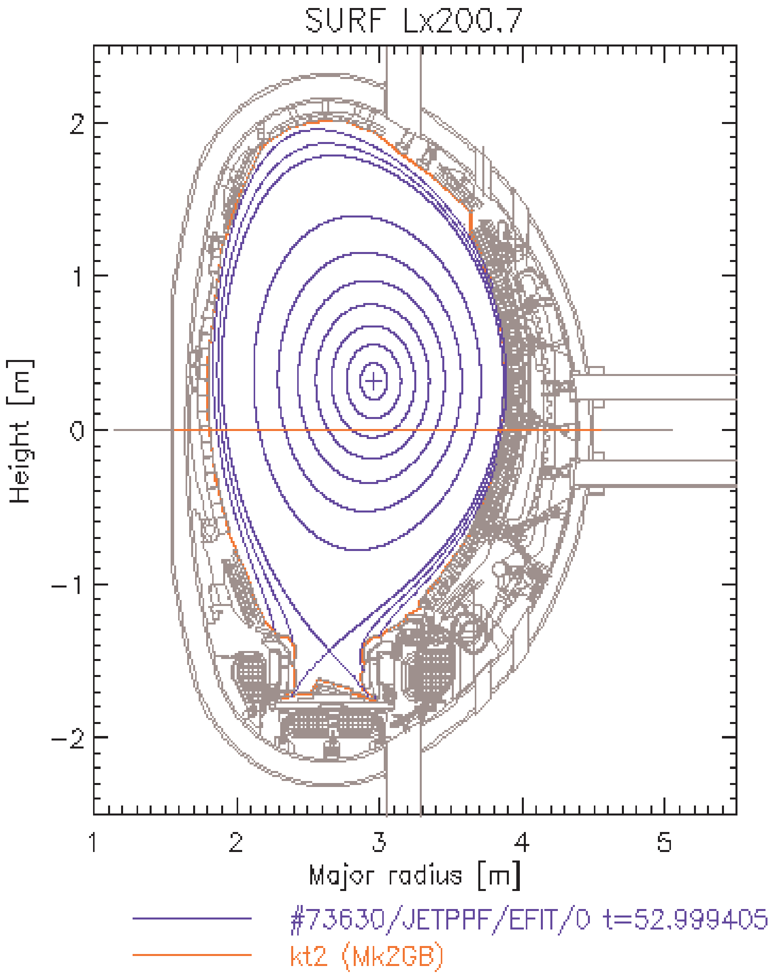
Impurity data analysis using UTC

K-D Zastrow and M O'Mullane

A tokamak with flux surfaces and a line of sight



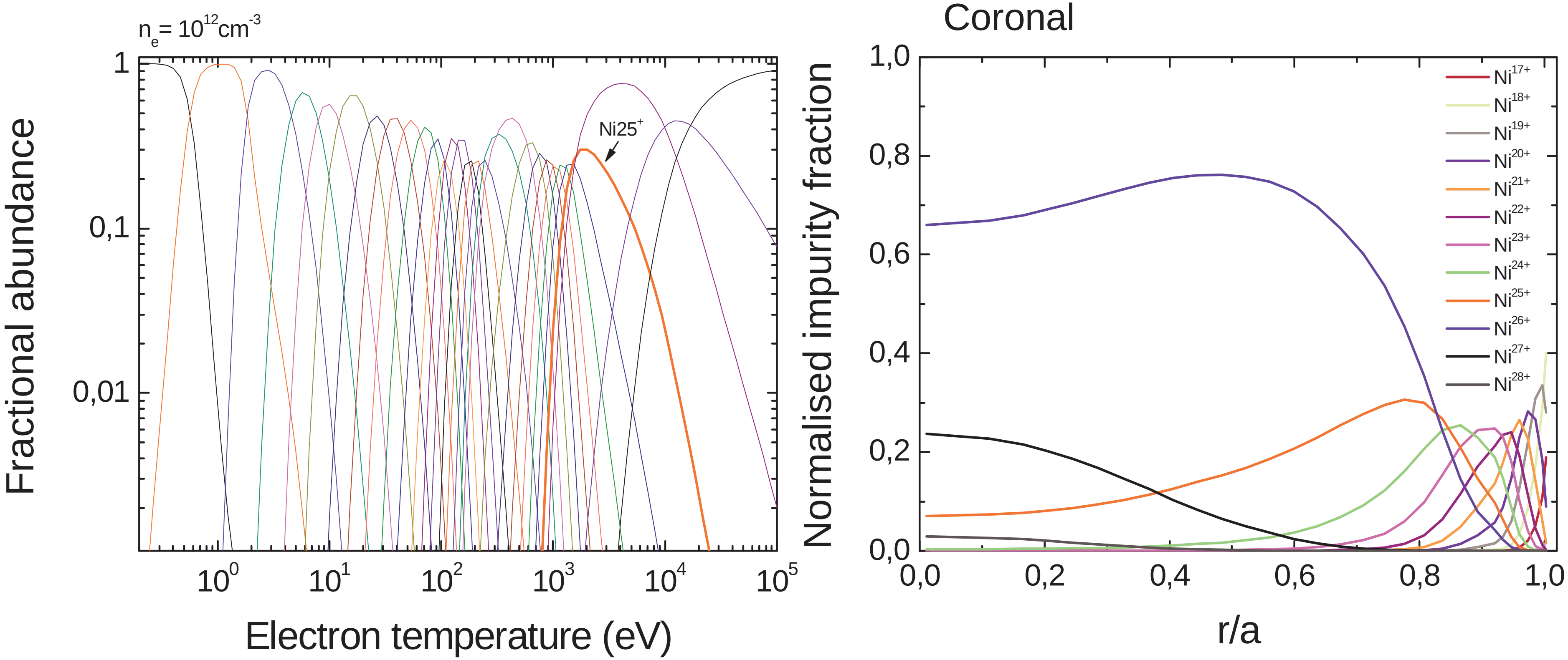
Neutrals and ions emit characteristic spectral lines from regions of the plasma where they can exist ("just the right environmental conditions")

Electrons and ions follow field lines that map out a flux surface defined by constant pressure (p_e+p_i).

Transport along a field line is fast, transport perpendicular to it is slow.

As a result, temperatures and densities are themselves constant on flux surfaces. The 3D transport problem is reduced to 1D by use of a flux surface label as radial co-ordinate.

Example Ni - Coronal balance?



f(Ni^{q+}) is function of T_e.

T_e is function of r.

f(Ni^{q+}) is also a function of r. But is it given by T_e(r) as shown here?

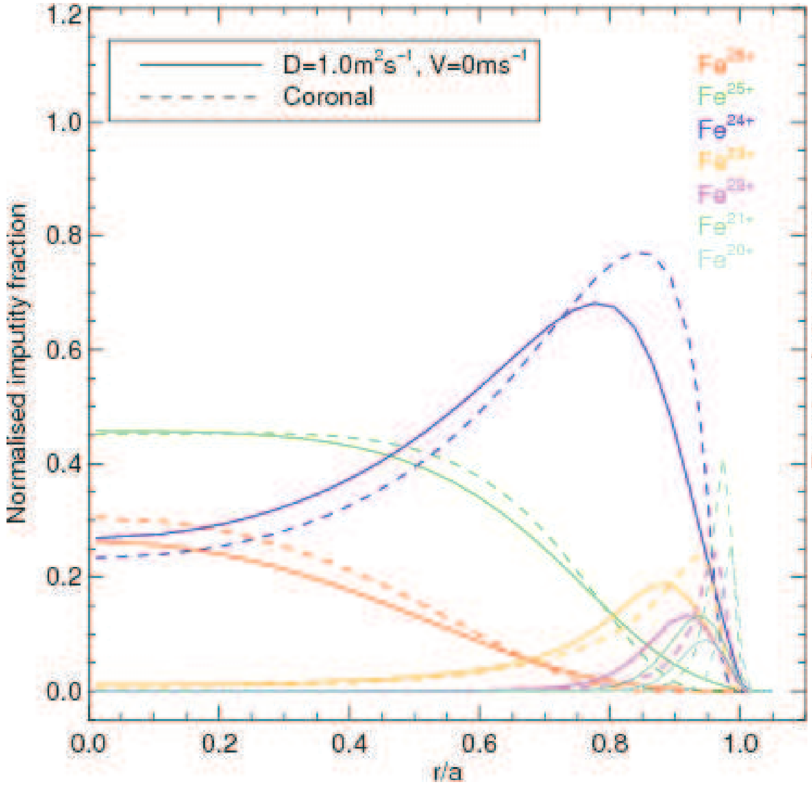
Timescales for transport and atomic processes

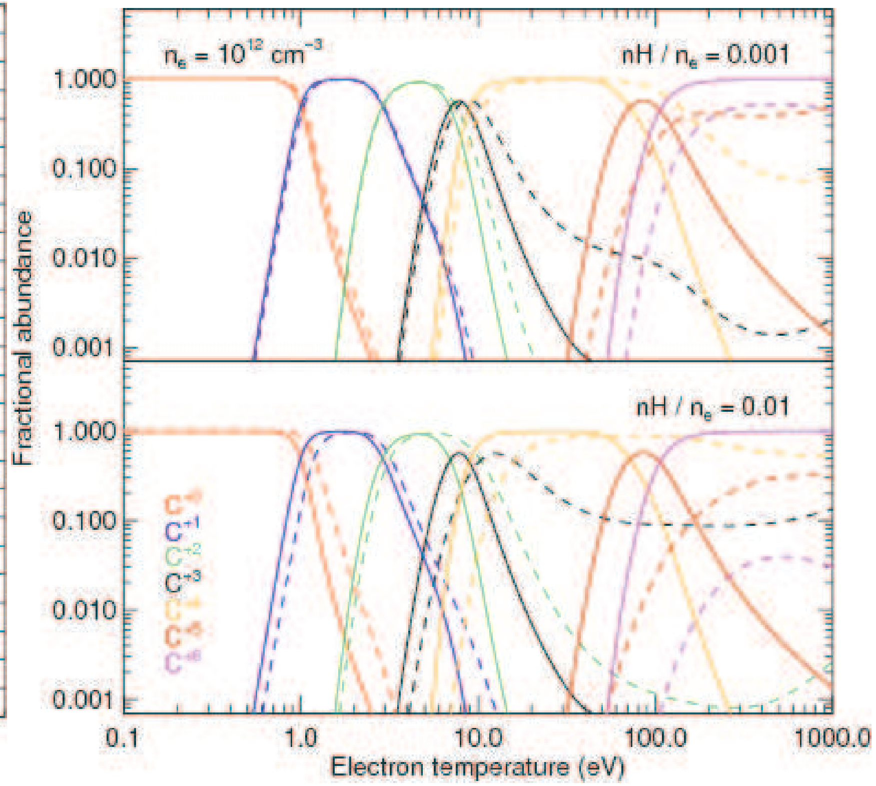
Emission	$n_e X \approx 10^{20}\ \mathrm{m}^{-3} \times 10^{-12}\ \mathrm{m}^3/\mathrm{s} \approx 10^8/\mathrm{sec}$
Ionisation	$n_e S \approx 10^{20}\ \mathrm{m}^{-3} \times 10^{-14}\ \mathrm{m}^3/\mathrm{s} \approx 10^6/\mathrm{sec}$
Diffusion	$D/(0.1\ a)^2 \approx 1\ \mathrm{m}^2/\mathrm{sec}\ /\ 0.01\mathrm{m}^2 \approx 100/\mathrm{sec}$
Convection	$v/(0.1\ a) \approx 1\ \mathrm{m/sec}\ /\ 0.1\mathrm{m} \approx 10/\mathrm{sec}$
Recombination	$n_e \alpha \approx 10^{20}\ \mathrm{cm}^{-3} \times 10^{-20}\ \mathrm{m}^3/\mathrm{s} \approx 1/\mathrm{sec}$

- Emission is a local process
- Timescale for transport is slower than ionisation but faster than recombination, therefore density profile of individual ionisation stage is determined non-locally

Answer: No!

Coronal equilibrium not a safe assumption





Neither is setting $n(H^0)=0$

Equations for particle transport
The "standard model"

Particle conservation with empirical ansatz for Γ_Z

$$\frac{\partial n_z}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_z) + \sigma_z; \quad \forall z \in [1, Z]$$

$$\Gamma_z = -D_z \frac{\partial n_z}{\partial r} + v_z n_z$$

Task: measure $D_Z(r,t)$, $v_Z(r,t)$.

Turn photon fluxes into densities.

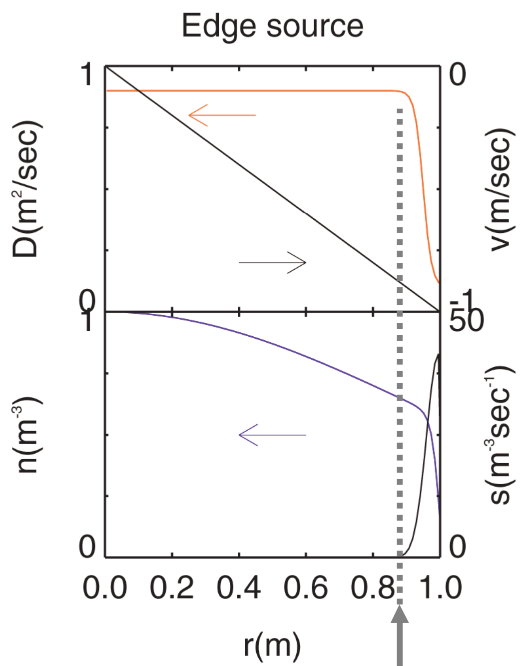
Sources and sinks $\sigma_Z(r,t)$: electron and neutral collisions

$$\sigma_z = n_e\left(n_{z-1}S_{z-1,z} + n_{z+1}\alpha_{z+1,z}\right) + n_{D_0} n_{z+1} CX_{z+1,z}$$

Some comments on the edge model

- For r/a>1.0 the code (SANCO) also requires parameters for calculations
  - Electron temperature and density
  - Neutral particle source rate $\Gamma_0(t)$
  - Neutral particle velocity for influx $\Rightarrow$ mean free path λ
  - SOL loss rate given by parallel confinement time $-n_Z/\tau_{||}$
  - Diffusion and convection continue from last defined value in the core
  - Recycling coefficient (not recommended…)
- These parameters are all meaningless and should not be interpreted as physics results.
- The only thing that's meaningful is the outermost measurement (whatever it is) and how well this is matched.
- It is worth checking that a change in these parameters does not affect the results in the core.
  - Change in particle velocity will change required influx rate but should change nothing else within reason
  - SOL density, temperature and particle velocity should combine so that the SOL is easily penetrable
  - Parallel loss rate, D_{SOL} and v_{SOL} should combine to a perfect sink

The ambiguity problem in steady-state



- Steady state profile shape in source free region given by

$$n(r) = n(r_S)\exp\left(-\int_r^{r_S} \frac{v(r)}{D(r)}\,dr\right)$$

$$n(r_S) = \frac{\Gamma_0 \lambda}{D(r_S < r < a)}$$

- Same solution obtained for $2\times\Gamma_0$, $2\times D$ and $2\times v$ etc.
- We need transient experiments to resolve D and v separately

Three types of impurity transport modelling

Sensitivity study

- Measurement of concentration or influx from spectroscopic observations
  - Impurity transport code is needed for interpretation but transport coefficients cannot be derived.
- Measurement of impurity transport coefficients
  - Coefficients in an empirical ansatz with diffusion and convection are fitted to data (success criteria?)
- Integrated plasma modelling including impurities
  - Theory based or empirical expressions are used, the main interest is to predict dilution and radiative power as well as other more exotic effects.

Testing against data

Choosing data to fit against

- A short time window after a gas puff (laser blow off, ELM, sawtooth crash….) carries transient information, so D can be determined from the relaxation of the profile.
  - Often not enough data to determine both v and D.
- A long quasi steady-state time window gives good statistics to determine v/D, as well as data on recycling from rate of decay.
  - Ambiguity problem.
- The choice of time window will not only influence the accuracy of the results but also what exactly is measured.

Usable data and modelling needs

Data		Diagnostic	Post-processing
Fully ionised impurity density	Z>1	Charge Exchange Spectroscopy	
Resolved spectral lines	Z>1	Visible, VUV, XUV, X-ray spectroscopy	Photon emissivities l-o-s integration
Tomography	Z>1	Soft X-ray diodes Bolometers	Filtered radiated power coefficients
Unresolved emission	Z>1	Soft X-ray diodes Bolometers	Filtered radiated power coefficients l-o-s integration

Confronting data and model

Parameterise coefficients $D(r,t)$, $v(r,t)$, $\Gamma_0(t)$

Model all data and adjust parameters by eyeballing

Estimate data errors, calculate χ^2

Generate derivatives by changing one parameter at a time

Improve solution using covariance
(Levenberg-Marquardt Method)

Least squares fit

Practicalities of fitting a model

- The fitting program (UTC) is a wrapper that generates input files for a transport code (SANCO) and collects the output files.
- UTC executes all post processing, including instrumental time and space resolution.
- For each data point UTC generates a value from the model and derivatives with respect to each fit parameter.
- UTC operates on the “house number” of the data point, where each data point has a weight.

$$\chi^2 = \sum_{n=1,N} w_n \left(f_n - y_n \right)^2$$

Levenberg-Marquardt Method

$$\chi^2 = \sum_{n=1,N} w_n \left(f_n - y_n \right)^2$$

$$\mathbf{M} \cdot \Delta\mathbf{p} = \mathbf{b}$$

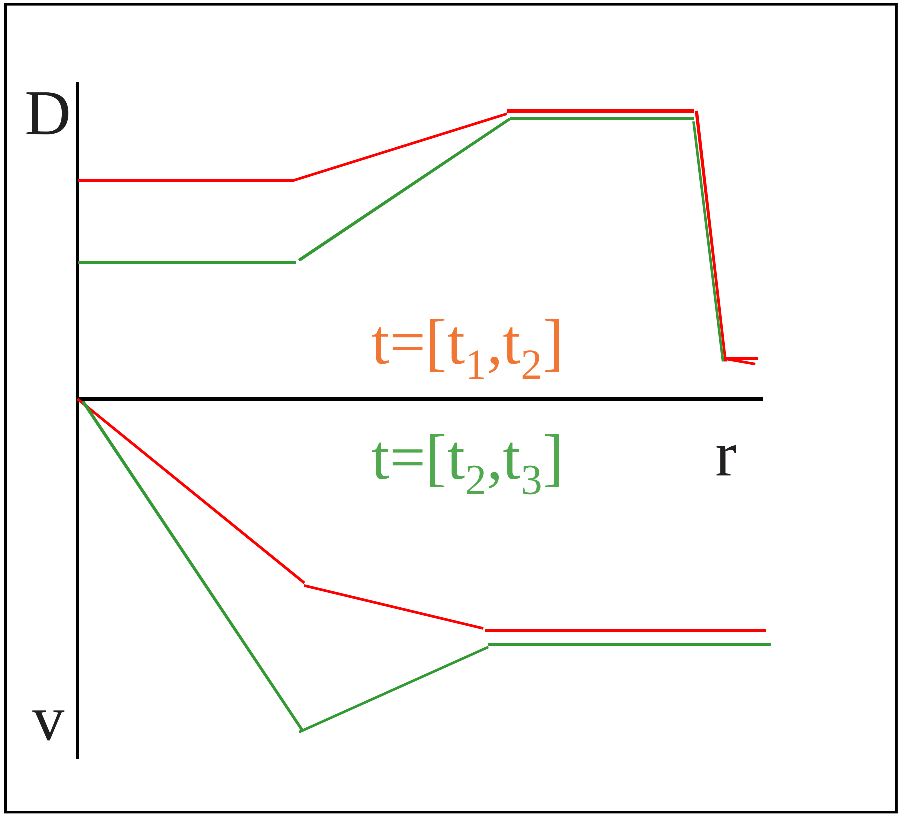
$$b_i = -\sum_{n=1,N} w_n \frac{\partial f_n}{\partial p_i} \left(f_n - y_n \right)$$

$$M_{ij} = \left(1 + d_{i,j}^2\right) \sum_{n=1,N} w_n \frac{\partial f_n}{\partial p_i} \frac{\partial f_n}{\partial p_j}$$

$$d_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

- Data point house number ***n***
- Data vector ***y***
- Model vector ***f*** described by parameter vector ***p***
- Co-variance matrix ***M***
- Improve solution by changing ***p*** iteratively
- Far from the solution, ignore co-variance terms and slow down rate of ~~improvement~~ change by multiplying diagonal of ***M***
- In every iteration, try several damp factors ***d*** and pick the best
- For every iteration, damp factor should be decreased to optimise speed

Model parameterisation



- D and v on a radial and time grid.
- Analogy: diagnostic with finite resolution.
- Practical number of grid points depends on the resolution of the data.
- Fit will not converge if information is not present in the data.
- The model needs parameters in regions where there are no measurements

Errors of transport parameters

$$M_{ij} = \sum_{n=1,N} w_n \frac{\partial f_n}{\partial p_i} \frac{\partial f_n}{\partial p_j}$$

$$\mathbf{C} = \mathbf{M}^{-1}$$

$$\sigma_i = \sqrt{C_{ii}} \qquad \forall i \in [1, m]$$

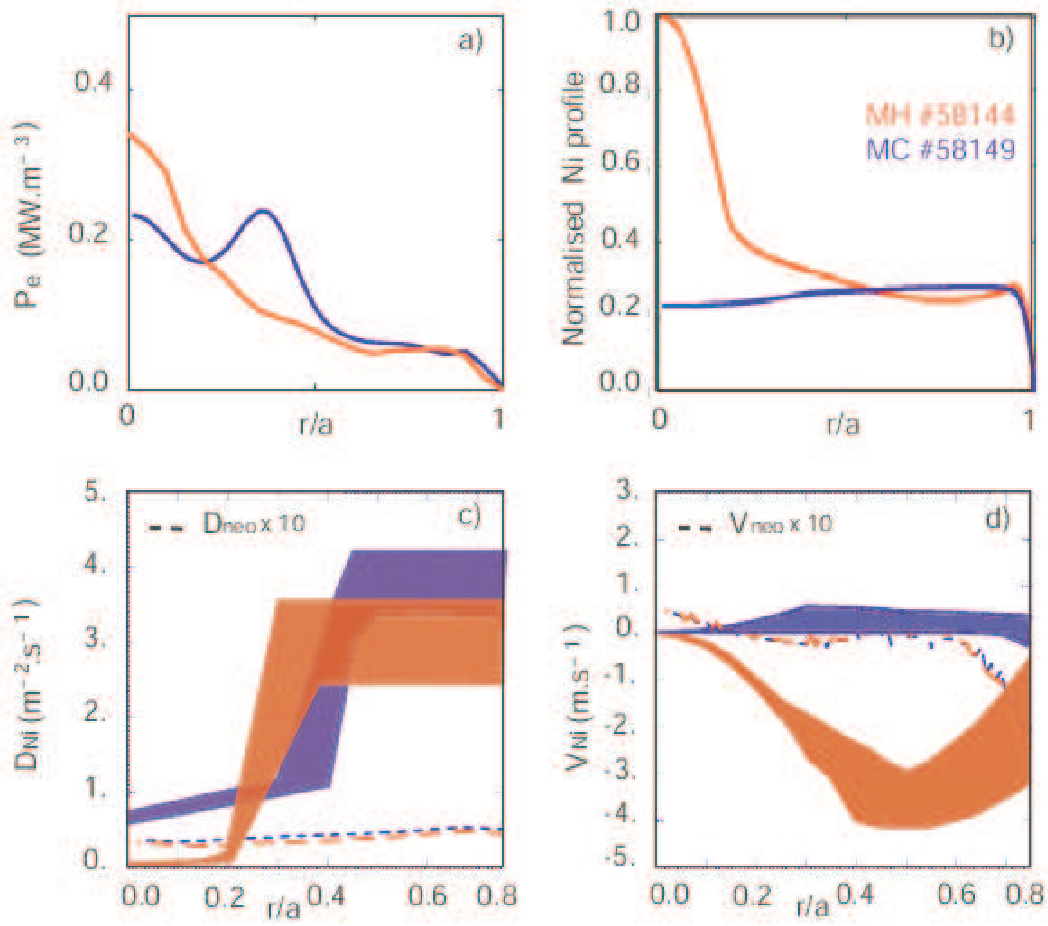
$$\rho_{ij} = \frac{C_{ij}}{\sqrt{C_{ii} C_{jj}}}$$

- Covariance of errors in fit parameters returned. If large then both parameters do the same job (ambiguity)
- Assumes $\chi^2 \approx N-m$.
- Assumes model and weights to be correct
- Errors (weights) are taken to be uncorrelated. For correlated errors a UTC extension exists but is not part of the code
- Same matrix as in least squares fit but without damp factor $(1+d^2)$ in Levenberg-Marquardt

What UTC and SANCO need from the user

- Plasma background data ($T_e(\rho)$, $n_e(\rho)$)
- Plasma geometry
  - Mapping local parameters (ρ) on lines of sight (x,y,z)
  - Plasma volume changes with radius
- Diagnostic information
  - What is measured (physics, ADAS)
  - What are the instrumental parameters (sensitivity, geometry, time and space resolution)
- Transport model parameterised – influx, core and edge transport including “nuisance” parameters

Ni in JET ICRH heated plasmas



C Giroud, 2006 IAEA

UTC and SANCO on other fusion plasmas but JET?

- SANCO is a stand alone code. Only reads and writes files.
- UTC interface with JET is through a small number of data access routines that need changing
  - Already converted for MAST by A Foster
  - For other machines collaborate with JET