Data requirements for simulating vapor shielding with radiation-hydrodynamic and collisional-radiative modeling

IAEA Consultancy Meeting on Vapor Shielding
in Fusion Devices

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Outline

- Where do collisional-radiative models fit in a radiative-hydrodynamics code?
- What requirements are put on the models?
- Examples
  - Hydrogen edge plasma w/ optical depth effects
  - Li data set for pellet injection
  - Sn data set for EUV generation

Note: My experience has been gained primarily with laser-produced plasmas

Collisional-radiative (CR) models in radiative-hydrodynamic codes

- At high densities ($n_i > 10^{20}$ cm^{-3})
  - Plasma can be optically thick to continuum radiation
  - Radiation is coupled strongly to free electrons
  - Absorbed radiation is redistributed thermally
  - Energy transferred between radiation and matter:

$$\int \left(\underbrace{\alpha_\nu}_{\text{absorption coefficient}} \overbrace{J_\nu}^{\text{angle-integrated intensity}} - \underbrace{\eta_\nu}_{\text{emission coefficient}} \right) d\nu$$

- At low densities ($n_i < 10^{18}$ cm^{-3})
  - Plasma can be optically thick to line radiation
  - Radiation is coupled strongly to bound electrons
  - Radiation is coupled indirectly to free electrons
  - Absorbed radiation is redistributed within line profiles
  - Radiative excitation / de-excitation rates:

$$\sigma_{ij} \times \bar{J}_{ij}, \left(\bar{J}_{ij} + \frac{2h\nu_{ij}^3}{c^2} \right) \quad \bar{J}_{ij} = \int \overbrace{\phi_\nu}^{\text{line profile}} J_\nu d\nu$$

The physical regime determines the use of CR models

- High density: averaged material information
  - Radiative properties: broadband absorption and emission coefficients
  - Equation of state: ionization balance, internal energy
- Low density: detailed material information
  - Radiative properties: absorption and emission profiles
  - Equation of state: populations
- Both regimes require "full" atomic models
  - All significant transitions between coupled states induced by collisions w/ electrons and photons: excitation, ionization + autoionization
  - Low temperature → collisions w/ ions and neutrals + molecules

The use determines the content of atomic models

- High density:
  - Extensive state space / configuration coverage
  - Multiple excitations from valence shell (can extend to inner shells)
  - Collisional broadening → detailed structure less important
  - Autoionizing state coverage more important than autoionization / DR

- Low density:
  - Most ionizations / excitations directly out of ground state
  - Detailed structure + line profiles important for radiation transfer
  - High-n excited states important for charge exchange
  - Autoionizing states critical for dielectronic recombination (DR)

Non-LTE Code Comparison Workshops have been extremely valuable in identifying requirements for atomic models

Plasmas at the tokamak edge are optically thick to line radiation on length scales < 1 cm

- Absorption coefficient for thermally-broadened Lyman α:

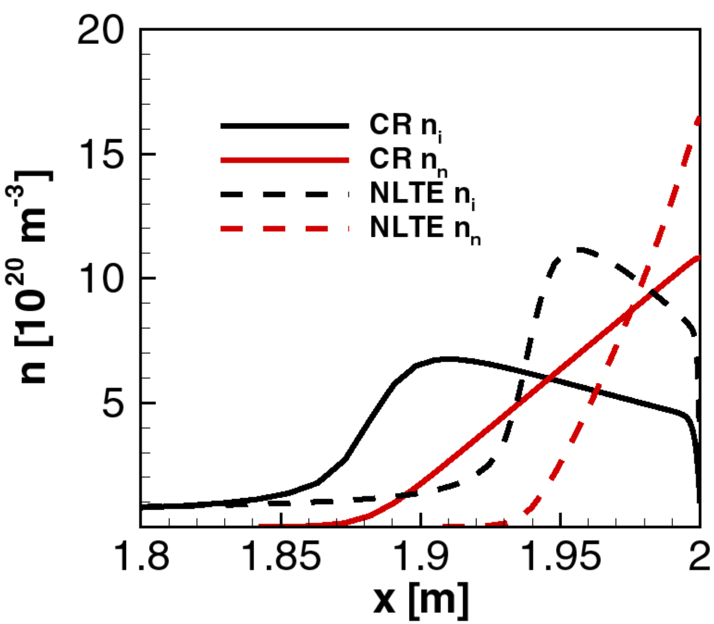
$$\alpha = n_o \frac{\pi e^2}{mc} f \frac{1}{\Delta\nu\sqrt{\pi}} \approx \frac{0.3}{\sqrt{T_{\mathrm{ev}}}} \left(\frac{n_o}{10^{14}} \right) \mathrm{cm}^{-1}$$

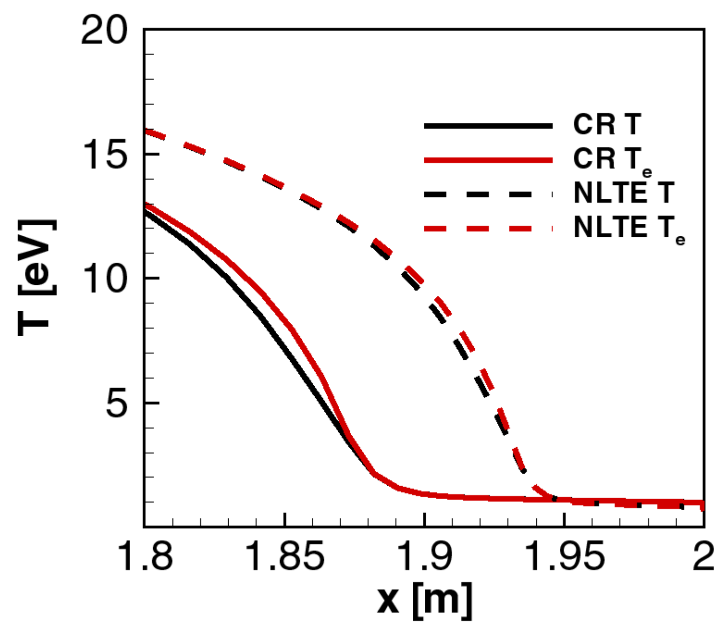
- Simulations show large effects from radiation fields
- PIP: Self-consistent treatment which includes
  - partially-ionized plasma transport
  - non-LTE atomic kinetics
  - line radiation transport
  - excited state transport
  - magnetic effects on line profiles

H.A. Scott and M.L. Adams, "Incorporating Radiation Effects into Edge Plasma Transport Models with Extended Atomic Data Tables", EPS Conference on Plasma Physics, 2004

Detached divertor simulations exhibit large radiation effects

Specifications: $L=2$ m, $N=10^{20}$ m^{-3}, $q_{in}=10$ MW/m^2, $b=0.1$

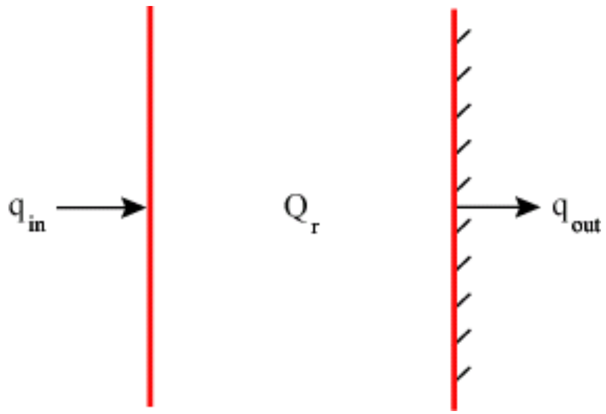




Qualitative description of the detached divertor region remains unchanged.

Quantitative details of the particle and power balance change dramatically.

Optically-thick hydrogen lines affect divertor power balance



Flux	q_{in}	Q_r	q_{out}
CR	**+1.000**	**-0.805**	**+0.195**
NLTE	**+1.000**	**-0.555**	**+0.445**

q_{in} : incident heat flux

Q_r : radiative heat flux

q_{out} : particle heat flux on target plate

CR : PIP w/ optically-thin collisional-radiative model (tabulated data)

NLTE : PIP w/ collisional-radiative model with full line transfer

Radiation effects <u>increased</u> the divertor target plate incident heat flux by a factor 2.3

Atomic data in plasma transport codes

- Plasma transport models explicitly treat ion and (ground state) neutral atoms
- Excited states are assumed to be in equilibrium on transport timescales:

$$n_x = f_x^g n_g + f_x^i n_i \quad , \quad f_x^{g,i} = f_x^{g,i}(n_e, T_e)$$

- Transport model uses effective ionization / recombination and energy loss coefficients which account for excited state distributions, e.g.

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{V}_i) = P_i n_n - P_r n_i \quad , \quad \frac{\partial n_n}{\partial t} + \nabla \cdot (n_n \mathbf{V}_n) = -P_i n_n + P_r n_i$$

- Tabulated coefficients are evaluated with a collisional-radiative code in the coronal (optically-thin) limit

In the coronal limit, coefficients depend only on n_e and T_e

Atomic data is condensed into effective rates: P- and H-rates

- P-rates are constructed from the atomic rate equations:

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{N}_t \\ \mathbf{N}_x\end{pmatrix} + \nabla\cdot\begin{pmatrix}\mathbf{N}_t\mathbf{V}_t \\ \mathbf{N}_x\mathbf{V}_x\end{pmatrix} = \begin{pmatrix}\mathbf{A}_{tt} & \mathbf{A}_{tx} \\ \mathbf{A}_{xt} & \mathbf{A}_{xx}\end{pmatrix}\begin{pmatrix}\mathbf{N}_t \\ \mathbf{N}_x\end{pmatrix}$$

$\mathbf{N}$: number density
$\mathbf{A}$: atomic rate matrix

$$\frac{\partial}{\partial t}\mathbf{N}_x = \mathbf{A}_{xt}\mathbf{N}_t + \mathbf{A}_{xx}\mathbf{N}_x = 0 \Rightarrow \mathbf{N}_x = -\mathbf{A}_{xx}^{-1}\left(\mathbf{A}_{xt}\mathbf{N}_t\right) \equiv \mathbf{B}_{xt}\mathbf{N}_t$$

$$\frac{\partial}{\partial t}\mathbf{N}_t + \nabla\cdot\left(\mathbf{N}_t\mathbf{V}_t\right) = \mathbf{A}_{tt}\mathbf{N}_t + \mathbf{A}_{tx}\mathbf{N}_x = \left(\mathbf{A}_{tt} + \mathbf{A}_{tx}\mathbf{B}_{xt}\right)\mathbf{N}_t \equiv \mathbf{P}\mathbf{N}_t$$

t : transported state
x : excited state

- H-rates are constructed from the electron energy equation:

$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_i T_e\right) + \nabla\cdot\left[\frac{5}{2}n_i\mathbf{V}_i T_e + \mathbf{q}_e\right] - \mathbf{V}_i\cdot\nabla\left(n_i T_e\right) + \frac{3 m_e n_i\left(T_e - T\right)}{M\tau_{ei}} = \sum_{j,k\neq j} N_j A_{jk}\Delta E_{jk}$$

$$\sum_{j,k\neq j} N_j A_{jk}\Delta E_{jk} = \sum_{t,t'\neq t}\left(\mathbf{A}_{t't}\Delta E_{t't} + \mathbf{A}_{t'x}\Delta E_{t'x}\mathbf{B}_{xt}\right)\mathbf{N}_t \equiv \sum_t \mathbf{H}_t\mathbf{N}_t$$

This generalized the approach of Stotler, Post and Reiter (1993)

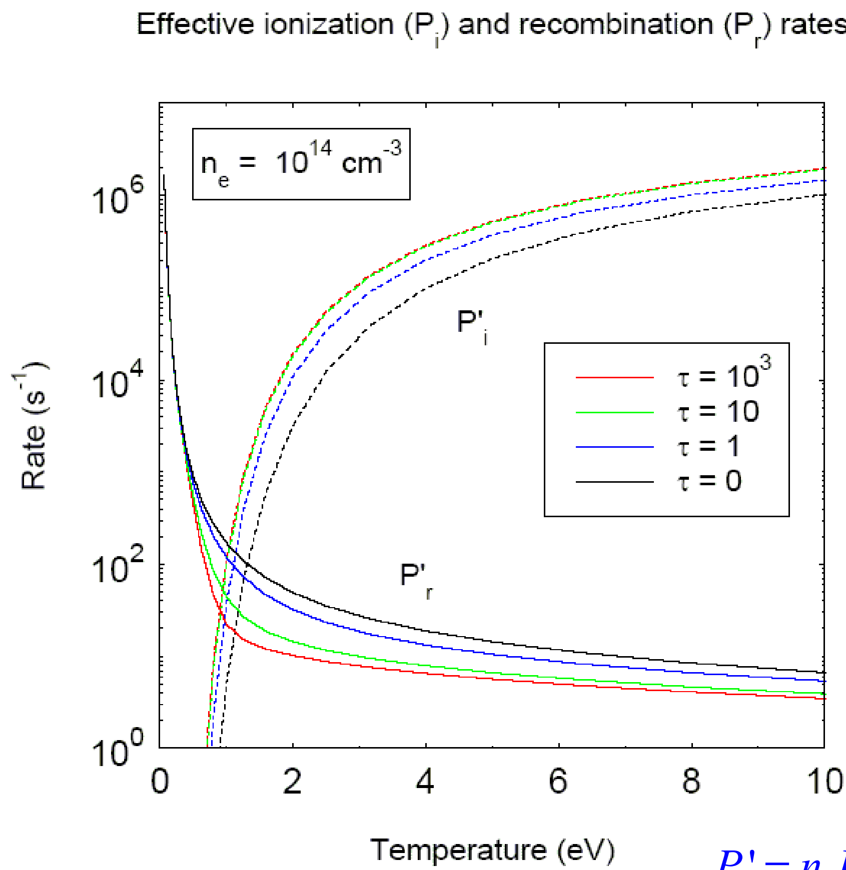
Radiation effects are incorporated through the P- and H-rates

- Radiation introduces spatial dependence into the atomic rates through the radiation field
- Rates are parameterized by the (approximate) optical depth of Lyman α:

$$P(n_e, T_e) \rightarrow P(n_e, T_e, \tau),$$

$$\tau = \int_0^s 10^{14} n_n(s')ds'$$

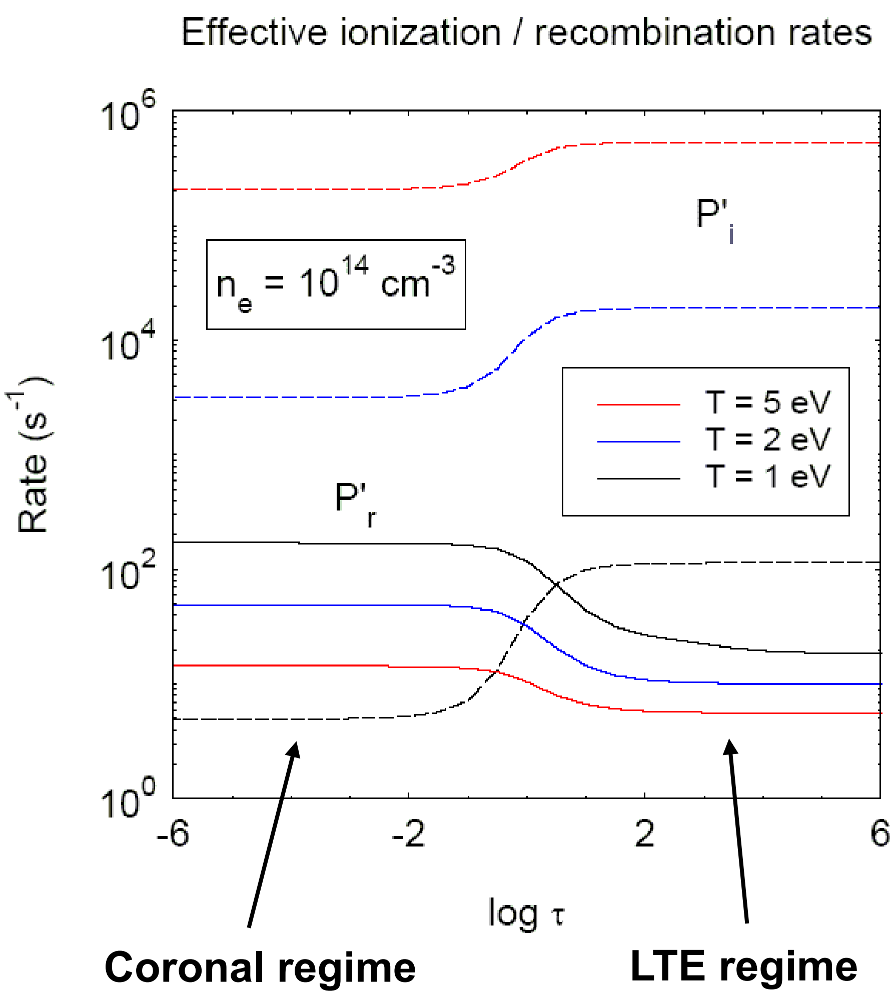
- Tabulated values generated with escape factors for midpoint of uniform plasma of depth 2τ
- Can be applied in arbitrary multi-dimensional geometry

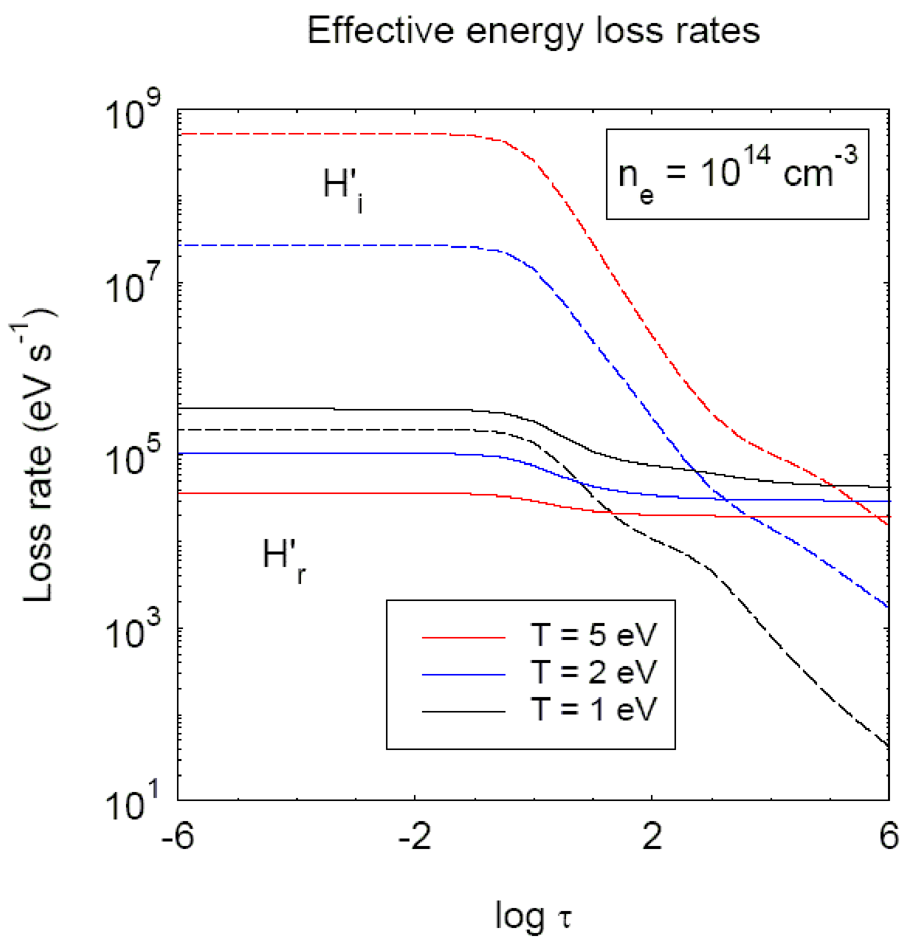


$P' = n_e P$

Parameterized tables were tested in UEDGE

Optical depth parameterization allows coverage from coronal to LTE regimes





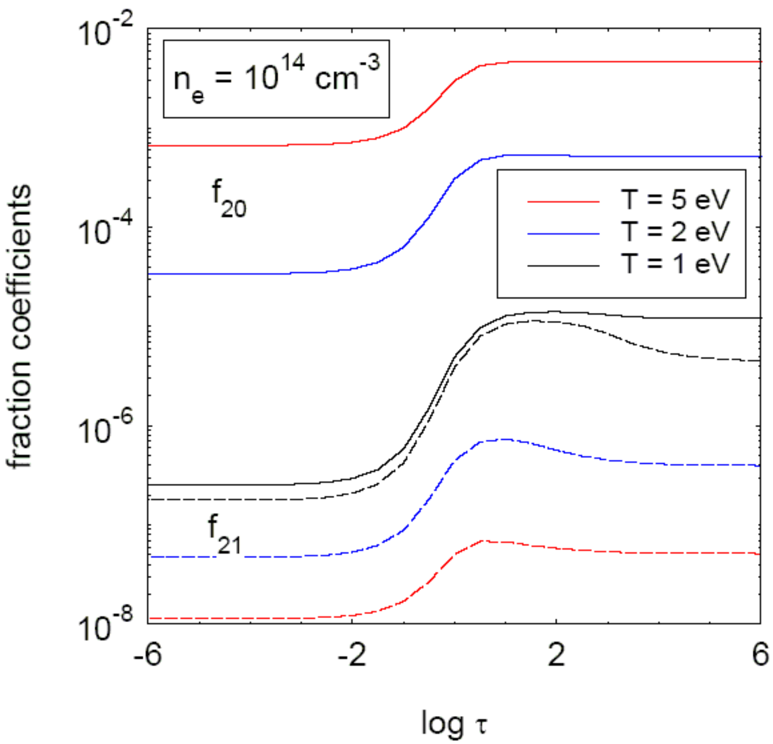
$$H'_{\mathrm{r,i}} = -n_e \left(H_{\mathrm{r,i}} \pm 13.6\,\mathrm{eV} \times P_{\mathrm{r,i}} \right)$$

Excited state populations follow from effective rates

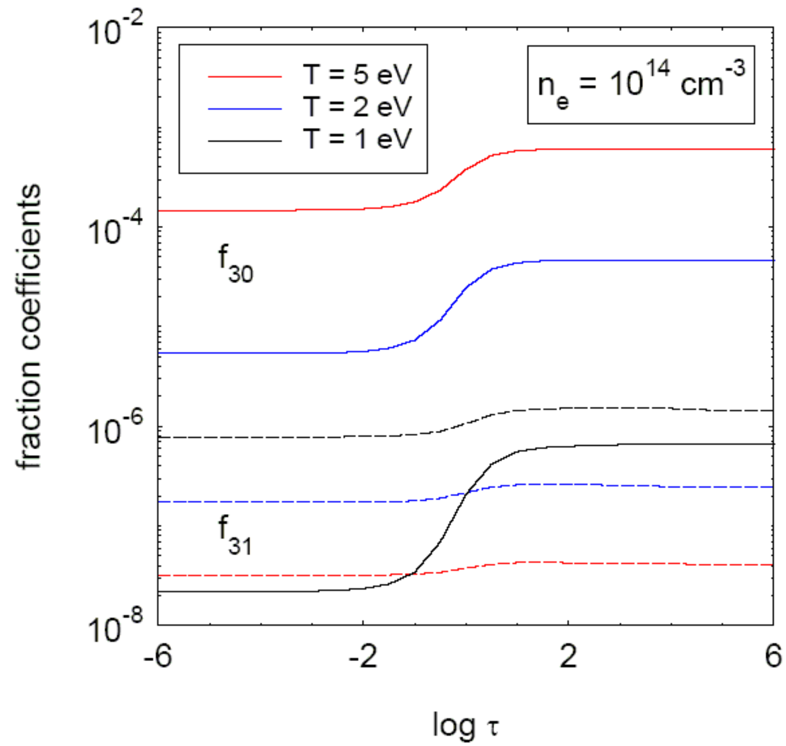
- Determined from ground state and ion densities

  $n_2 = f_{20} n_i + f_{21} n_g \,,\; n_3 = f_{30} n_i + f_{31} n_g$

n=2 excited state



n=3 excited state



Optical depth can change populations by orders of magnitude

H data for edge plasma

- Constructed from semi-classical formulas
- Johnson-Hinnov collisional rates
- Doppler + collisional + (approximate) Stark broadening
- No fine structure

Comments

- Ly-α fine structure splitting negligible compared to broadening
- Stark line shapes did not affect energetics, but are important for diagnostics
- Zeeman splitting due to a large magnetic field might decrease τ enough to matter

Li data for killer pellets (for P. Parks of GA)

- Fine structure data calculated with FAC (Flexible Atomic Code)
- Single excitations to n=8, double excitations to n=5
- E1, M1, E2 radiative transitions

H-like:	64 levels,	1.1e3 transitions
He-like:	252 levels,	1.1e4 transitions
Li-like:	270 levels,	1.2e4 transitions

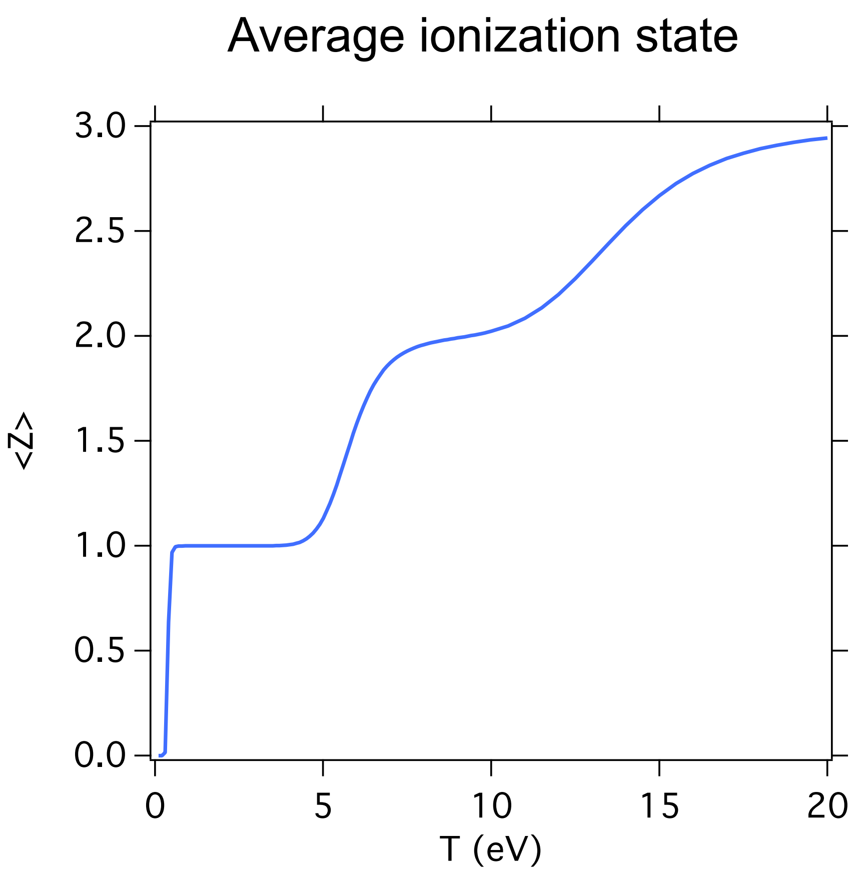
Comments:

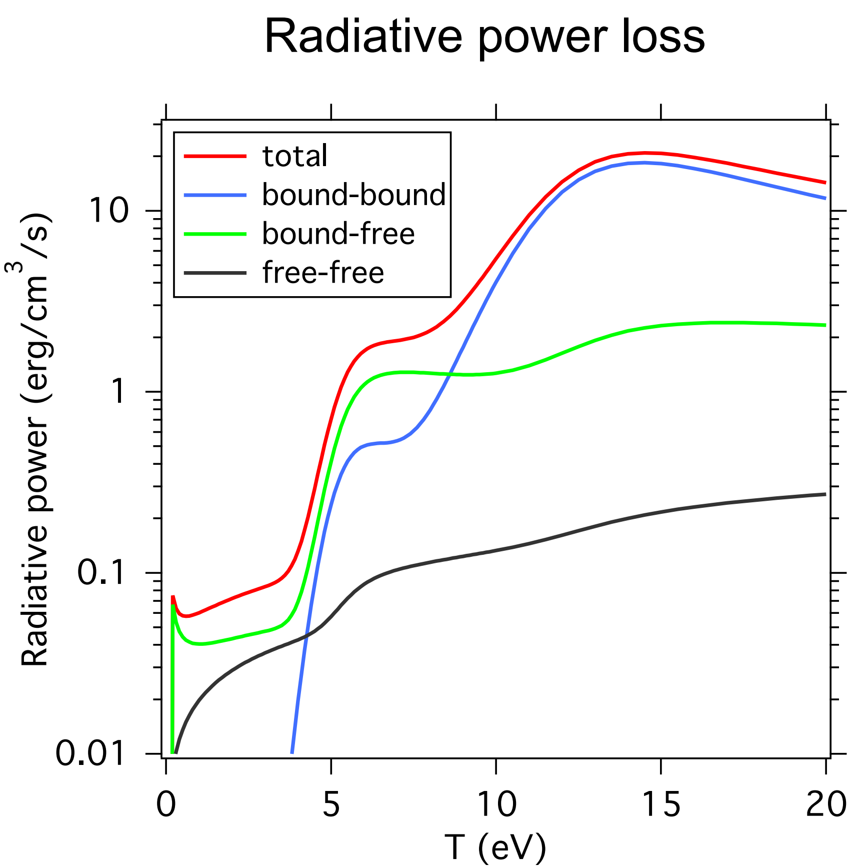
- FAC and similar codes are quite accurate for low-Z elements (except neutrals?)
- Datasets remain reasonably compact and fast for low densities

  – but –

- Including enough DR channels could be problematic

Li evaluation @ $n_e = 10^{15}$ cm^{-3}



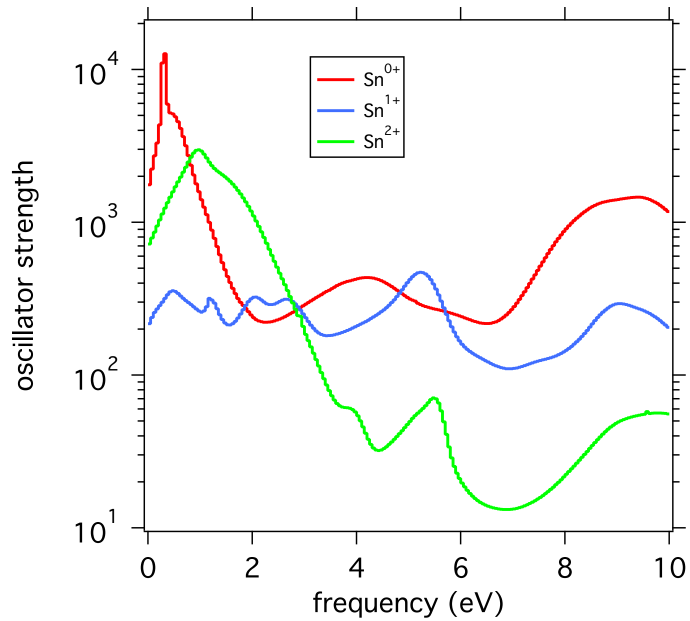


Sn data for EUV generation (from J. Colgan of LANL)

- Fine structure energy levels / oscillator strengths from LANL code
- Special attention paid to configuration interaction
- Dataset restricted to structure + oscillator strengths for 33-50 electrons
  - Sufficient structure for low densities (except for DR channels)

Comments:

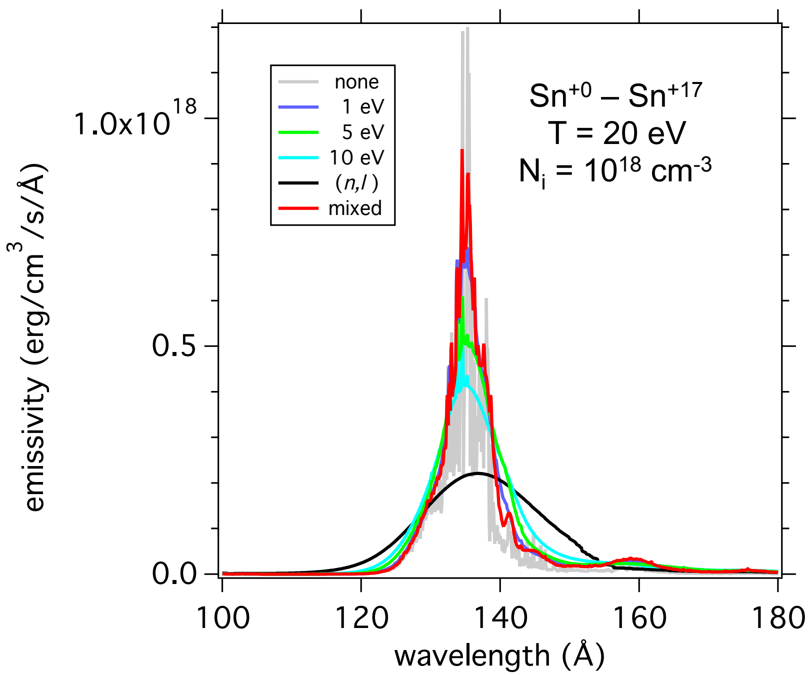
- High-fidelity calculations of complex ions are difficult but possible
- Adding other transitions for NLTE work increases expense greatly but might be done with semiclassical methods



J. Colgan, *et al*, HEDP **23** (2017) 133-137

(LTE) Radiative emission of averaged models

- Combine levels by configuration and energy spread
- Averaged transitions between combined levels
- Aim to maintain oscillator strength distribution in each charge state



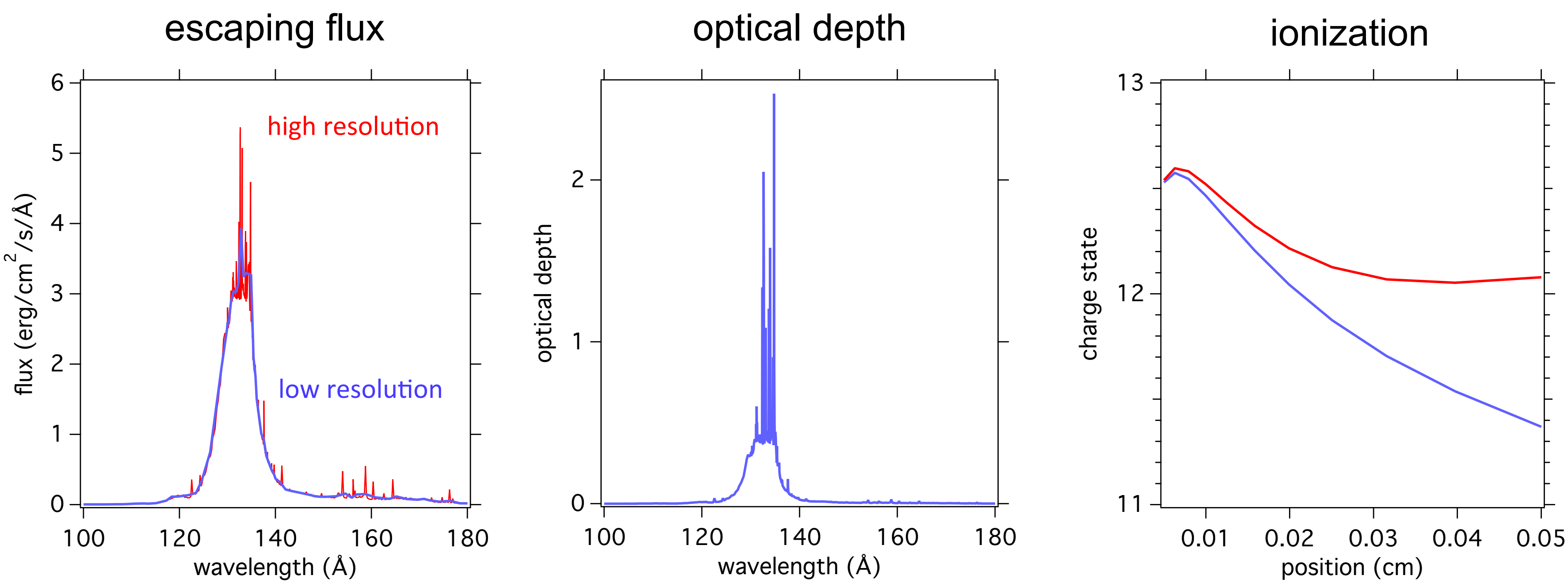
Data from fine-structure model of J. Colgan

averaging	energy levels	transitions
none	1.85e6	4.6e8
1 eV	29668	4.4e6
5 eV	8471	5.2e5
10 eV	5091	2.2e5
(n,l)	1258	2.0e4
mixed	11072	1.1e6

Carefully averaged data maintains the spectral structure

Testing averaged models with radiation transport

- NLTE atomic kinetics + radiation transport for 1 eV-averaged model
- $T = 30$ eV + maximum $N_i = 10^{18}\ cm^{-3}$
- Density profile $N_i \propto r^{-2}$ (fit from rad-hydro simulation)



Bandpass flux is insensitive to frequency resolution

Questions / Suggestions

- What are expected density / temperature ranges?
  - will help set model parameters
- Which molecular reactions can occur?
  - use a complete set of transitions or a chemistry model?
- Do non-thermal electrons play any role?

- Comparisons of data + simulations are both helpful

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