**Kinetic Neoclassical Calculations** 

of Impurity Radiation Profiles\*

D. P. Stotler, D. J. Battaglia, R. Hager, K. Kim (KAIST),

## T. Koskela (LBL), G. Park (NFRI), and M. L. Reinke (ORNL)

Princeton Plasma Physics Laboratory

NSTX-U Results Review September 21 – 22, 2016





\*This work supported by US DOE contracts DE-AC02-09CH114466 (PPPL) and DE-AC05-00OR22725 (ORNL).

#### Summary

- Modify drift-kinetic code XGC0 to include transport, ionization, and recombination of impurities.
- Use to simulate C and Ne in NSTX H-mode.
- First, demonstrate approach to coronal equilibrium.
- Then, isolate impacts of neoclassical effects on radiated power profile.
- Orbit squeezing & inward pinch result in increased core  $P_{rad}(\psi)$ ,
  - & changes to ratios of charge state emissions at given  $T_e$ .

### Objective: Do a Better Job of Simulating Radiated Power Distribution

- Fluid impurity transport models miss kinetic & non-local neoclassical effects.
- $\Rightarrow$  Extend full-f, drift-kinetic XGC0 PIC code to resolve impurity charge states,
  - Particle push integrates guiding center Hamiltonian equations of motion,
  - $E_r$  obtained via Ampere's Law averged over closed flux surfaces.
  - Also: realistic recycling, linear Fokker-Planck operator, ....
  - Had two *fixed* charge impurities,
    - \* Add ionization & recombination using ADAS rates.

## **Approach to Coronal Equilibrium**

- Comparing with CE  $\Rightarrow n_e \& T_e$  fixed for all runs.
- This run: disable all physical processes except ionization & recombination.
- Profiles from NSTX H-mode 139047.
- All C<sup>+</sup> initially.



- Dashed  $\Rightarrow$  rate computed from local  $n_e, T_e$ .
- Solid ⇒ actual rate after Monte Carlo collisions.

## **Time Evolution of** L<sub>rad</sub>



- Emulate Carolan (1983), Post (1995).
  - $n_e$  & time enter only as  $n_e \tau$ .
- *T<sub>e</sub>*, *n<sub>e</sub>* variation is actually radial variation along profile.
  - $n_{\rm COTE} = 6.8 \times 10^{19},$
  - $-n_{\rm SOL} = 3.1 \times 10^{18} \, {\rm m}^{-3}.$

$$L_{\mathsf{rad}}(T_e, n_e) = \left(\sum_{q} P_{\mathsf{rad},q}\right) / \left(n_e \sum_{q} n_q\right);$$
$$P_{\mathsf{rad},q} = n_q n_e P_{\mathsf{ion},q}(T_e, n_e) + n_{q+1} n_e P_{\mathsf{rec},q+1}(T_e, n_e)$$

## Add NC Effects $\Rightarrow$ Modest Increase in $P_{rad}(\psi)$ & Large Changes in $P_{rad}^{q+1}(\psi)/P_{rad}^{q}(\psi)$



- In CE:  $P_{rad,tot} = 0.18$  MW,
- With neoclassical effects:  $P_{rad,tot} = 0.24$  MW.
- Ne: similar, with 65% increase.



- Recycling source keeps  $C^+ \leftrightarrow C^{2+}$ &  $C^{2+} \leftrightarrow C^{3+}$  nontrivial.
- $C^{\geq 3+}$  shifted inward.

#### **Future Work**

- Include kinetic electrons & effects of  $P_{rad}$  on energy balance.
- Include diffusive anomalous transport & core particle, momentum, energy sources ⇒ simulate individual discharges.
- Replace simple neutral model with DEGAS 2,
- Accurate treatment of SOL via XGCa.

# **BACKUP SLIDES**

## XGC Code Family Continues to Mature within EPSi

- XGC0: Full-f, drift-kinetic, multi-species PIC transport code.
- XGCa: Axisymmetric variant of XGC1 (Churchill P.2.23),
- XGC1: 5-D edge gyrokinetic PIC code.



XGC0 D<sup>+</sup> and C<sup>6+</sup> velocity distributions [Battaglia 2014].



XGCa bootstrap current calculations [R. Hager, K. Ma]

#### **Implementation of Impurity Ionization & Recombination**

- Add q/Z to list of phase space parameters.
  - For low-Z, include all charge states,
  - Will require "bundled" representations for high-Z.
- Evolve q via Monte Carlo ionization & recombination,
  - Generalized collisional radiative rates from ADAS,
    - \* All are "96" files; C files dated Nov. 4, 1999, Ne are June 11, 2014.
  - Loaded into DEGAS 2 & accessed by new interface.
  - Electrons created, removed, cooled, etc., but  $T_e$ ,  $n_e$  fixed here.
- Evaluate rates, etc. on 2-D mesh:
  - 50 surfaces  $0.4 \le \psi_n \equiv \psi/\psi_{sep} \le 1$ ; 4 poloidal divisions each.
  - 5 SOL cells each above & below X-point,  $1 \le \psi_n \le 1.05$ ,
  - 1 PFR cell.
  - $\Rightarrow$  relatively simple model of open field lines.
  - XGCa will provide more detailed treatment.

## q = 1 Source from Neutral Ionization // Coulomb Collisions

- Monte Carlo ionization of 2-D neutral density profile:
  - $n_0(\psi, \theta)$  from Monte Carlo calculation using fluid plasma background.
  - Source of neutrals: recycling with user specified rate,
    - \* Spatial profile = poloidal distribution of  $D^+$  lost to walls.
    - \* 99% recycling rate for impurities here.
    - \* 3 eV thermal energy distribution.
  - Impurity neutrals only undergo ionization,
- Linear Fokker-Planck collision operator:
  - 1. "Background" species loop  $\rightarrow$  loop over species & charge states,
    - For each, do Monte Carlo Coulomb collisions with all other "test" species → species & charge states.
  - 2. Apply "restoring" force on background particles.
  - 3. Enforce particle, momentum, and energy conservation.

#### **Apply to NSTX H-Mode Plasma**

- Electron & carbon profiles input to XGC0,
  - Similar to NSTX H-mode discharge 139047 at 580 ms.
  - No initial toroidal rotation.
  - Initial D<sup>+</sup> density computed from quasi-neutrality.
- For comparison with coronal equilibrium, fix  $T_e$ ,  $n_e$  in all simulations.



## **Neoclassical Effects on** L<sub>rad</sub>

- Initialize each run with CE charge state distribution.
- Add effects in stages:



- 1. Particle push &  $E_r$ 
  - $\Rightarrow$  orbit width & squeezing.
- 2. Impurity source via recycling,
  - Replace orbit- & X-loss,
  - Transient except for SOL.
- 3. Collisions,
  - Pitch angle scattering moves ions from confined to loss orbits,
  - $\Rightarrow$  steady source of C<sup>+</sup>.
  - Anomalous transport would have same effect.
  - Inward pinch increases C<sup>4+</sup>, C<sup>5+</sup> in core,
  - $\Rightarrow$  more realistic  $E_r$  profile.

#### **Neon Simulation Similar**



#### Ne Radiation Density $\sim 2\times$ CE in Core



- In CE:  $P_{rad,tot} = 0.95$  MW,
- With neoclassical effects:  $P_{rad,tot} = 1.57$  MW.



- Ne<sup>+</sup> & Ne<sup>2+</sup> trivial in CE,
- Ne<sup>+</sup> in neoclassical case also.