Bundled charge states: A practical example

X. Bonnin, D. Coster, L. Horton, H. Summers, M. O'Mullane

- ## Implementation in SOLPS5.0

  – Technical requirements

- ## First test case

  – AUG #16151 benchmark case: D+Ar

  – Full 21 species description *vs.* « natural » bundling

  – Impact on the solution

  – Remaining issues:

    - Role of intra-bundle CX reactions
    - Need of more bundling choices to test sensitivity

Implementation in SOLPS5.0
(version 01.001.024)

✓Full backward compatibility and user transparency

  ▪ Old species data format: Z_a, Z_n, A_m, Z_a^2

  ▪ New data format: $Z_{a,min}$, $Z_{a,max}$, Z_n, A_m

✓Full recovery of old results

✓New ADAS rate arrays $Z_a(n_e, T_e)$, $Z_a^2(n_e, T_e)$, $E_i(n_e, T_e)$

✓Now need n_e saved in plasma state file and properly updated! (Quasi-neutrality equation becomes recursive)

✓Conversion tools to change between bundling schemes

✓No bundling allowed with neutrals (too different physics)

D+Ar test case

- **AUG #16151**

  - Reference: All charge states:

    - D_0, D^+, Ar_0, Ar^{+1}, Ar^{+2}, ..., Ar^{+18}

  - « Natural » bundling:

    - D_0, D^+, Ar_0, Ar^{+1}, Ar^{+2-+6}, Ar^{+7}, Ar^{+8}, Ar^{+9-+14}, Ar^{+15}, ..., Ar^{+18}

  - Both cases:

    - Identical boundary conditions and transport
      - Core: $n_{D+} = 5e19$, $n_{Ar+18} = 1e17$ m^{-3}, zero flux all others
      - $D = 0.5$ m^2/s, $\chi_i = 0.5$ m^2/s, $\chi_e = 0.5$ m^2/s
    - Fluid neutrals
    - Converged to machine accuracy

Bundled atomic physics rates
$(Z_a, E_i, <\sigma v>_{ion}, <\sigma v>_{rec})$

Z_a

E_i

$<\sigma v>_{rec}$

$<\sigma v>_{ion}$

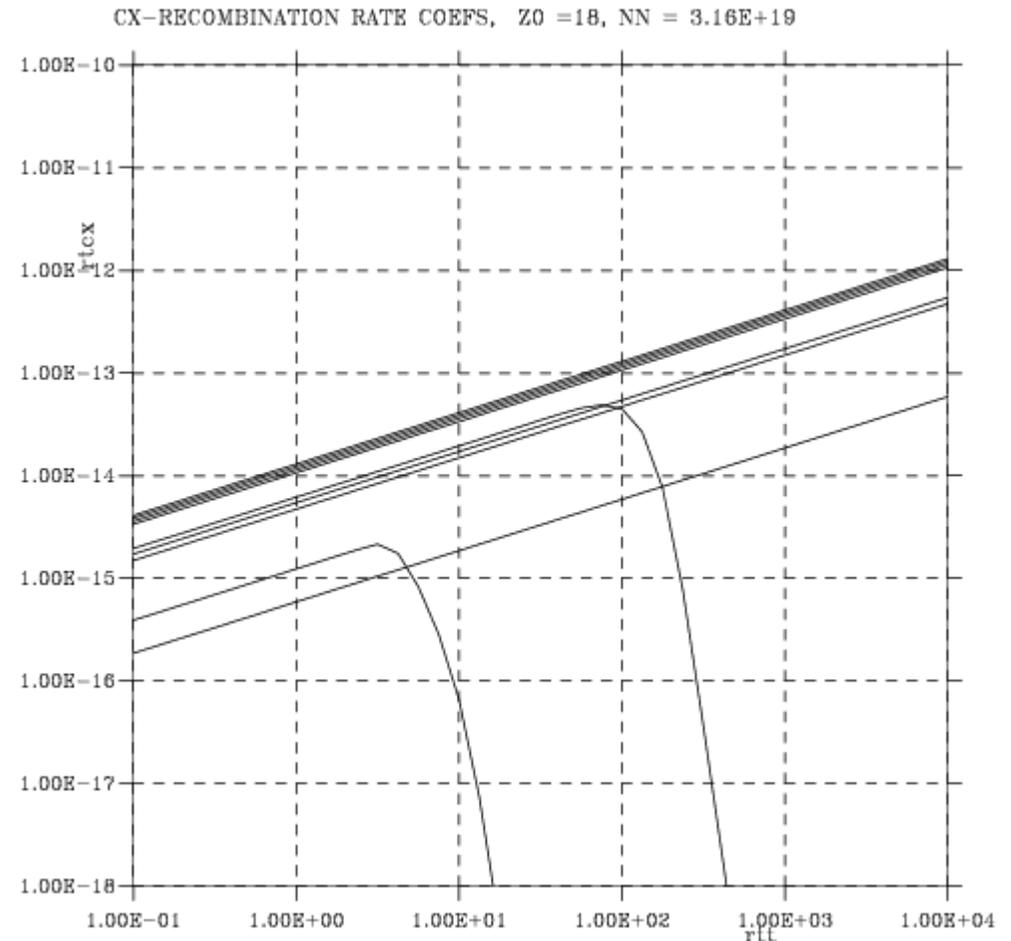**ADAS Workshop, Ringberg, 10-12 october 2007**
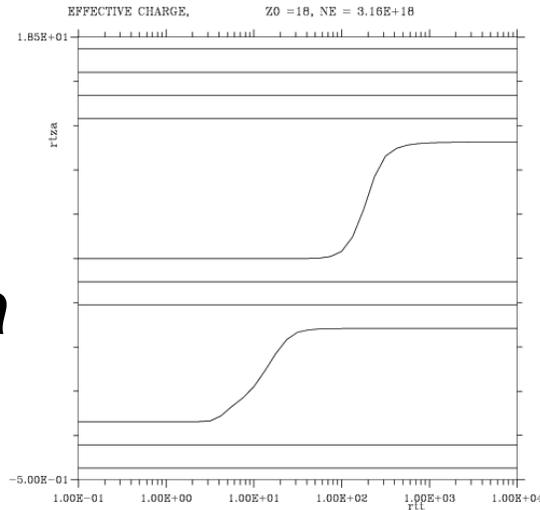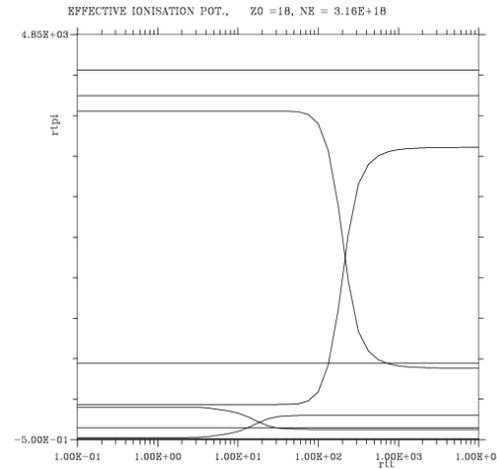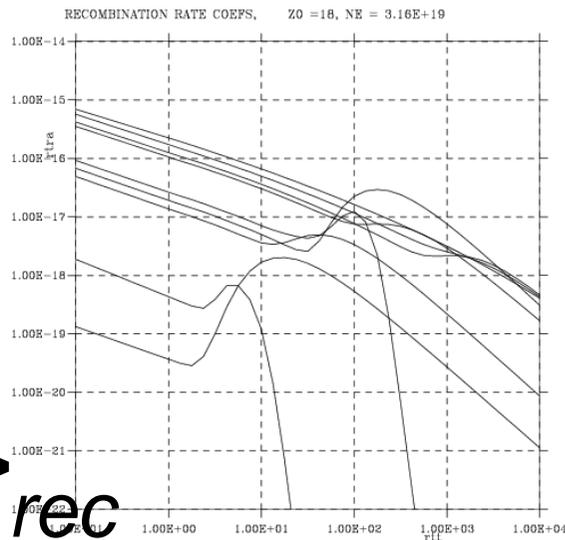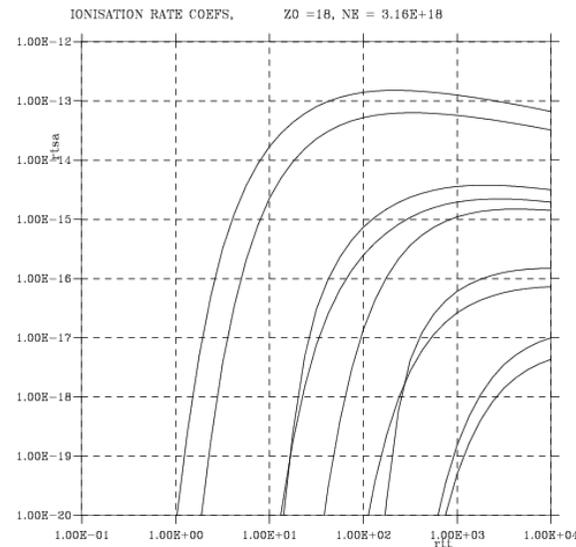
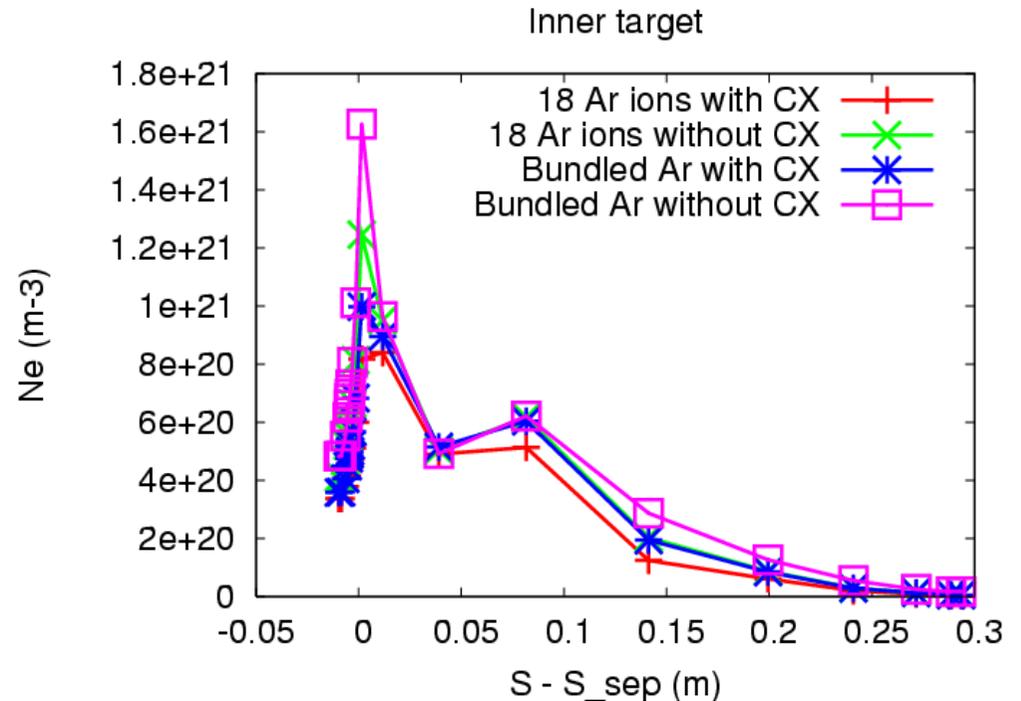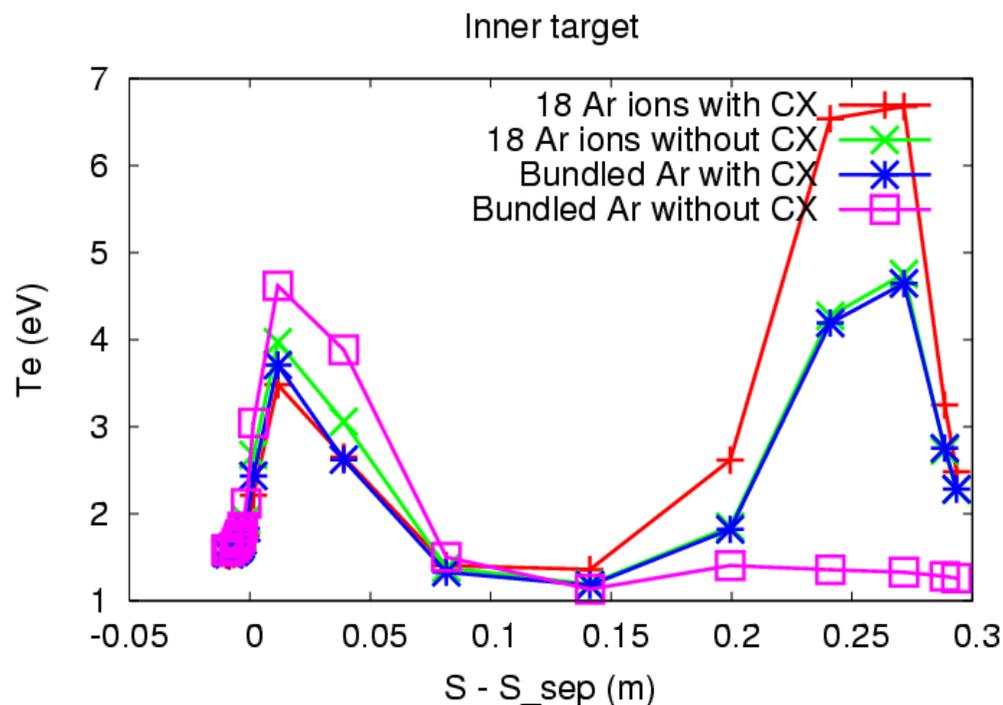# Results comparison (OMP T_e and n_e, targets)
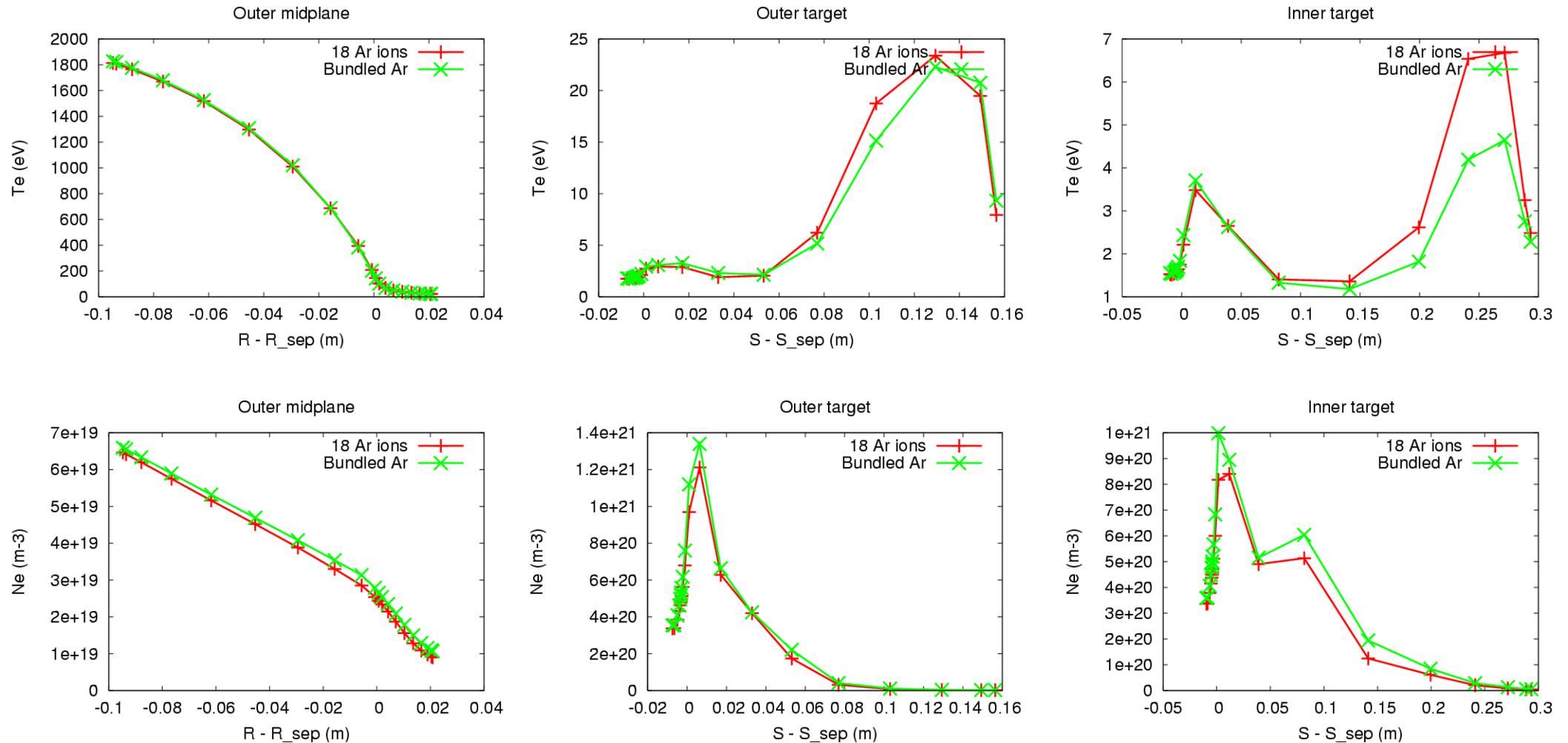
Bundling yields quite a good approximation !

Charge-exchange

- Bundled rates neglect intra-bundle CX rates

  - $D_0 + Ar^{+3} \rightarrow D^+ + Ar^{+2}$

- Does this matter?

- Re-do cases without CX

CX-RECOMBINATION RATE COEFS, ZO =18, NN = 3.16E+19

Comparison without CX: turning off all Ar CX reactions

Neglect of CX has consequences of the same magnitude as bundling itself

Conclusions and perspectives

- Bundled charge states can now be used in SOLPS5.0

- Need to complete sensitivity study with more bundle choices to assess what is allowable

  – From « lightly » bundled to « totally » bundled:

    - Only pair bundles, to Ar^{+1-+18}

  – Find an « edge »-optimal bundle set:

    - Keep low charge states more individualized, aggressively bundle high charge states

- Need to settle CX rates issue

  – One possibility, make bundle rates dependent on three variables: n_e, T_e and n_0