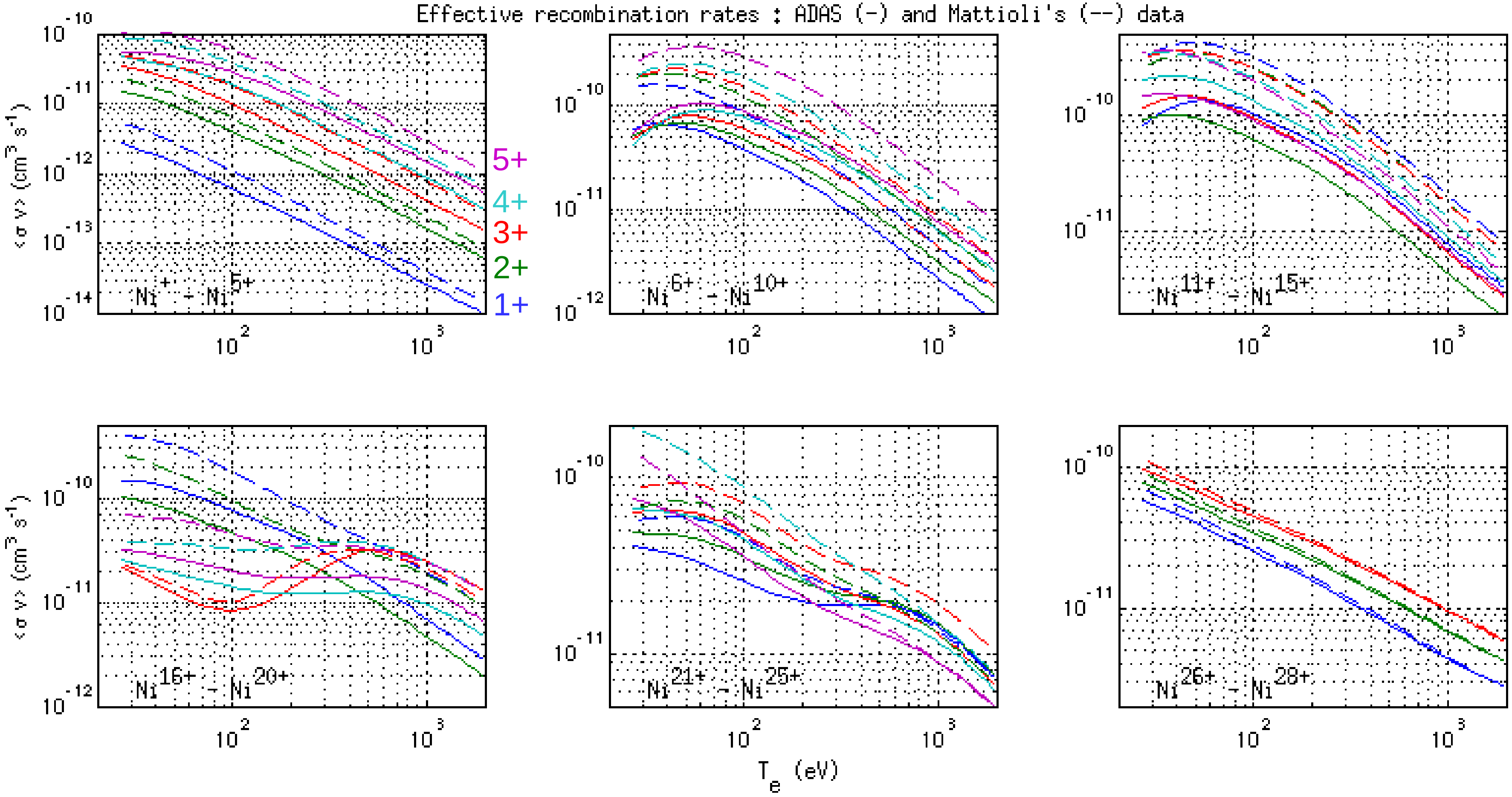
- **ADAS (solid) :** ADAS408 on ADF03 atompars/atompars#ms_ni.dat:
  Dielectronic : adjusted Burgess general formula or R-matrix (Badnell)
  Radiative : analytic formula

- **Mattioli 1988 (dashed) :**
  Dielectronic from various authors:
  (H He) Arnaud & Rothenflug 1985 (Shull & Van Steenberg 1982)
  (Li O F) Roszman 1987, (Be) Badnell 1987,
  (B C N) Burgess 1965 - Merts 1976 + Badnell 1986
  (Ne) Chen 1986 + Smith 1985
  (Na Mg) Burgess 1965 - Merts 1976 + U. Connecticut 1984-7
  (Al and >) Burgess 1965 - Merts 1976 ~ A-R

  Radiative from formulae ~ Arnaud & Rothenflug 1985

1.2. Recombination rate coefficients

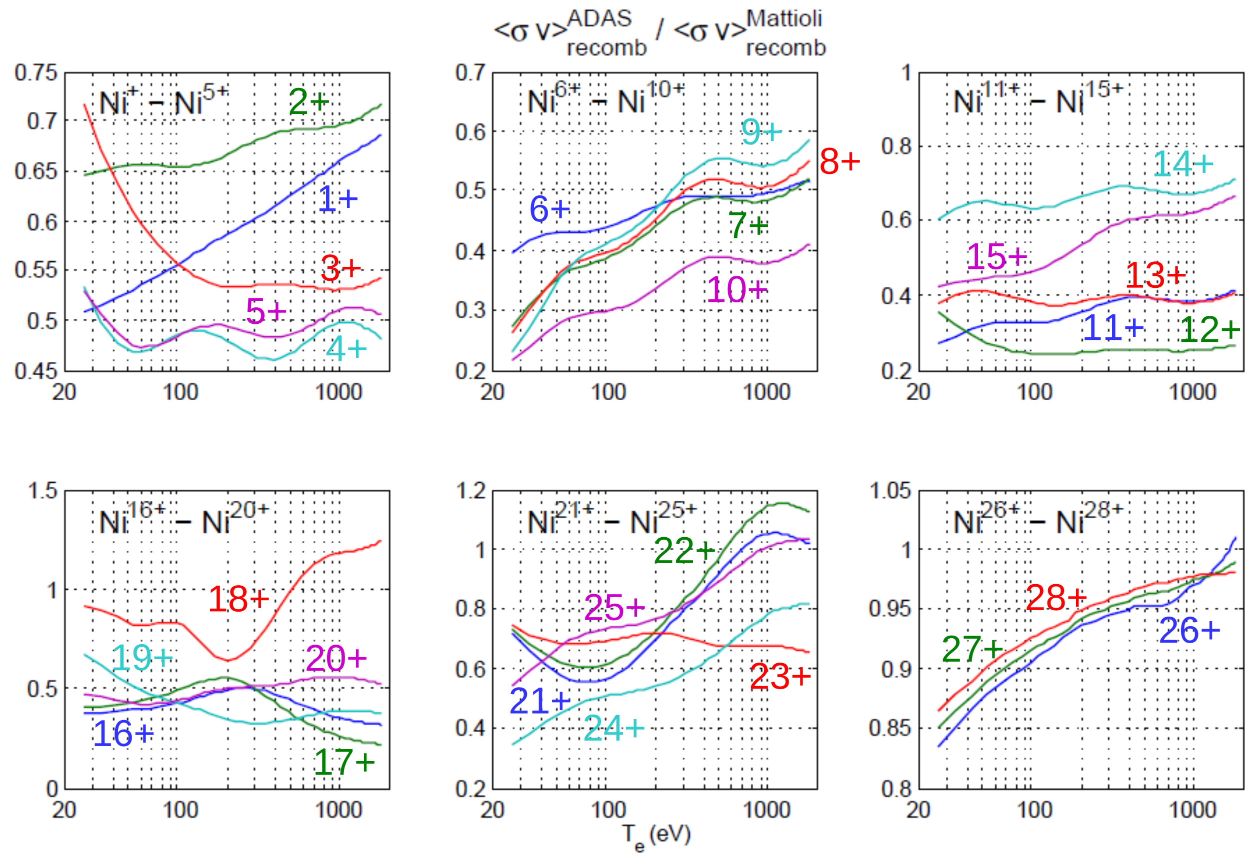
- **ADAS (solid), Mattioli (dashed) :**



- T_e dependences very similar
- Differences not much more than factor 2, very small for He-like to fully stripped

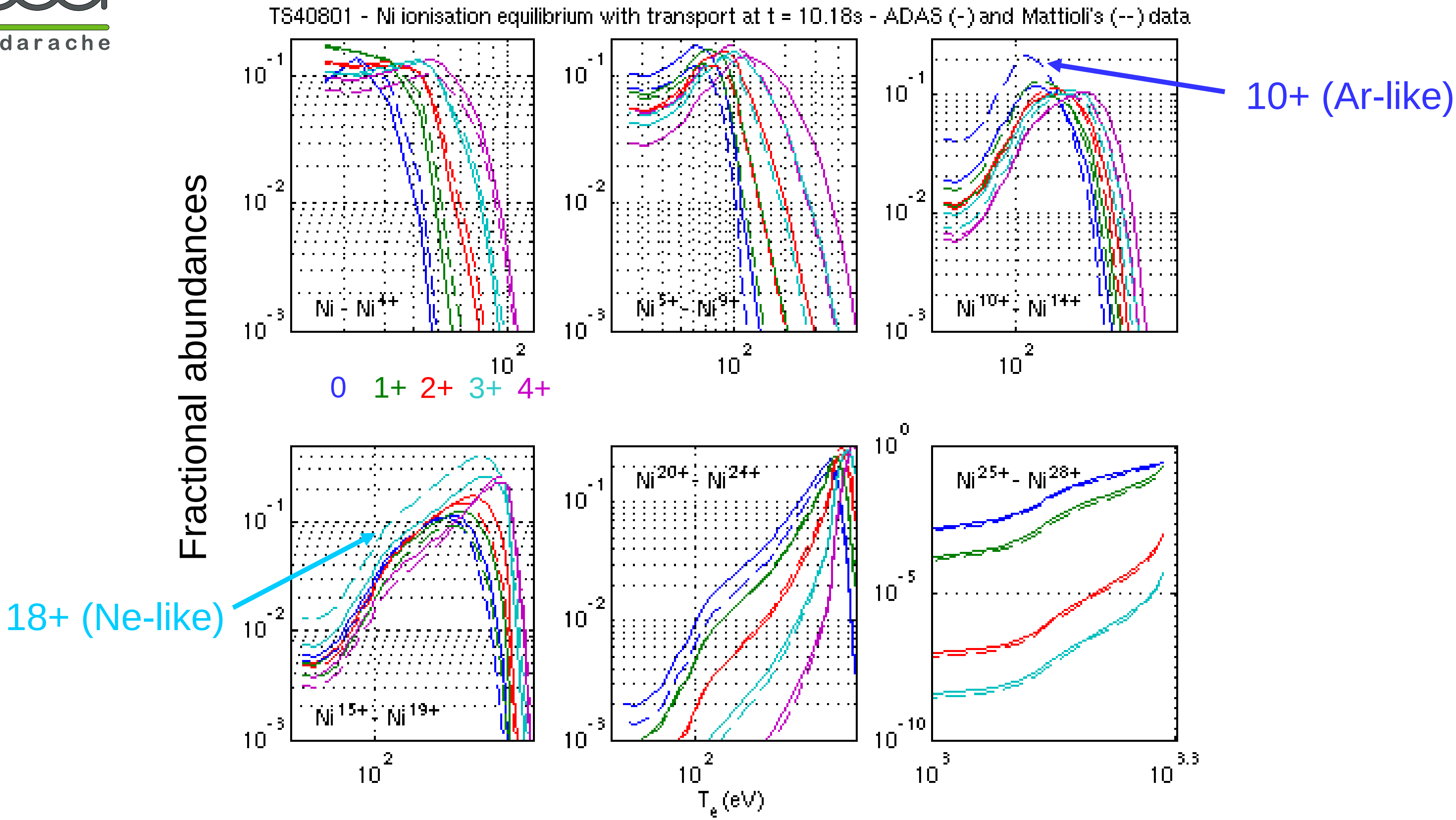
1.2. Recombination rate coefficients

Ratios ADAS / Mattioli



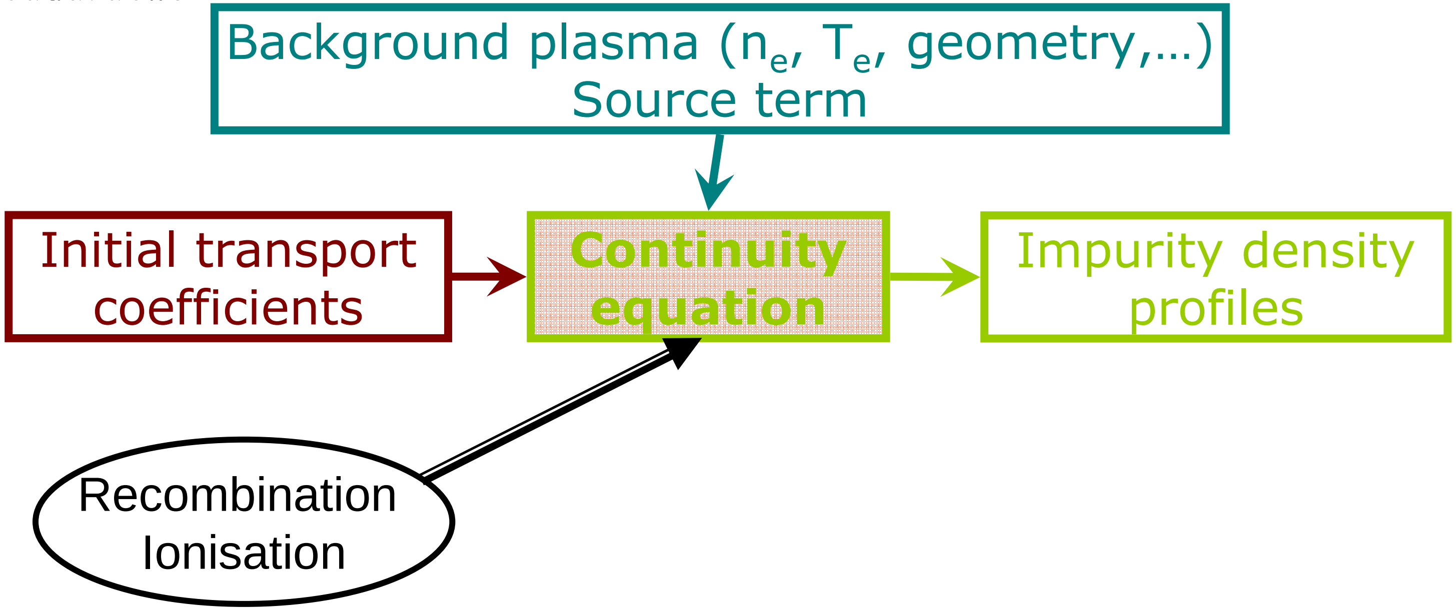
ADAS data always smaller than Mattioli but by a factor ≤ 2

1.3. Ionisation equilibrium (including transport)

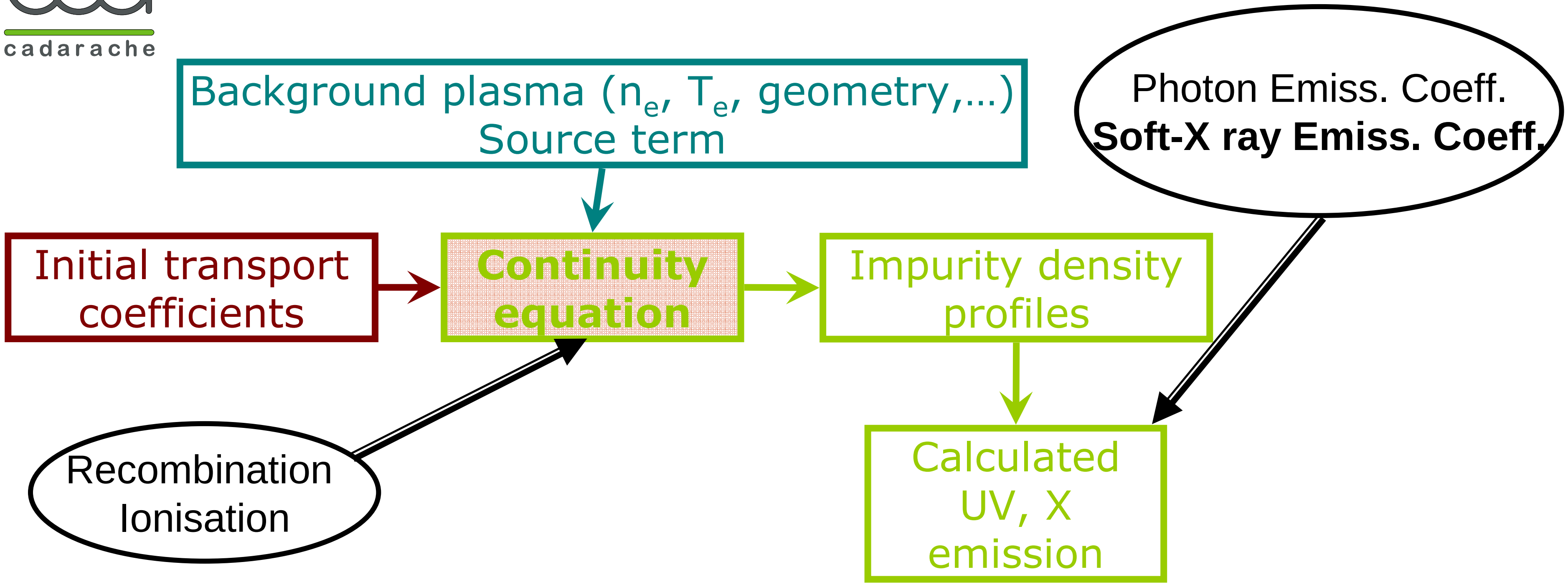


- Ionisation equilibrium not very different
- Ar-like and Ne-like, enhanced by ‘Mattioli’ data

2. Method : match calculated emission with measts

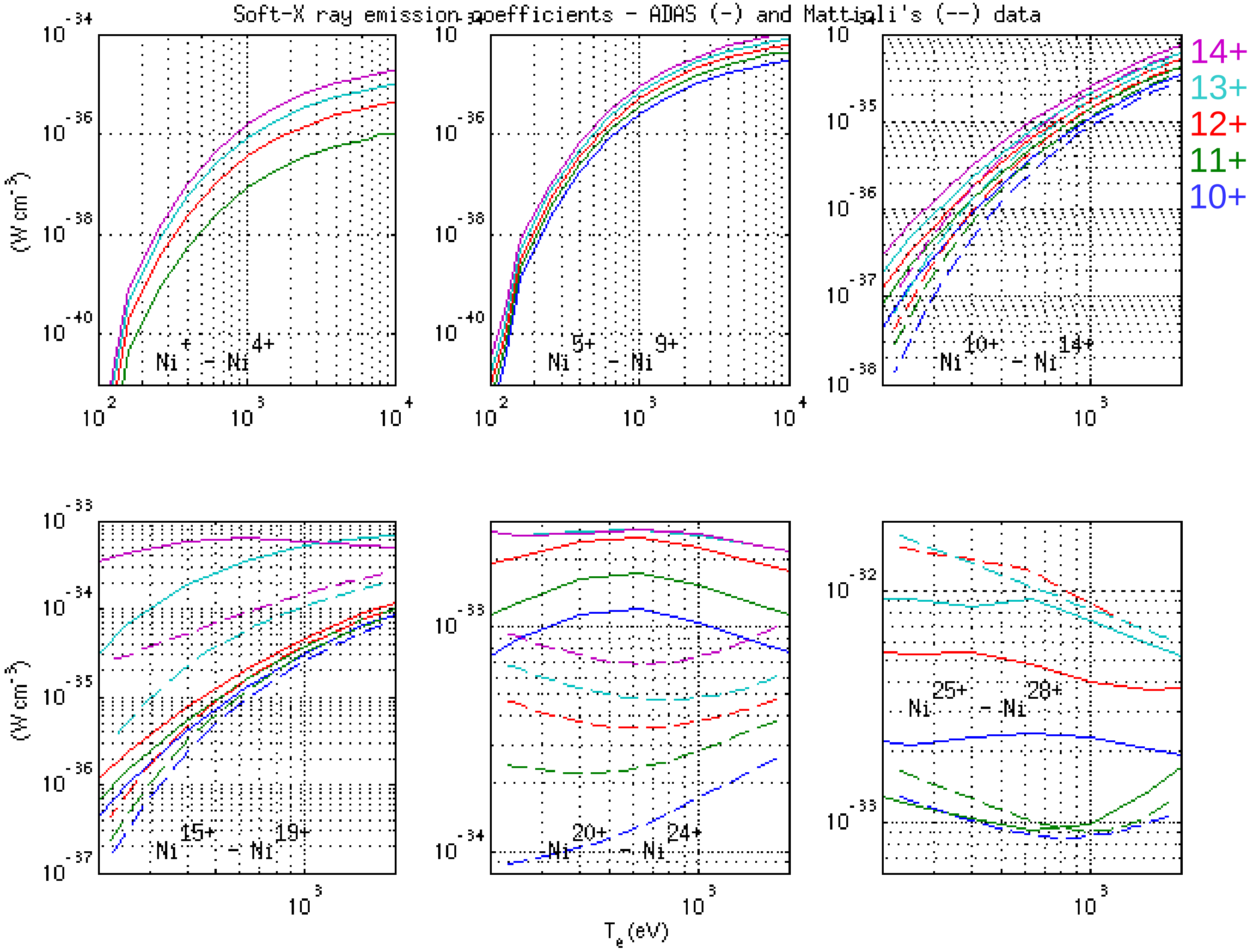


2. Method : match calculated emission with measts



2.1. Soft-X ray emission rate coefficients

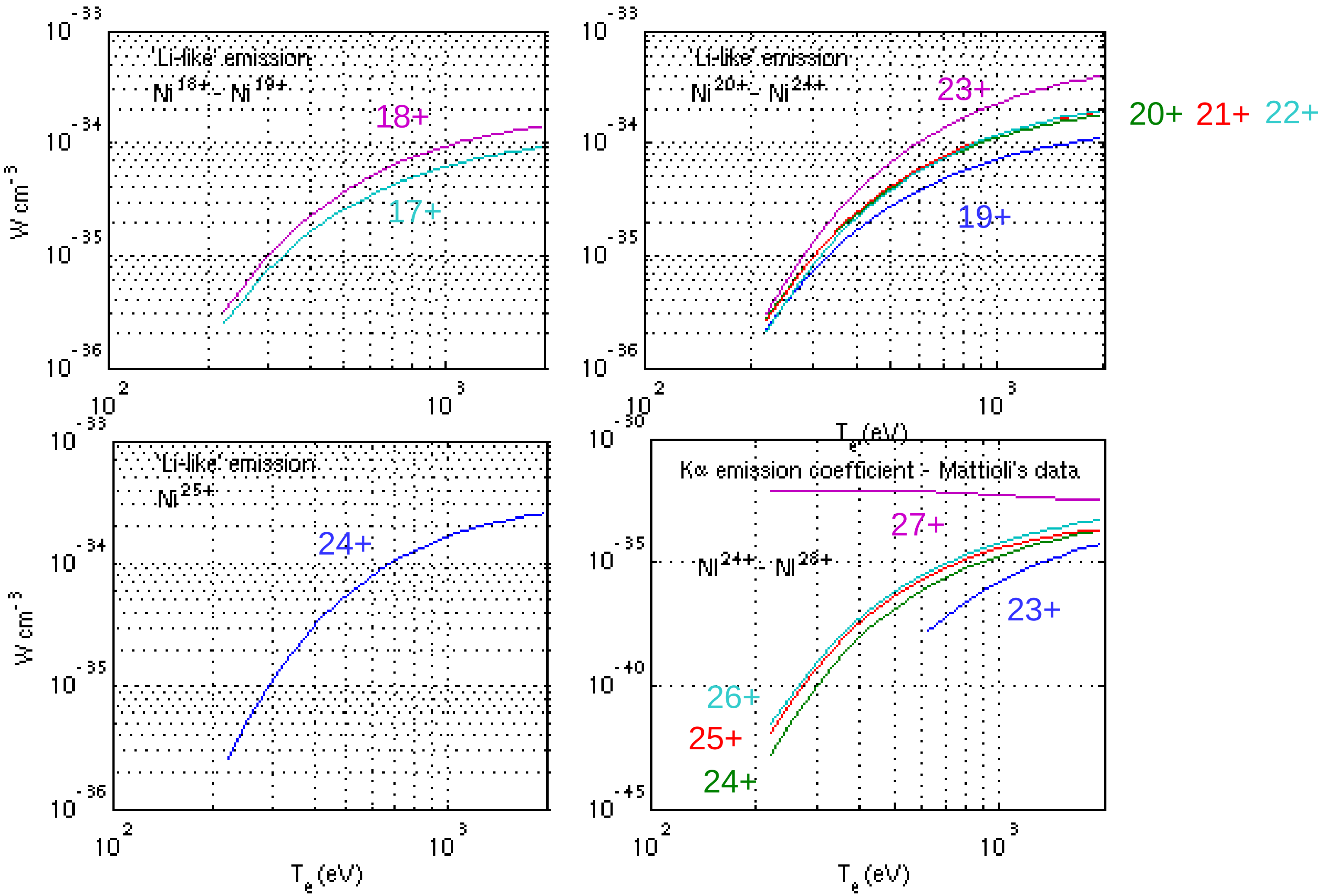
- **ADAS (solid), Mattioli (dashed)**



Large differences from 18+ (Ne-like) up

2.1. Soft-X ray emission rate coefficients

• **Mattioli : separate Kα and L spectrum contributions**



2.2. Soft-X ray emission rate coefficients: detail

Mattioli :

- Bremsstrahlung : known formulae + Hummer 1988, Carson 1987 (KL 1961)
  Mattioli's code consistent with :

$$P_Z^{Brems} \propto \frac{n_e n_Z}{\sqrt{kT_e}} g_{ff} e^{-h\nu/kT_e}$$ (proportionality coefficient?)

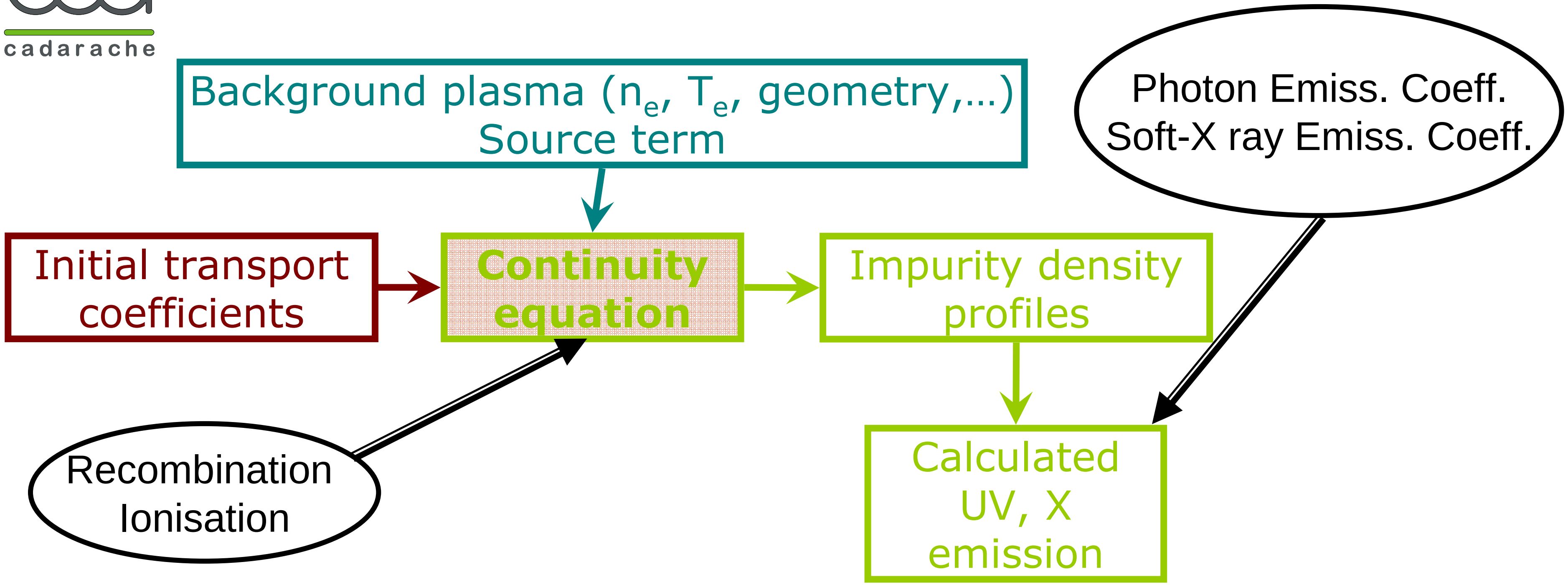
- Recombination: Burgess & Summers 1987 (KL 1961)

- Kα: Clark 1982 H-like Lyα
  He-like w
  Bombarda 1988 He-like (x+y+z)/w
  He-, Li-, Be-, B-like satellites
  H-like recombination contrib. to x, y, z, w

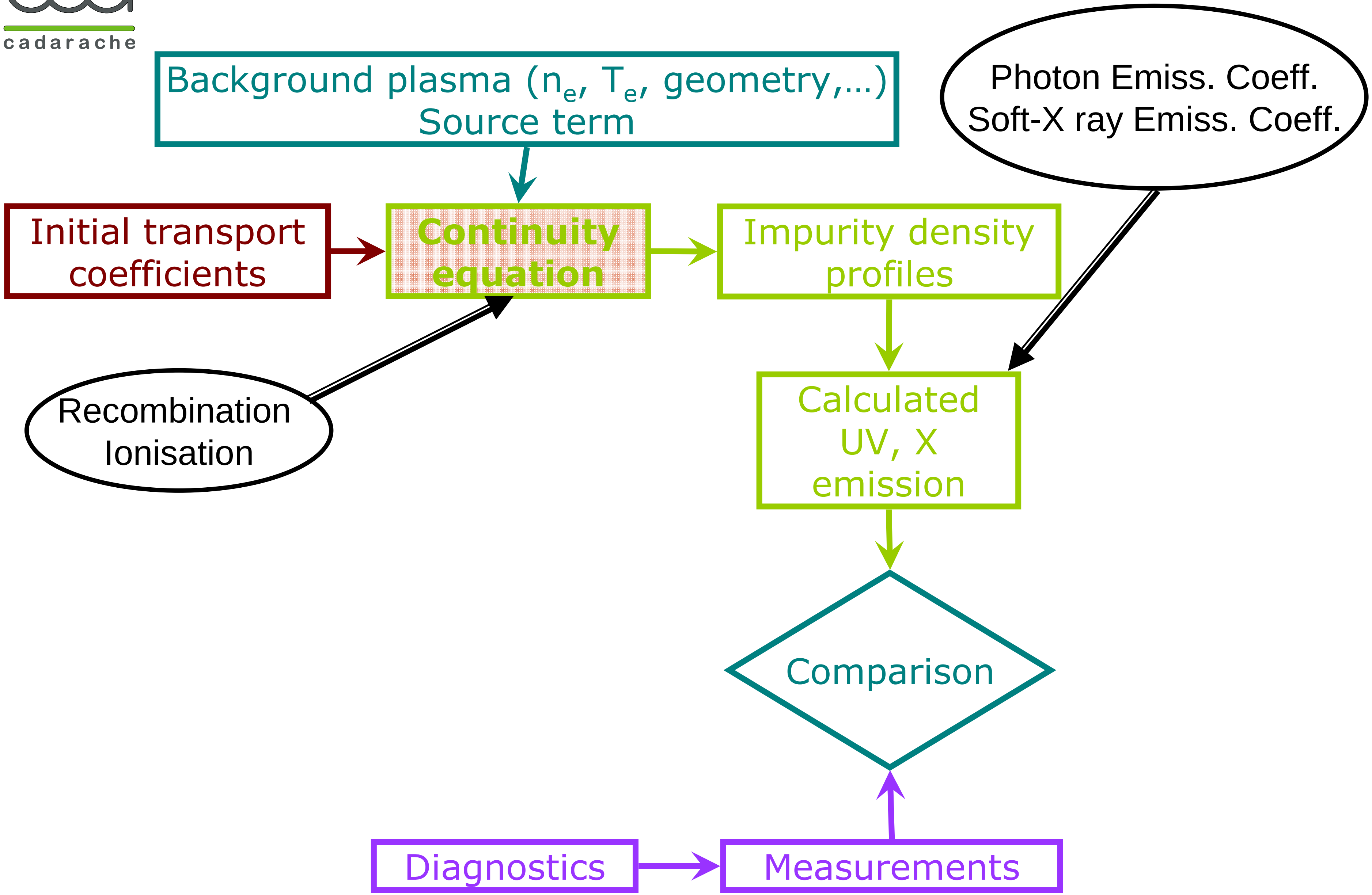
- L series: 2-3 transitions for Li- to Ne-like → analytic formula
  B-, C-, N- and Ne-like : Bhatia 1985-89
  Li-like : Cochrane 1983

ADAS :

2. Method : match calculated emission with measts

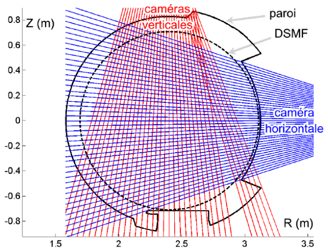


2. Method : match calculated emission with measts



3.1. Effect of ionis./recomb. coefficients in emission calculations

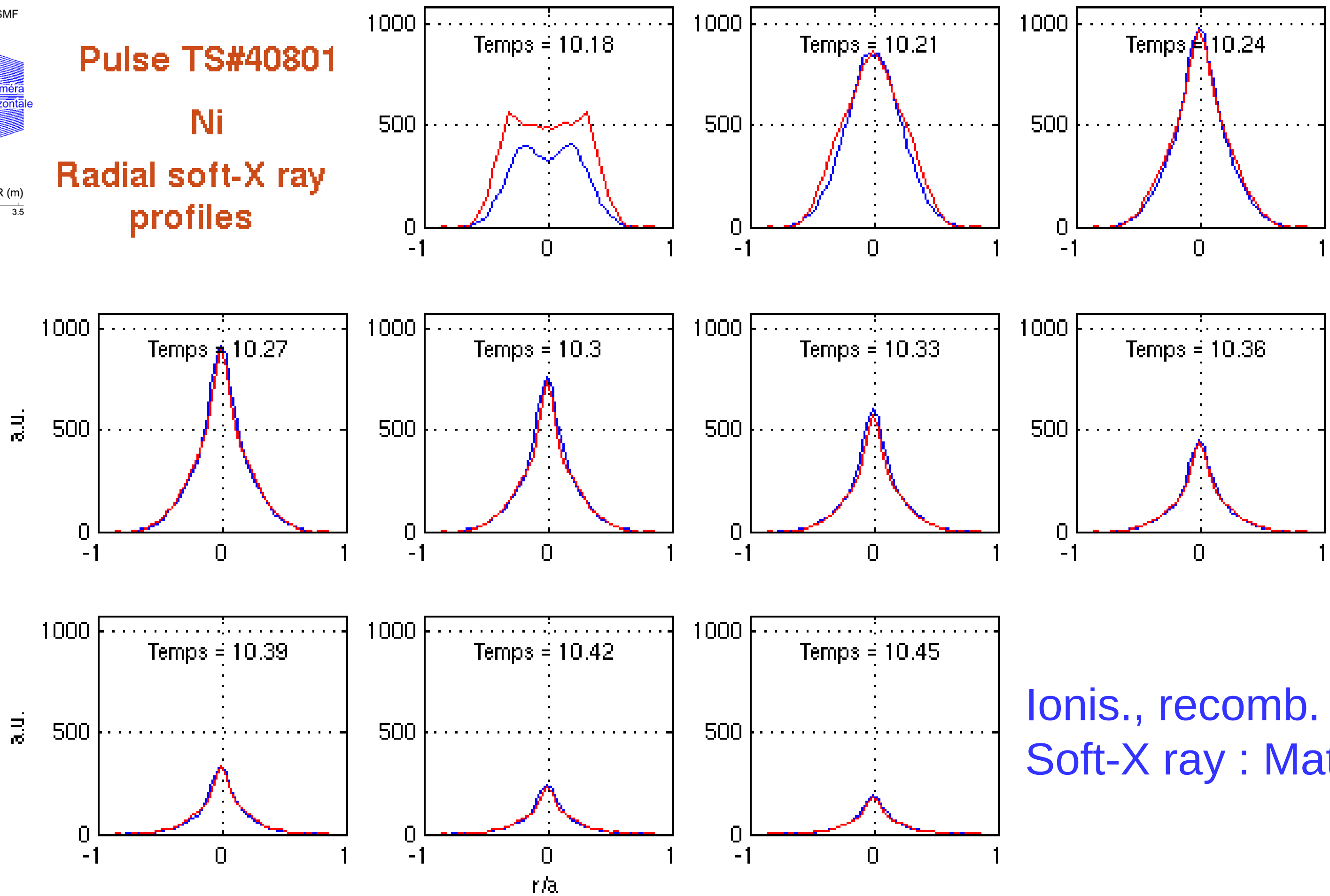
- Opimisation of the transport coefficients has been performed with ‘Mattioli’ data



Pulse TS#40801

Ni

Radial soft-X ray profiles



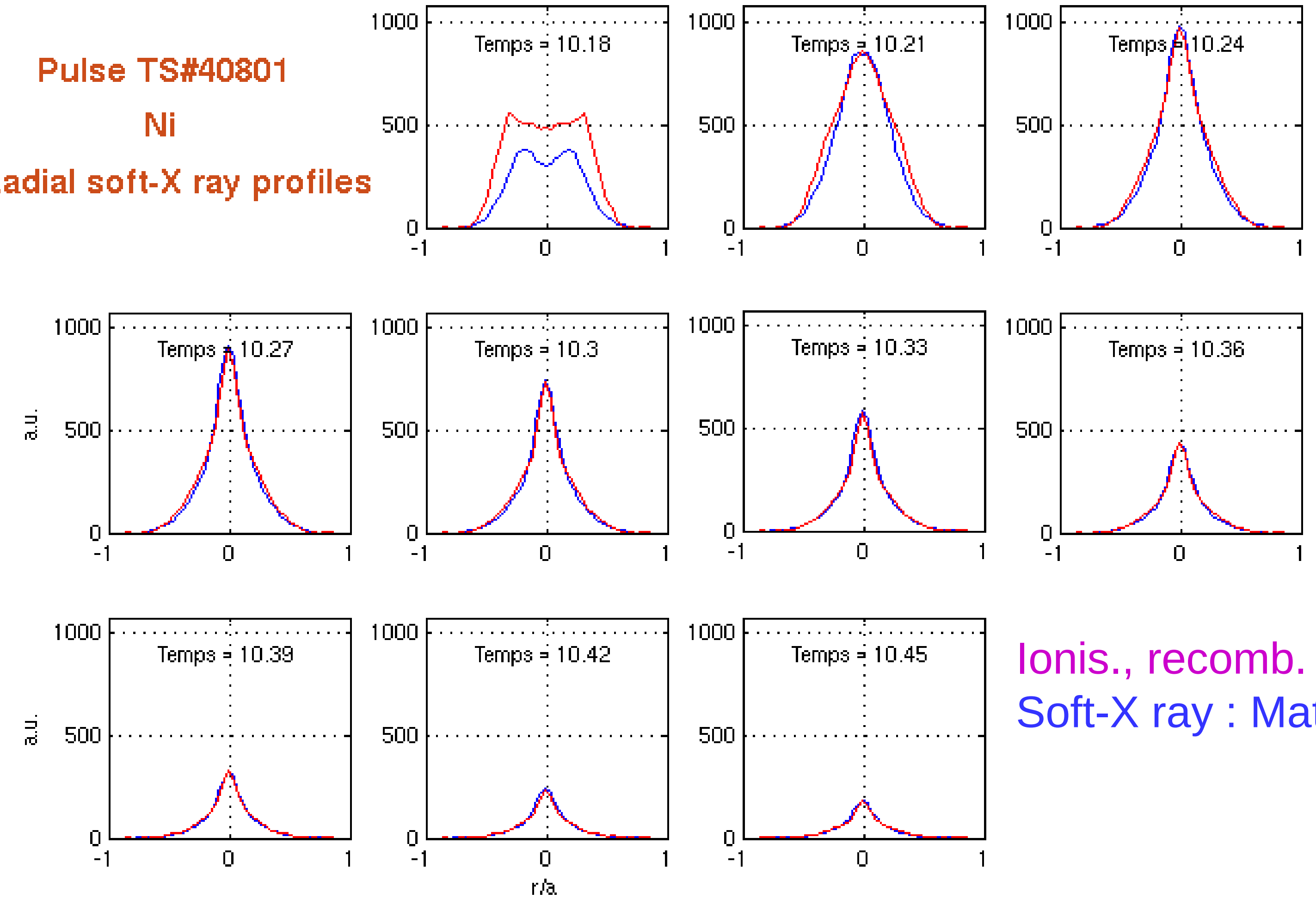
Ionis., recomb. : Mattioli
Soft-X ray : Mattioli

3.1. Effect of ionis./recomb. coefficients in emission calculations

Pulse TS#40801

Ni

Radial soft-X ray profiles



Ionis., recomb. : ADAS

Soft-X ray : Mattioli

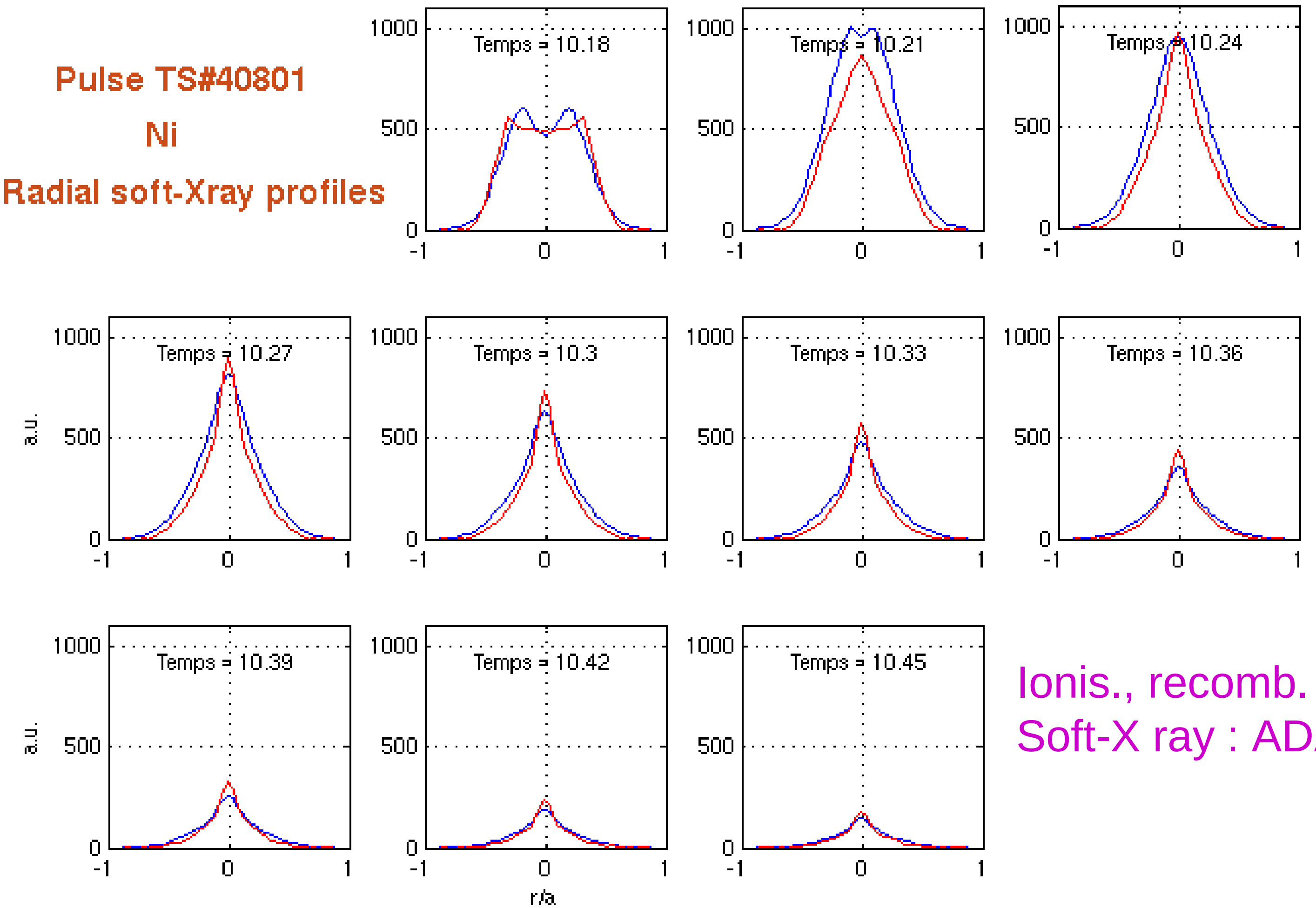
Calculated emission weakly sensitive to ionisation equilibrium (coefficients within factor 2)

3.2. Effect of soft-X ray coefficients in emission calculations

Pulse TS#40801

Ni

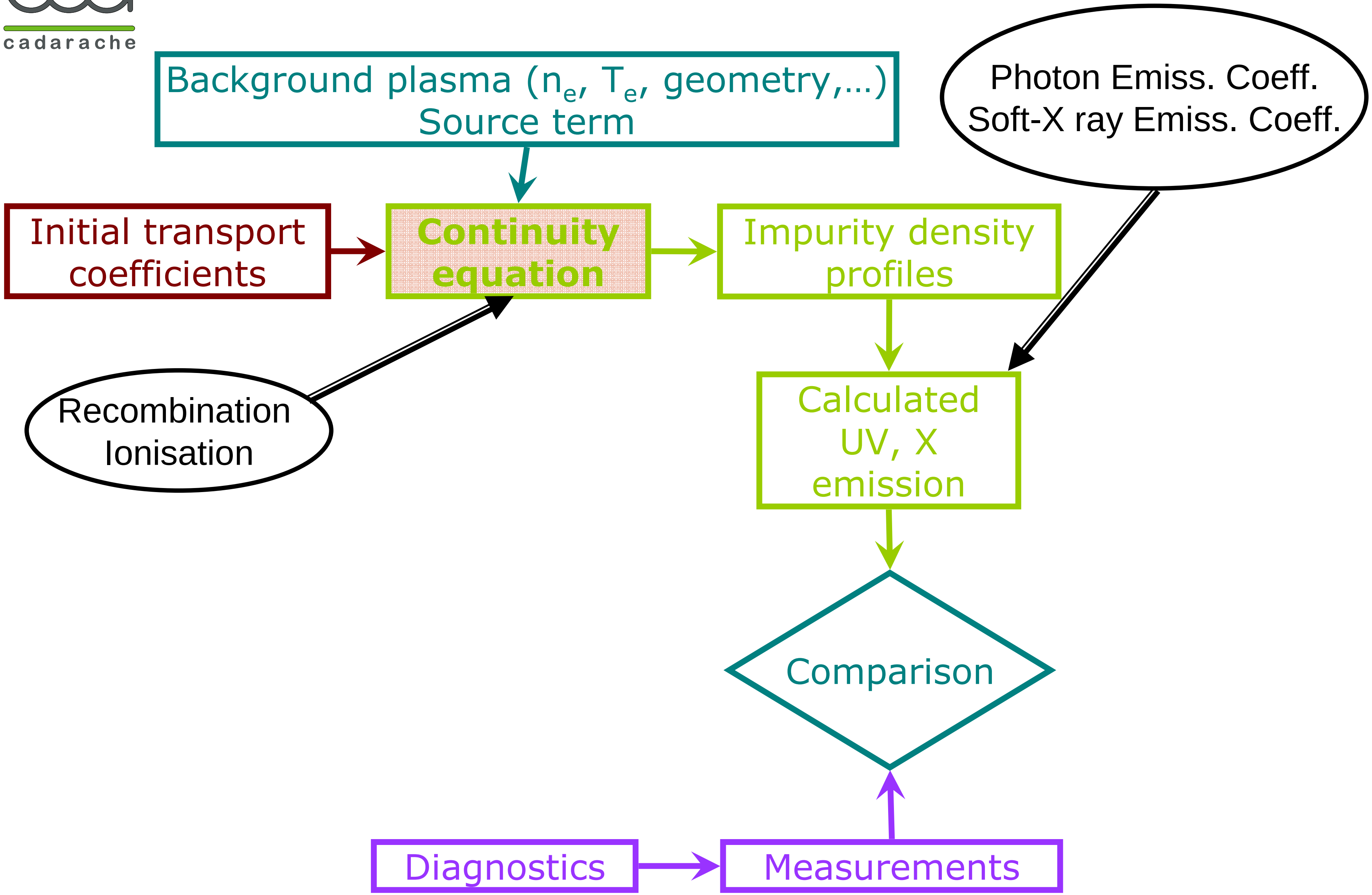
Radial soft-Xray profiles



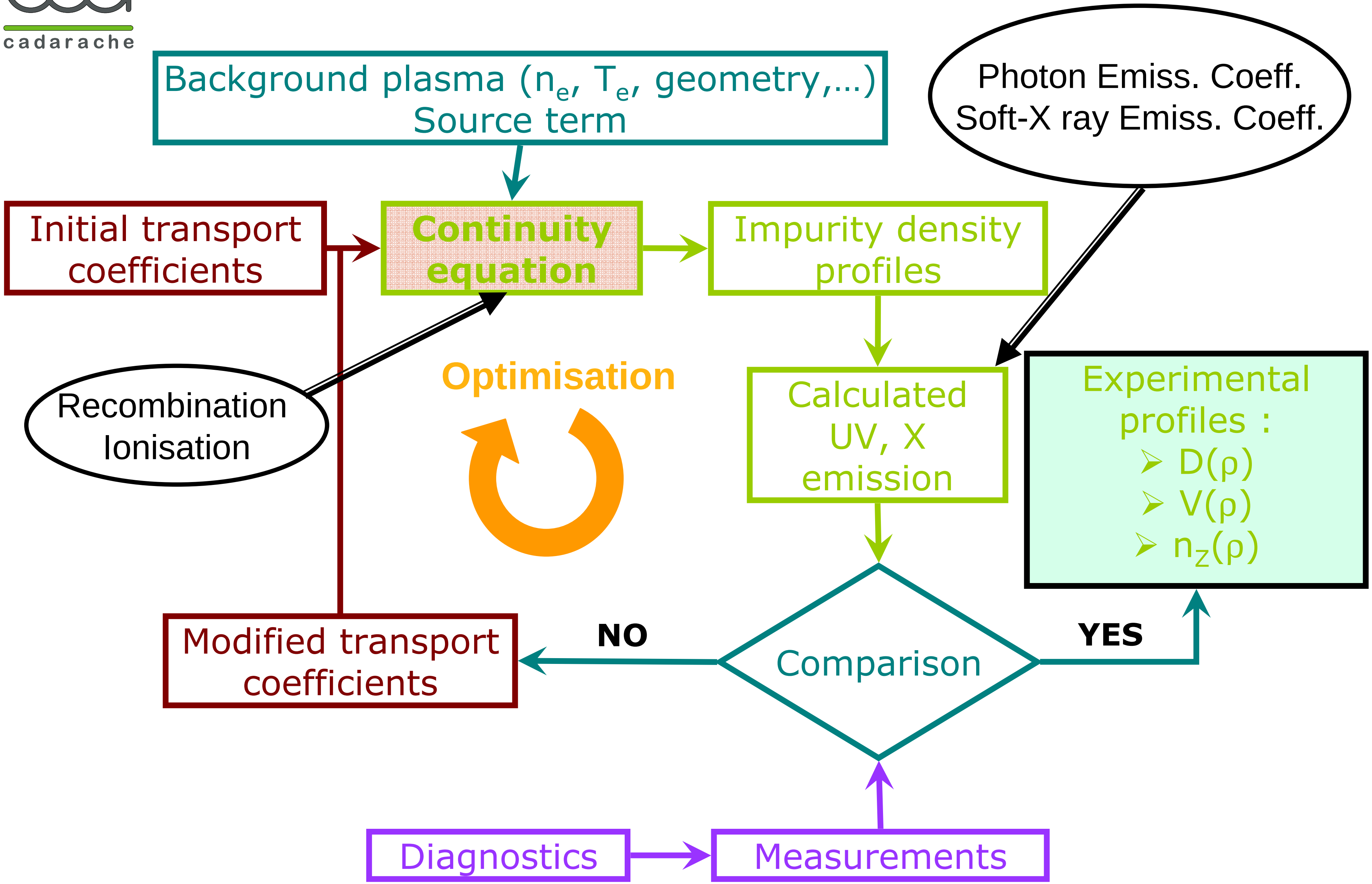
Ionis., recomb. : ADAS
Soft-X ray : ADAS

Calculated emission very sensitive to soft-X ray emission coefficients

2. Method : match calculated emission with measts



2. Method : match calculated emission with measts



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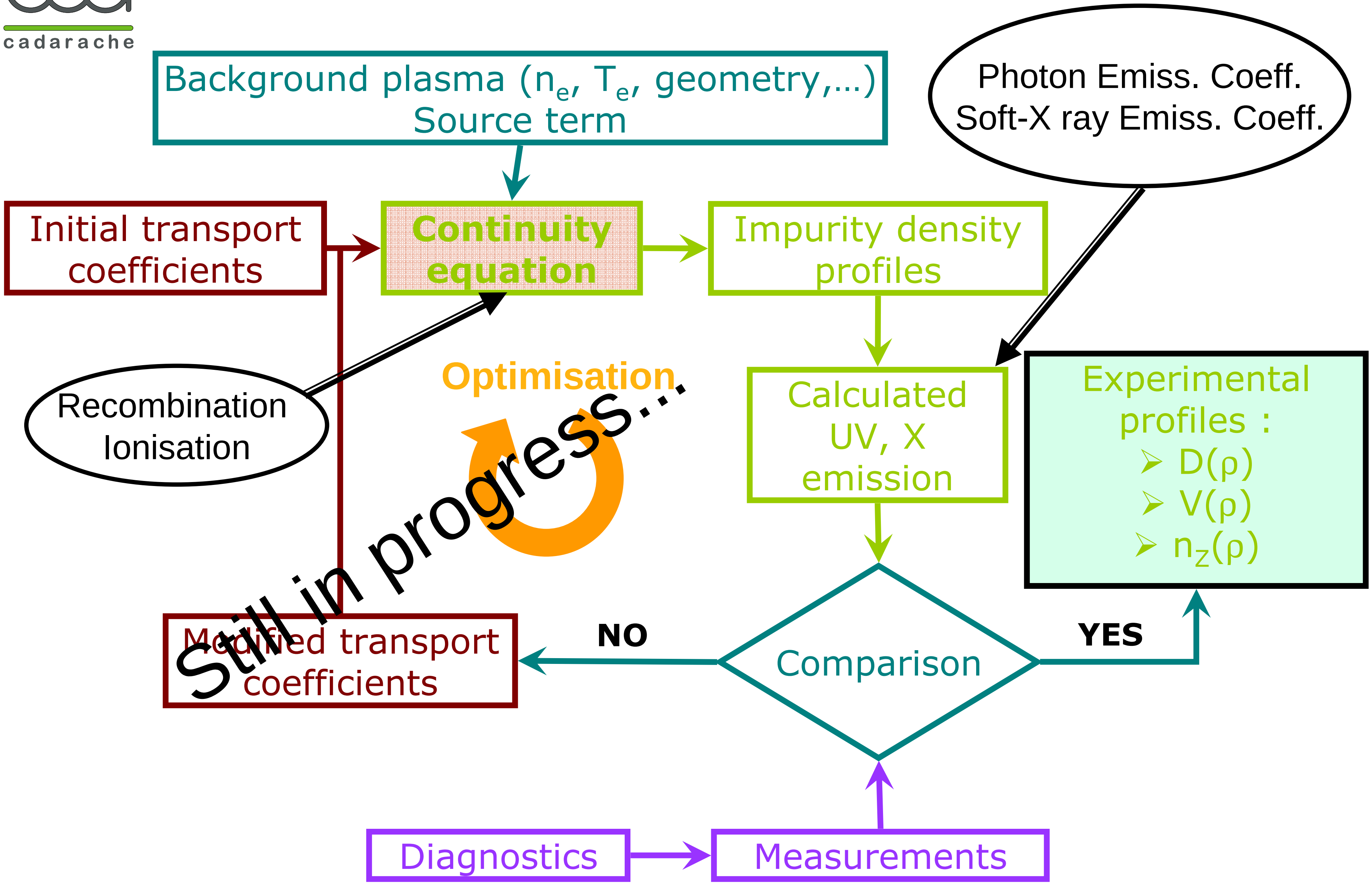

Conclusions

Atomic physics:

- Ionisation
  Factors up to 5 between ADAS and 'Mattioli' rate coefficients
  Difference smaller for higher charge states

- Recombination
  ADAS rate coeff. smaller by a factor 1-3

  → Ionisation equilibrium : Mattioli's coefficients favour Ar- and Ne-like

- **Soft-X ray emiss. coefficients: large differences (~ 10) for Ne-like and above**

Transport:

- **Soft-X ray emission coefficients essential** (value + T_e dependence)

- Small differences in ionisation equilibrium have a weak effect on calculated emission (soft-X ray, UV)

- UV PEC T_e dependence relatively unimportant for emitters confined on narrow layers, absolute values must be consistent with soft-X ray coeff.

➥ In progress : **propagation of atomic physics uncertainties to transport**

Mattioli's bibliographic database (1)

- Ionisation rate coefficients

  M.S. Pindzola et al., Physica Scripta T37, (1991) 35 *(includes inner shell excit. + autoionis.)*

- Recombination rate coefficients

→ *Dielectronic from various authors*:

(H He) Arnaud & Rothenflug, Astron. Astrophys Suppl.Ser. 60 (1985) 425
Schull & Van Steenberg, Astrophys. Suppl. Ser. 48 (1982) 95
(Li O F) Roszman, Phys. Rev. A 35 (1987) 2122
(Be) Badnell, J. Phys. B 20 (1987) 2081
(B C N) Burgess, Astrophys. J. 141 (1965) 1588
Merts, Los Alamos Scientific Lab. Report LA-6220-MS (1976)
Badnell, J. Phys. B 20 (1986) 3827
Roszman, Phys. Rev.A 35 (1987) 2138 & 3368
(Ne) Chen M.H., Phys. Rev. A 34 (1986) 994
Smith B.W., Astrophys. J. 298 (1985) 898
(Na Mg) Burgess – Merts
Lagatutta, Phys. Rev. A 30 (1984) 316
Dube, J. Quant. Spectrosc. Radiat. Transfer 33 (1985) 13
Dube, J. Quant. Spectrosc. Radiat. Transfer 38 (1987) 311
(Al and >) Burgess - Merts ~ A-R

→ *Radiative from formulae* ~ A-R

Mattioli's bibliographic database (2)

→ Radiative from formulae ~ A-R

Fully stripped : $\alpha_{rZ} = 5.2\times10^{-14} Z^2 \sqrt{\frac{I_H}{T_e}}\phi_1(\beta)$ with

$$I_H = 13.6eV$$

$$\beta = Z^2 \frac{I_H}{T_e}$$

$$\phi_1(\beta) = \sum_{n=1}^{\infty} \frac{\beta}{n^3} e^{\beta/n^2} E_1\left(\frac{\beta}{n^2}\right)$$

Others : $\alpha_{rZ} = 2.6\times10^{-14}(\alpha_1 + \alpha_2)$ with

$$\alpha_1 = Z^2 \sqrt{\frac{I_H}{T_e}} \frac{\xi}{n^3} \frac{I_{Z-1}}{T_e} e^{I_{Z-1}/T_e} E_1\left(\frac{I_{Z-1}}{T_e}\right)$$

$$\alpha_2 = 2Z^2 \sqrt{\frac{I_H}{T_e}} \phi_{n+1}\left(Z^2 \frac{I_H}{T_e}\right)$$

(ξ empty sites in valence shell n)

Mattioli's bibliographic database (3)

- Soft-X ray emission rate coefficients

- Bremsstrahlung: known formulae
  Hummer, Astrophys. J. 327 (1988) 477
  Karzas, Astrophys. J. Suppl. Ser. 6 (1961) 167
  Carson, Astronom. Astrophys. 189 (1988) 319

- Recombination: Burgess & Summers, Mon. Not. R. Astr. Soc. 226 (1987) 257

- Kα spectrum: Clark, Astrophys. J. 254 (1982) 412
  H-like Lyα
  He-like w

  Bombarda, Phys. Rev. A 37 (1988) 504
  He-like (x+y+z)/w
  He-, Li-, Be-, B-like satellites
  H-like recombination contrib. to x, y, z, w

- L spectrum: 2-3 transitions for Li- to Ne-like $\rightarrow$ analytic formula
  B-, C-, N- and Ne-like : Bhatia, ADNDT 32 (1985) 435, 35 (1986) 319, 35 (1986) 449, 36 (1987) 453, 43 (1989) 99
  Li-like : Cochrane, Physica Scripta 28 (1983) 25

Th. Puetterich, PPCF 2008

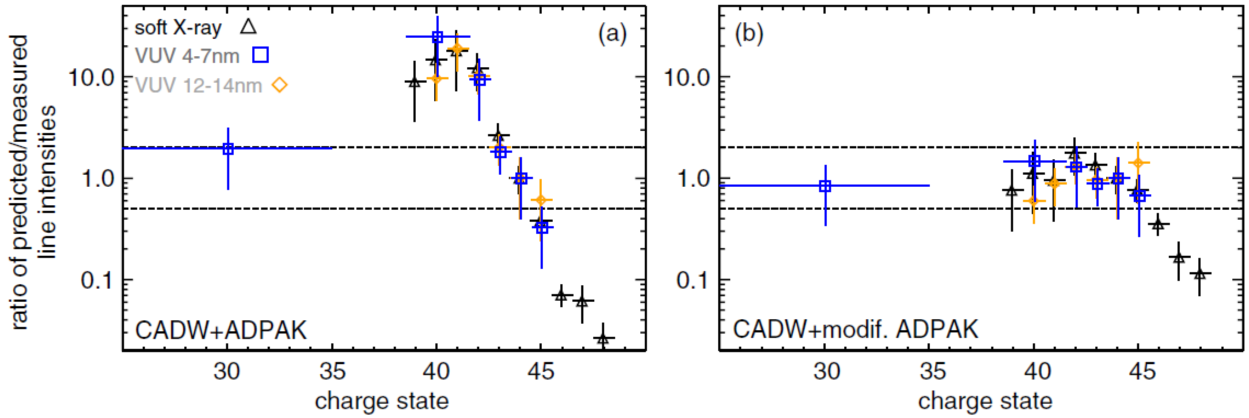

Figure 5. (*a*) Ratios of predicted to measured line intensities for different wavelength ranges versus ionization stage using the 'CADW+ADPAK' ion balance (see figure 6). Several lines of an ionization stage are summed in the model and in the spectrum to reduce the uncertainties that could occur for a single spectral line. (*b*) Similar data as (*a*), but using the data set 'CADW+modif. ADPAK' which is described in the text. Dashed lines correspond to 'factor of 2'-margin around 1 introduced to guide the eye.