Midplane neutral density measurements in NSTX-U and fueling studies via UEDGE and DEGAS 2 simulations

NSTX-U Monday Physics Meeting

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Neutral distribution is critical to characterize SOL and pedestal physics, particle sources, edge power balance

- Accurate measurements of edge neutral densities are critical to:
  - Estimate particle sources in edge plasmas
    - Fueling studies
    - Determination of radial transport coefficients in steep gradient region is limited by knowledge of ionization source
    - Extrapolation to future devices further complicated by possible opaqueness of edge plasmas to neutral penetration
  - Characterize power balance
    - Charge exchange losses can be important for edge power balance
    - Integrated modeling (e.g., TRANSP) uses assumptions on edge neutral densities to calculate NBI losses
  - Aid diagnostics interpretation
    - E.g., FIDA, thermal charge exchange from impurity ions

Neutral densities are commonly estimated from passive emission from neutrals excited by background plasma

- Many tokamaks have developed techniques for neutral density n_D estimation
  - Yet, neutral densities are still typically not a routine measurement

- Common method is to use passive emission from neutrals excited by background plasma
  - Visible (Balmer series) emission (e.g., DIII-D[1], NSTX[2], AUG[3], TEXT[4]): easy measurement and calibration, more complicated interpretation
  - VUV (Lyman series) emission (C-Mod [5], DIII-D): easier interpretation but more challenging to measure/calibrate

- Alternative methods such as laser induced fluorescence [5] or charge exchange recombination from impurity ions [6] have also been used

- Local and reliable T_e, n_e measurements essential for accurate n_D determination
  - Limits availability of direct n_D measurements to few poloidal locations
  - Edge modeling is required to fill in the gaps of the 2D (or 3D) neutrals distribution

[1] Colchin, NF 2000.
[2] Stotler, PoP 2015.
[3] Agostini, PPCF 2019.
[4] Boedo, RSI 1988.
[5] Boivin, RSI 2001.
[5] Galante, PoP 2014.
[6] Bell, APS 2017.

Edge n_D measurements would directly support NSTX-U Five Year Plan Objectives I and II

- NSTX-U 5 Year Plan - Objective I: Extend confinement and stability physics basis at low-A and high beta to lower collisionality relevant to burning plasma regimes
  - *"Identifying transport and stability mechanisms that determine core and pedestal profiles"*
    - Neutral densities will be needed to characterize ionization rate profiles and edge particle losses

- NSTX-U 5 Year Plan - Objective II: Develop operation at large f_{BS} and advance the physics basis required for non-inductive and low-disruptivity operation of steady-state compact fusion devices
  - *"The largest energy confinement on NSTX was realized through a reduction in the edge neutral density using lithium wall coatings. The focus of this thrust is to characterize and optimize the boundary solution that enables long pulse operation in high* f_{BS} *scenarios and full performance scenarios "*
    - Neutral density measurements will enable determination of neutral fueling sources and effect of wall conditioning on particle balance (also covered in Objective III) and discharge performance

Research carried out in NSTX/NSTX-U towards establishing routine measurements of neutral density profiles

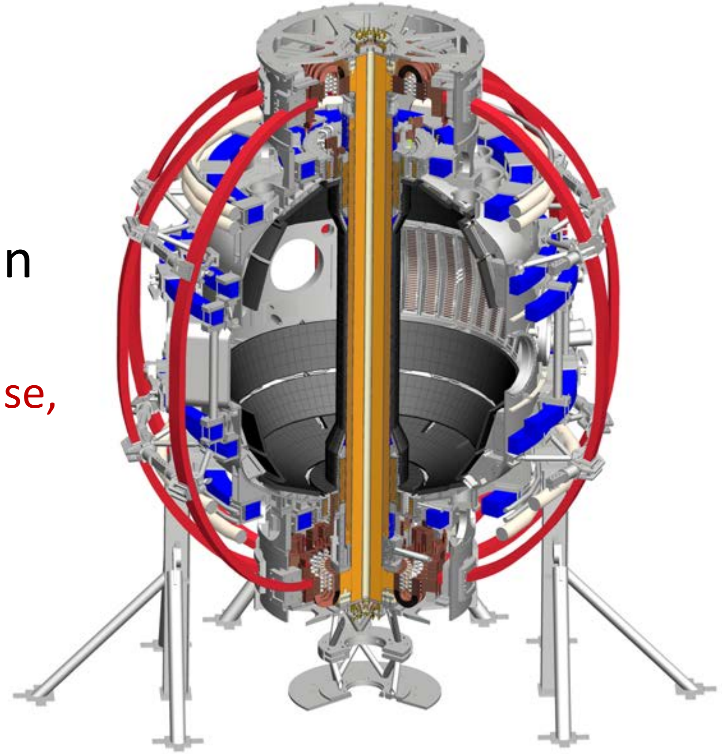
- Previous neutral density work in NSTX:
  - Original Edge Neutral Density Diagnostic (ENDD) diagnostic (D-β) installed in mid-2000 by P. Ross (PU grad. stud)
  - Took it over in 2010 (as PU grad. student) and photometrically/spatially re-calibrated
    - Initial ENDD/DEGAS 2 validation work from 2010 NSTX campaign in [Stotler PoP 2015, JNM 2015]
    - In 2011 ENDD port was reassigned by NSTX to a different diagnostic (never installed)
  - ENDD was moved to a more unfavorable location and redesigned for NSTX-U using some lessons learned from validation work and was operated in initial NSTX-U campaign (2015-2016)
- The goal of the work in NSTX-U was to establish ENDD as a standard diagnostics providing routine and (eventually) automated measurements of midplane n_D

- This work covers:
  - Determination of midplane n_D profiles and core ionization rate profiles in NSTX-U
  - Verification of assumptions in n_D derivation via MonteCarlo DEGAS 2 simulations
  - Interpretation of ENDD neutral density and ionization profiles via UEDGE and DEGAS 2 simulations

- Part of this work was performed towards the 2019 DOE-FES Joint Research Target milestone

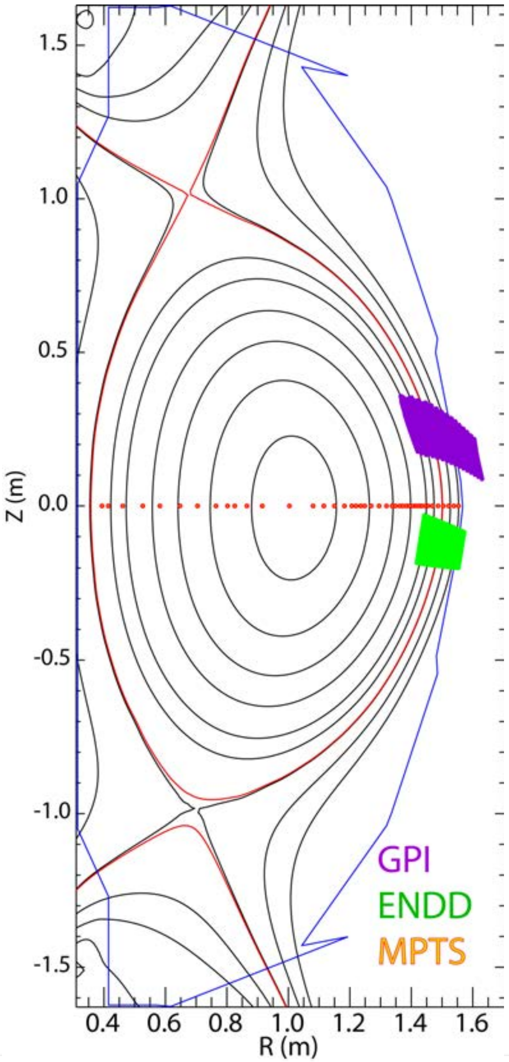
Measurements were taken during startup phase of first NSTX-U experimental campaign

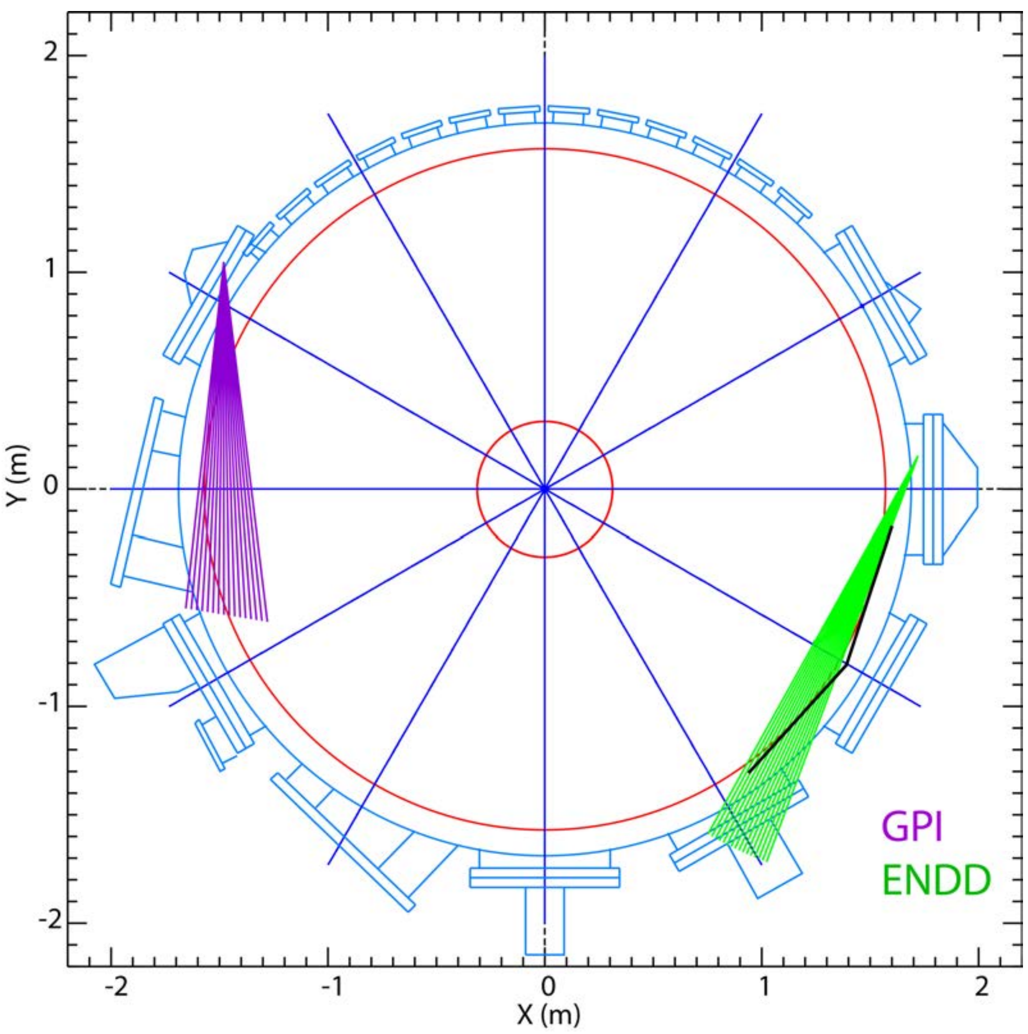
- NSTX-U operated Dec. 2015-May 2016
  - 10 weeks of operations
  - Startup tasks and initial discharge development
  - Up to I_p=1.0 MA, B_T=0.65 T
  - Pulse lengths ~1s H mode, ~2s L-mode
- Diagnostics needed for n_D determination were available throughout the run
  - ENDD view finalized ~mid "campaign", analyzed for ~400 discharges
    - No in-vessel time before campaign, alignment performed during initial operation phase, spatial and photometric calibration only post-run
  - Thomson scattering (MPTS) routinely available
  - CHarge Exchange (CHERS) routinely available (when 2nd beam not in use)
- Diagnostics needed for science and edge modeling unavailable in NSTX-U
  - No bolometers, Langmuir probes, heat flux measurements
  - Physics studies and edge modeling "challenging"



D_α line-integrated brightness monitored via two toroidally-separated tangential midplane 2D cameras

- ENDD:
  - 128x128 CCD camera
  - 1000x800 fiber bundle
  - Re-entrant view-port
  - D_α filter
  - 3.7 ms integration
  - Proximity to recycling surface (NBI armor)
- Passive GPI:
  - 64X80 fast CMOS
  - 1000x800 fiber bundle
  - D_α filter
  - 10 µs integration
  - No limiter surfaces nearby view
  - More challenging inversion
  - Lower S/N

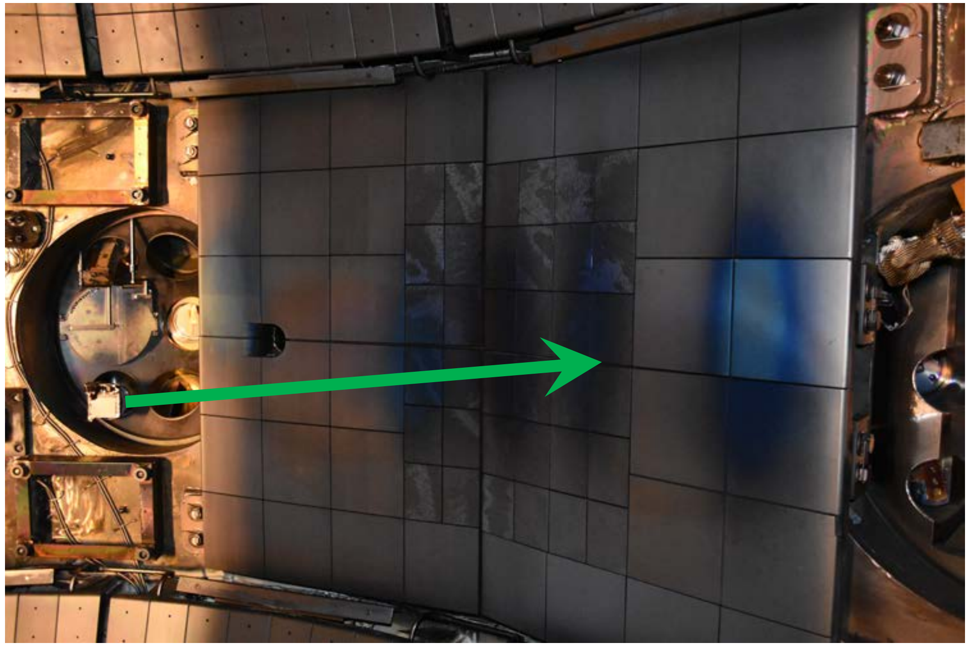


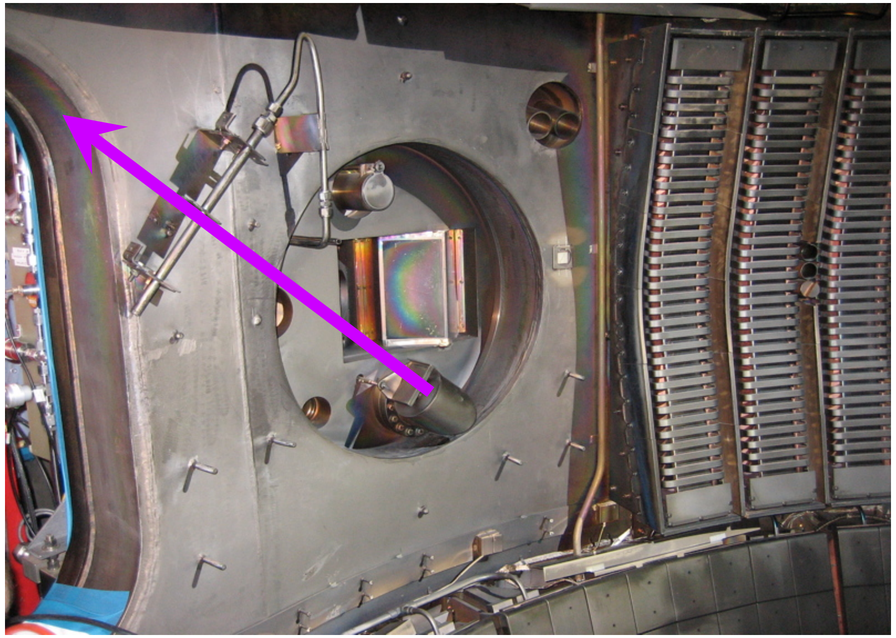


Hydrogenic emission monitored via two toroidally separated 2D cameras with tangential views

ENDD

view



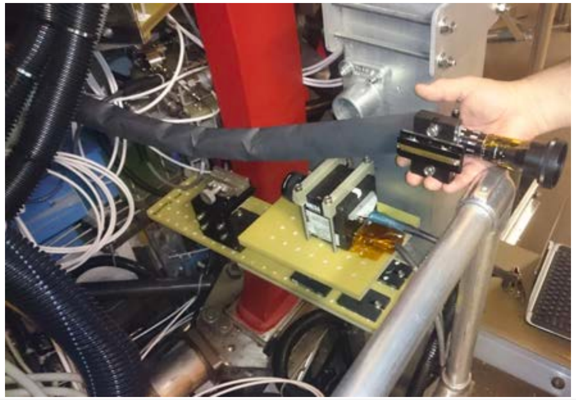


GPI

view

ENDD

window



ENDD

camera

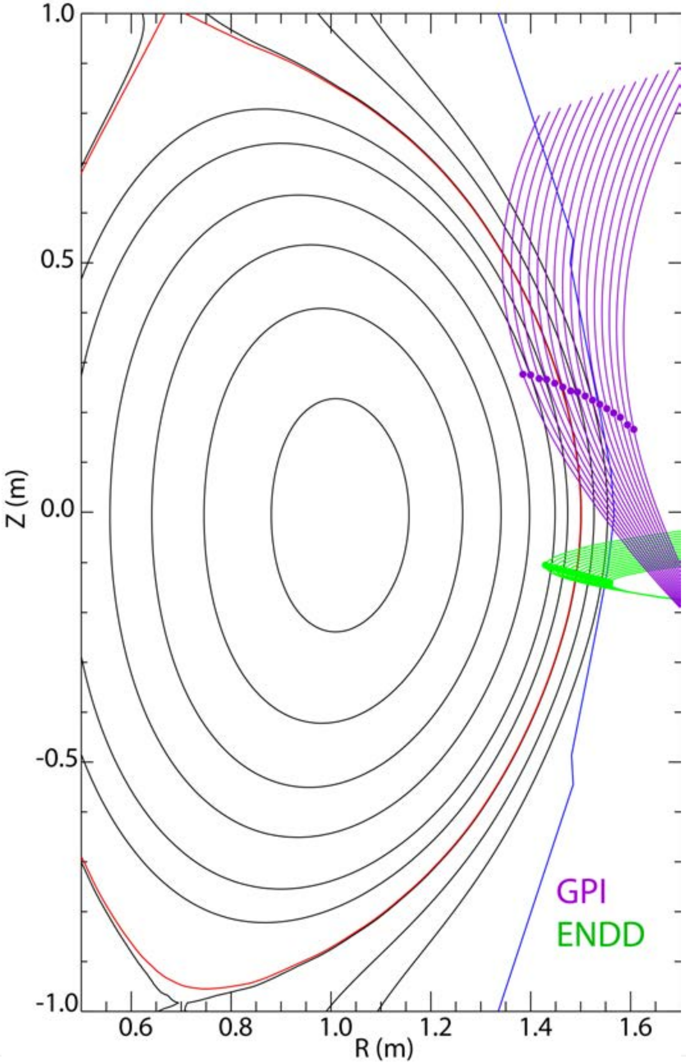
Inversion used to derive emissivity profiles from line integrated brightness in different views

- ENDD and passive GPI provide line-integrated measurements through a D_α filter
- Emissivity calculated from brightness using matrix inversion:
  - Length matrix calculated for 3D geometry using EFIT equilibrium
  - Assuming toroidal symmetry and constant emissivity along flux surface

$$4\pi B_i = \sum_j L_{ij} E_j \qquad E_j = 4\pi \sum_i L_{ij}^{-1} B_i$$

- Pixels are binned poloidally
- Tangency mapped to Z=0 for direct use of TS measurements

Inversion developed by R. Bell



Neutral density inferred from measured emissivity assuming only contribution from e- impact excitation

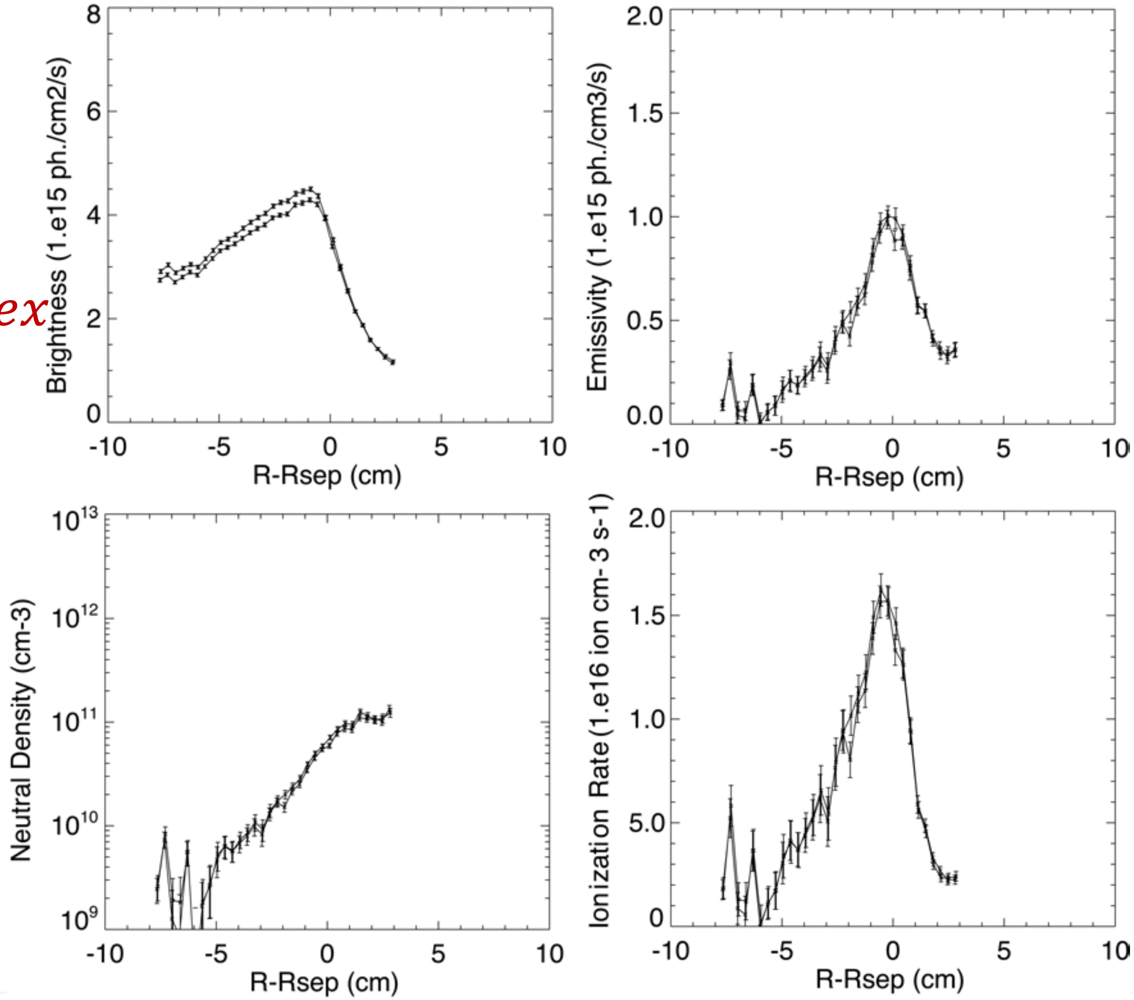
- n_D inferred assuming emission due to electron impact excitation
  - Using local T_e, n_e values (single profile) to estimate photon emission coefficients

$$E_{D\alpha} = n_e n_D(1s)\left[\frac{n_D(n=3)}{n_D(1s)}\right] A_{3\rightarrow 2} = n_e n_D(1s) \times PEC_{ex}$$

$$\Rightarrow n_D = \frac{E_{D\alpha}}{n_e PEC_{ex}}$$

- PEC produced by *collrad* (D. Stotler, ehr5.dat as used in DEGAS 2)
- Contribution from molecular processes expected dominant in SOL (neglected here)
  - n_D from ENDD will be an upper estimate of the actual n_D and expected to be accurate only inside the separatrix

NSTX-U L-mode discharge 204202



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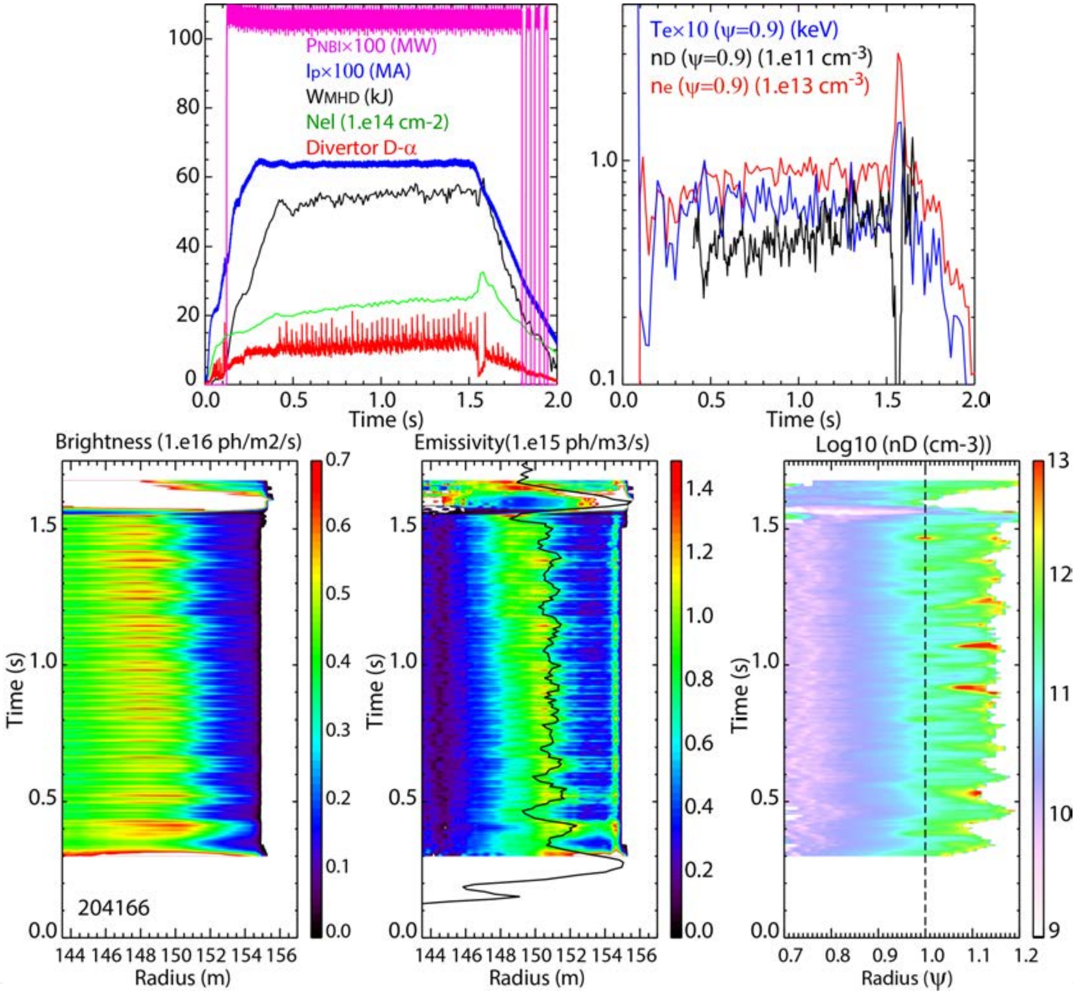
NSTX-U L-mode discharge 204166



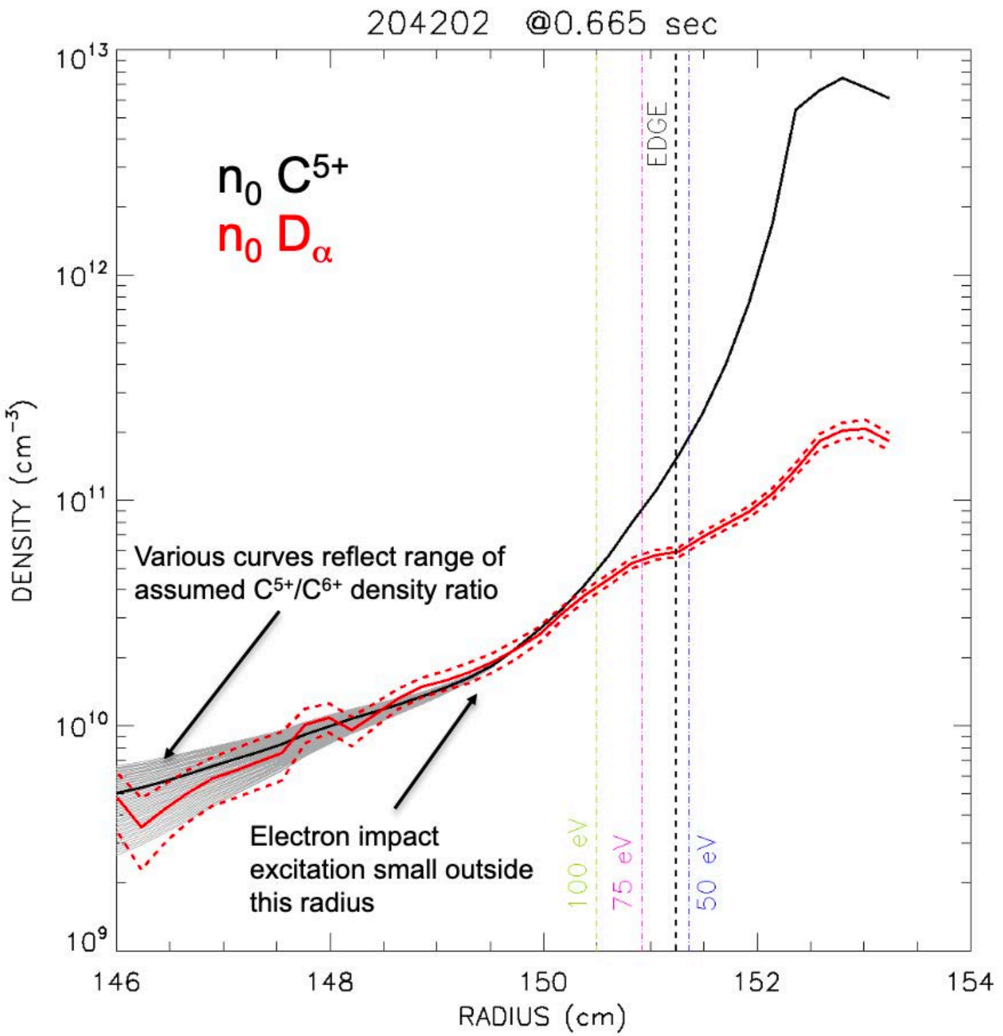
Alternative method by R. Bell to infer n_D from passive C^{5+} charge exchange emission compares positively with ENDD

- Method developed by R. Bell [R. Bell APS 2017]
- n_D inferred from background charge exchange emission from C^{5+}

$$E_{C^{5+}} = \underset{\underset{\text{Excitation}}{\uparrow}}{Q_{ex} n_e n_{C^{5+}}} + \underset{\underset{\text{Recombination}}{\uparrow}}{Q_{rec} n_e n_{C^{6+}}} + \underset{\underset{\text{Thermal Charge Exchange}}{\uparrow}}{Q_{cx} n_0 n_{C^{6+}}}$$

$$n_0 = \frac{E}{Q_{cx} n_{C^{6+}}} - n_e \left(\frac{Q_{ex}}{Q_{cx}} \frac{n_{C^{5+}}}{n_{C^{6+}}} + \frac{Q_{rec}}{Q_{cx}} \right)$$

- Needs C^{6+} from CHERS and assumptions on C^{5+}/C^{6+}
- Compares well with ENDD measurements inside separatrix

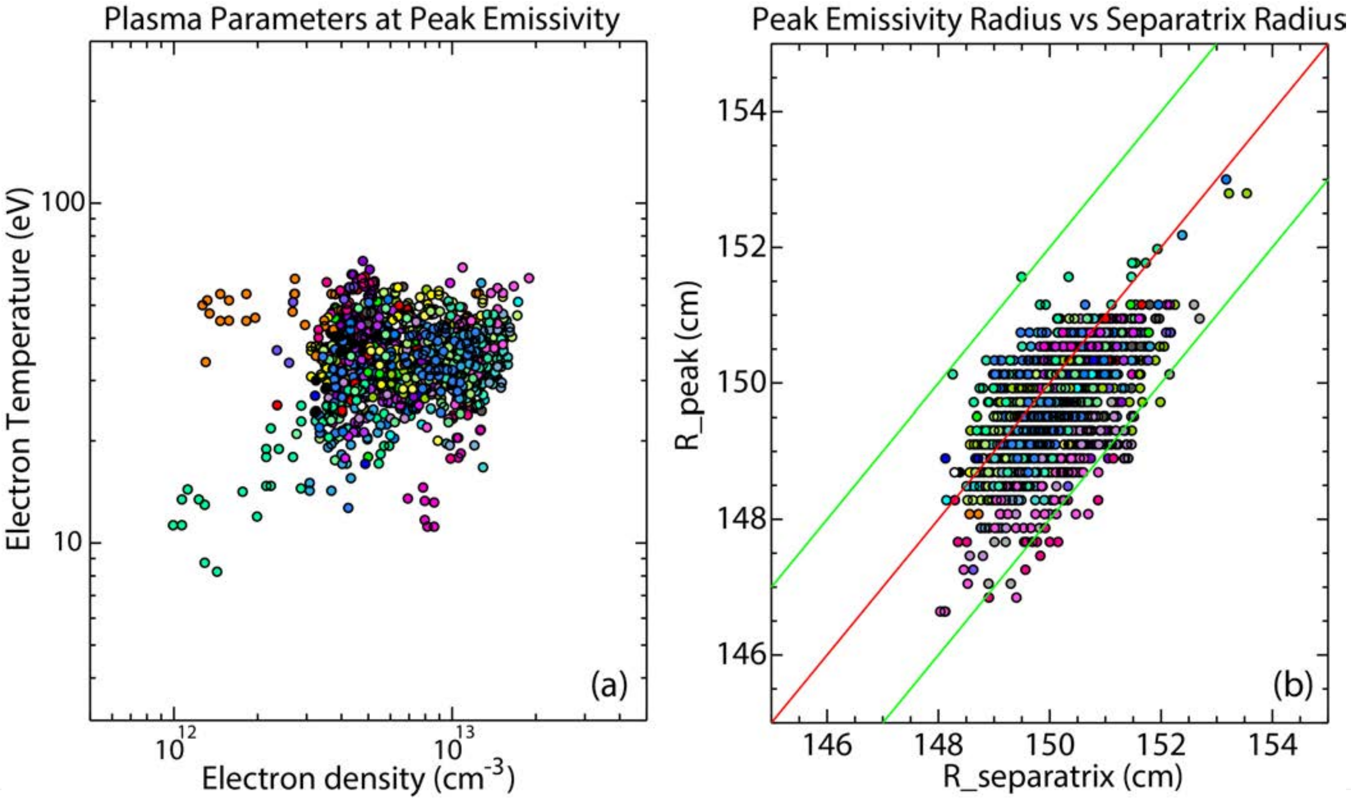


Various curves reflect range of assumed C^{5+}/C^{6+} density ratio

Electron impact excitation small outside this radius

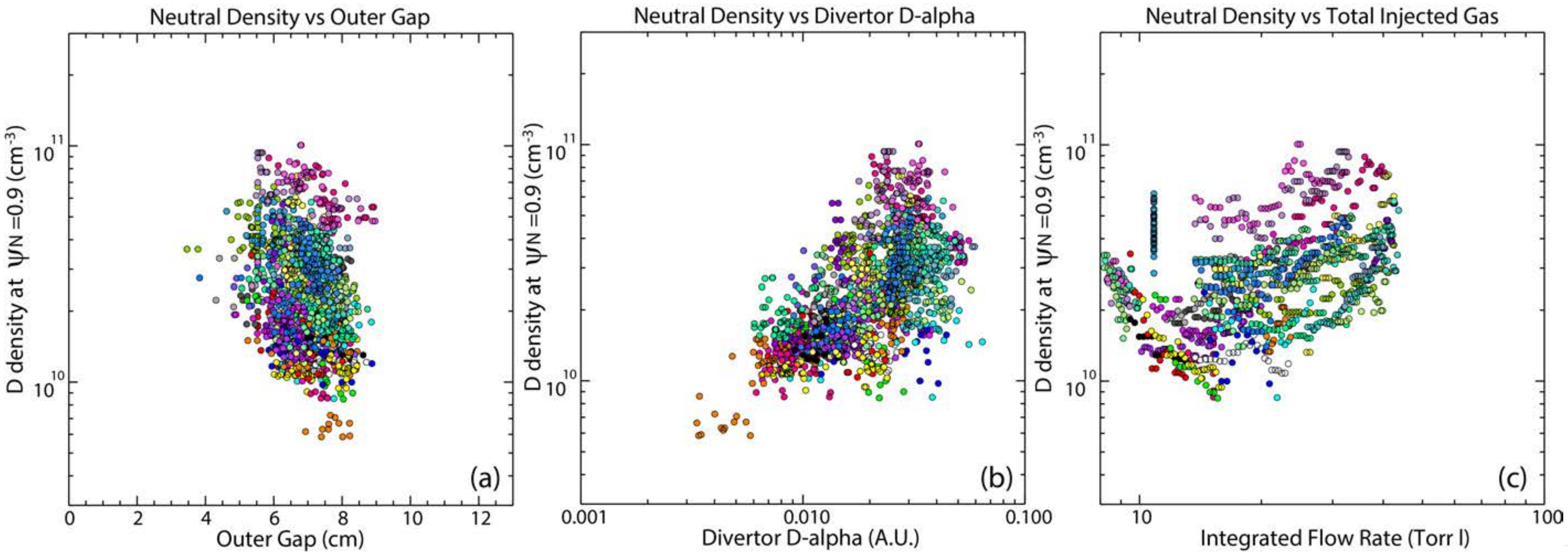
Profiles of D-α emissivity and n_D assembled for 60 L-mode discharges during current flat-top to assess main trends

- NSTX-U L-mode discharges, intervals during current flat-top, ENDD profiles at MPTS time points
  - 60 discharges, 1750 time points (points from each discharge in a different color)
- Peak emissivity localized at LCFS +/-1cm, follows T_e=25-45 eV



In L-mode plasmas, line density, divertor recycling, and LFS fueling correlate with midplane edge n_D

- Edge n_D derived at $\Psi_N=0.9$ to avoid molecular contribution
- Edge n_D well correlated with line avg. density and neutral pressure from pump duct ion. gauge
- Edge n_D correlated with divertor D-α, integrated injected gas from LFS injector suggesting possible role of divertor recycling and LFS fueling
  - All these quantities are correlated, DEGAS 2 simulations will later be used to investigate relative role



DEGAS 2 Monte Carlo neutral transport simulations used to validate assumptions in ENDD measurements

- n_D from ENDD represents an upper estimate of n_D
  - D_α emission due to excitation by molecular processes dominant outside separatrix

$$e + D_2 \rightarrow e + D(1s) + D^*(n=3),$$

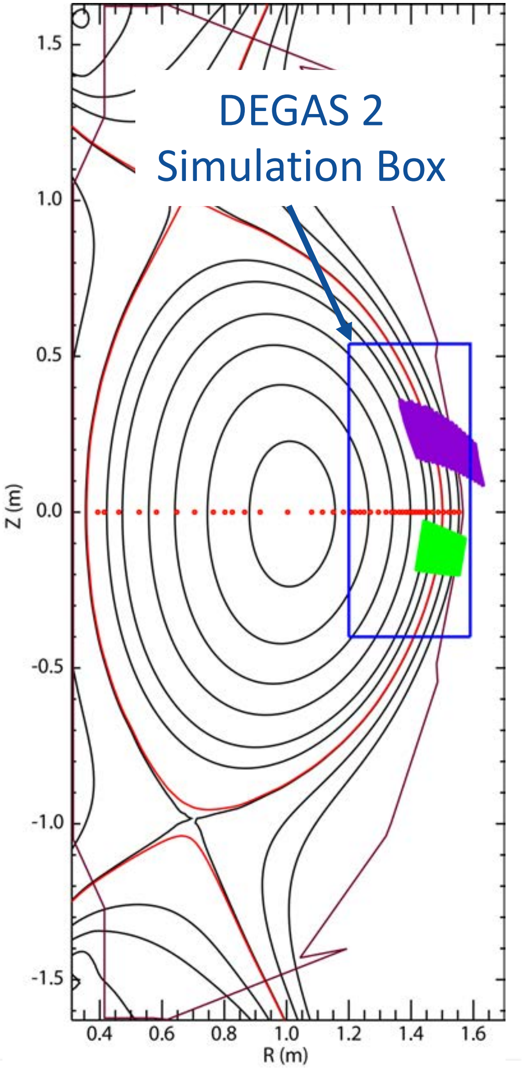
Dissociative excitation

$$e + D_2^+ \rightarrow e + D^+ + D^*(n=3),$$

$$e + D_2^+ \rightarrow D(1s) + D^*(n=3).$$

Dissociative recombination

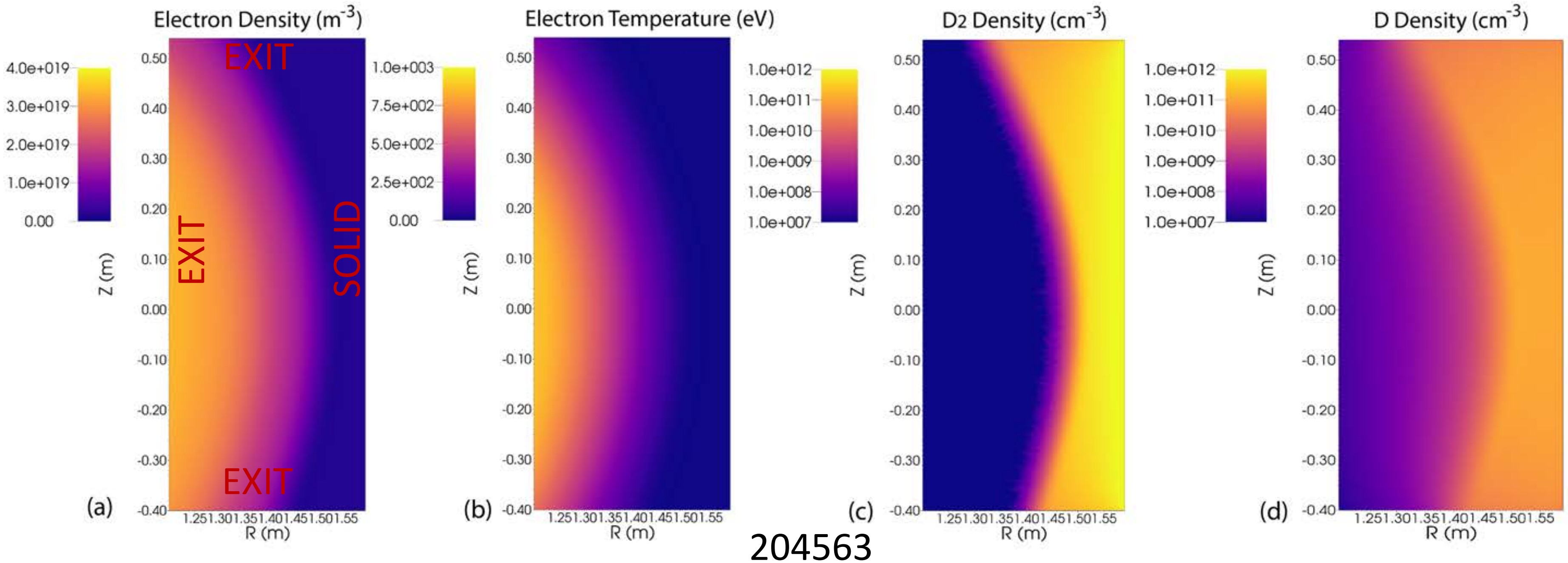
- DEGAS 2 Monte Carlo neutral transport simulations performed to model experimental D_α emissivity and contribution from molecular processes
  - Validate assumptions used for ENDD n_D derivation
  - Gain a better understanding of diagnostic measurements
  - Extract n_D and ionization profiles at radii where ENDD measurements are not available
  - Similar method initially applied for NSTX [Stotler, PoP 2015] using original D_β ENDD brightness via synthetic diagnostic



An automated workflow was developed to launch and post-process DEGAS 2/ENDD simulations

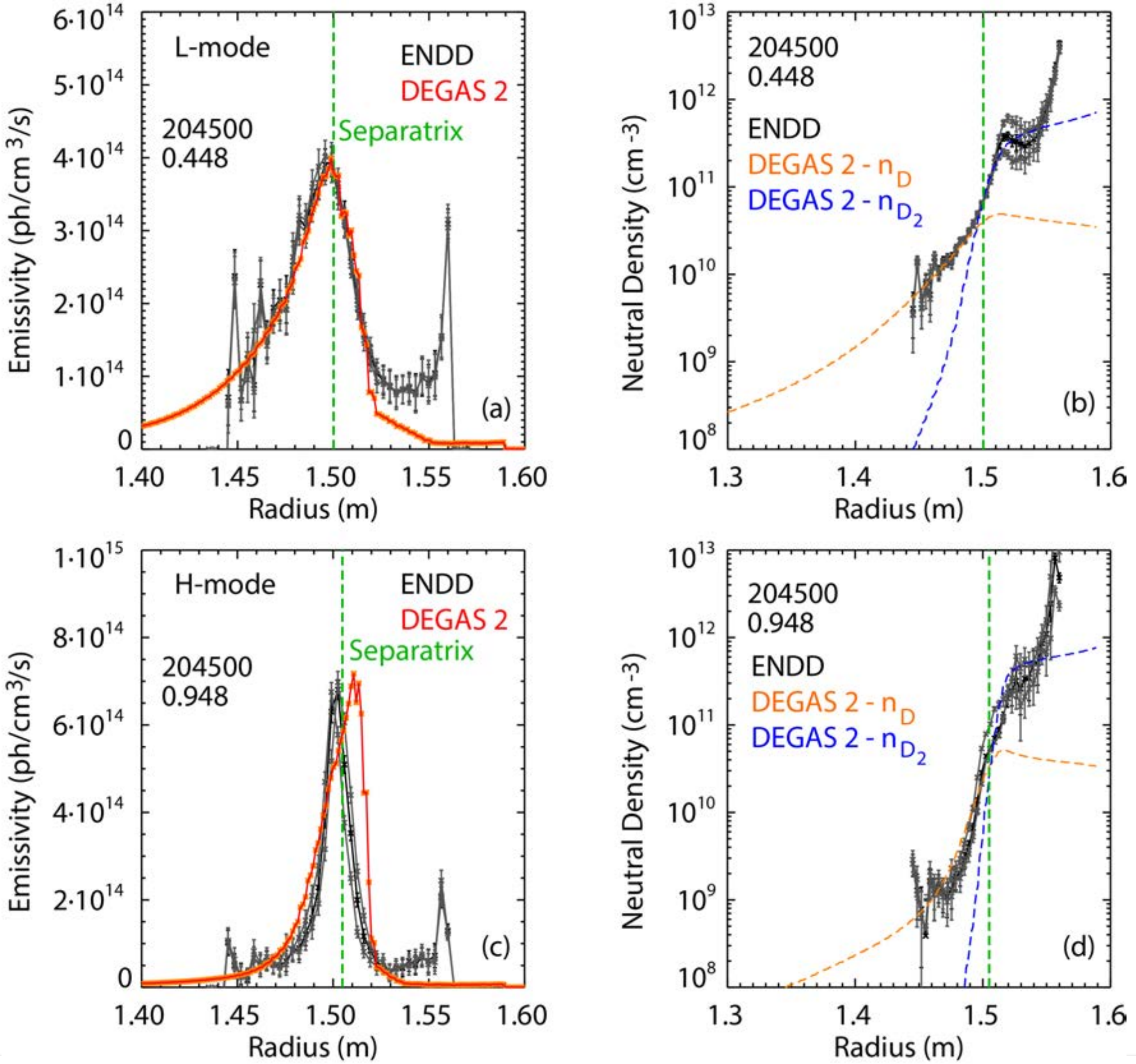
- Simulation box R = [1.2, 1.59] m , Z = [−0.4, 0.55] m: solid interface at R=1.59 m
- Simulation grid generated from EFIT02, T_e, n_e from single MPTS profile, T_i=T_e
- Test particles (4×10^6) launched from solid interface with uniform distribution
  - Sensitivity study on source location shows normalized emissivity profile shape unaffected by source location
- D-α emissivity, n_D, n_{D2} profiles calculated with DEGAS 2 (for a given wall source)

- DEGAS 2 D-α emissivity normalized to experimental ENDD emissivity
- Emissivity normalization is carried to n_D, n_{D2} calculated by DEGAS 2, allowing their absolute determination



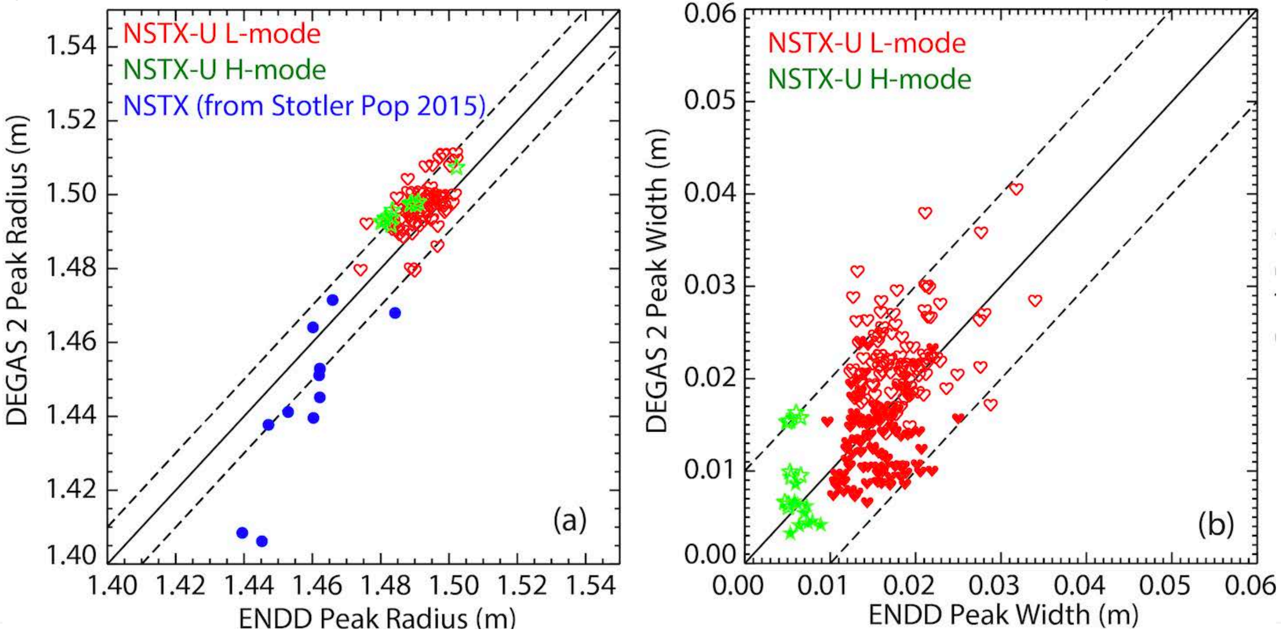
DEGAS 2 simulations match ENDD emissivity profile, ENDD n_D profiles accurate inside LCFS

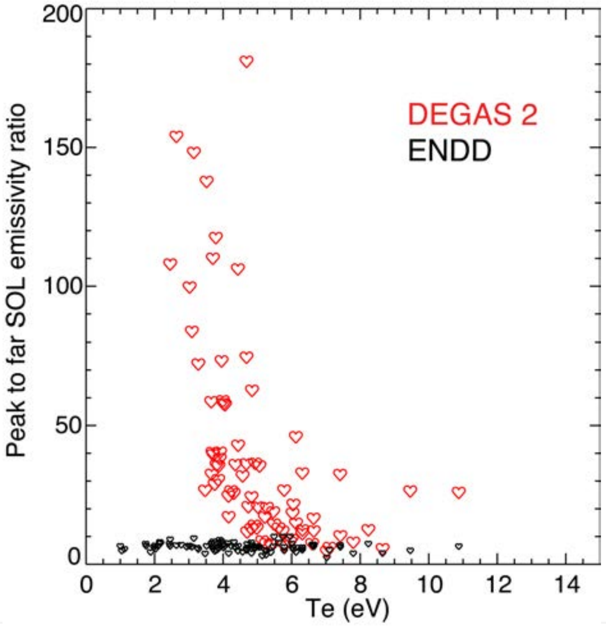
- Good agreement in midplane D_α emissivity profile shape
  - Better inside separatrix
  - Better in L-mode
  - Peak emissivity radius overpredicted
    - Especially in H-mode
  - Far SOL emissivity underpredicted
    - Especially in L-mode
- Great agreement in inferred neutral densities after emissivity normalization
- $n_{D\text{-}ENDD} \sim n_{D\text{-}DEG} + n_{D2\text{-}DEG}$
  - Inside LCFS $n_{D\text{-}DEG} = n_{D\text{-}ENDD}$
  - Emission dominated by e- impact excitation



DEGAS 2 simulations compared with ENDD data over large database of L- and H- mode discharges

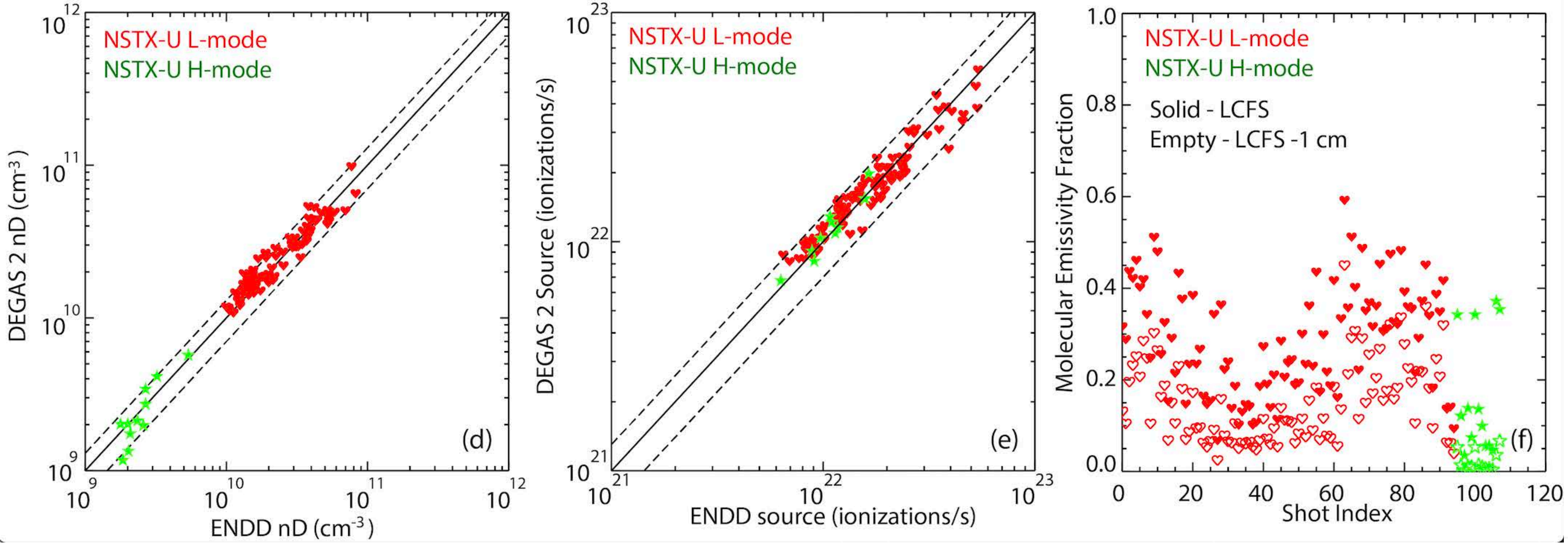
- ~110 DEGAS 2 simulations ran for different MPTS times in 15 L-mode and H-mode discharges
  - Profiles shapes and inferred densities and ionization rates are compared between sim. and experiment
- Peak emissivity radius on average overestimated by 4-5 mm in simulations
  - Worse in H-mode, due to overpredicted molecular emission outside LCFS
- Emissivity FWHM ~consistent with experiment, overpredicted inside LCFS, underpredicted in SOL
- Underprediction of far SOL emissivity scales inversely with SOL T_e

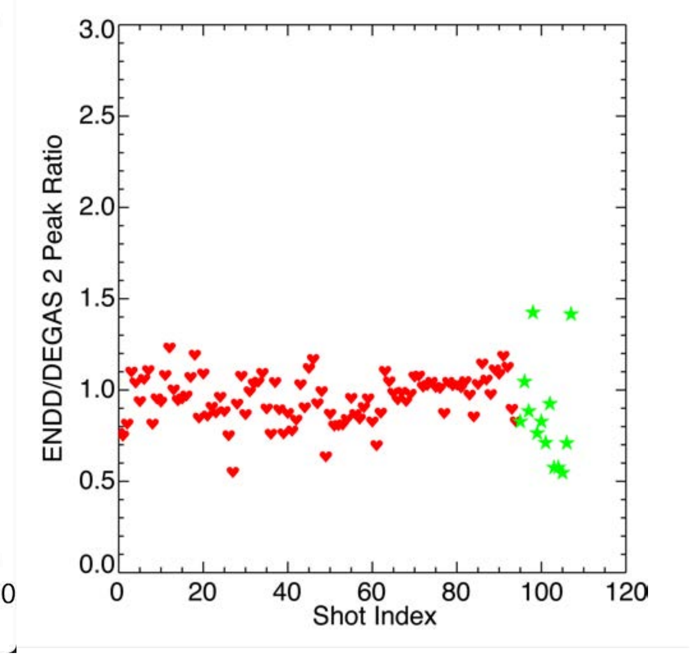




Good agreement inside separatrix between n_D and ionization source from ENDD and DEGAS 2

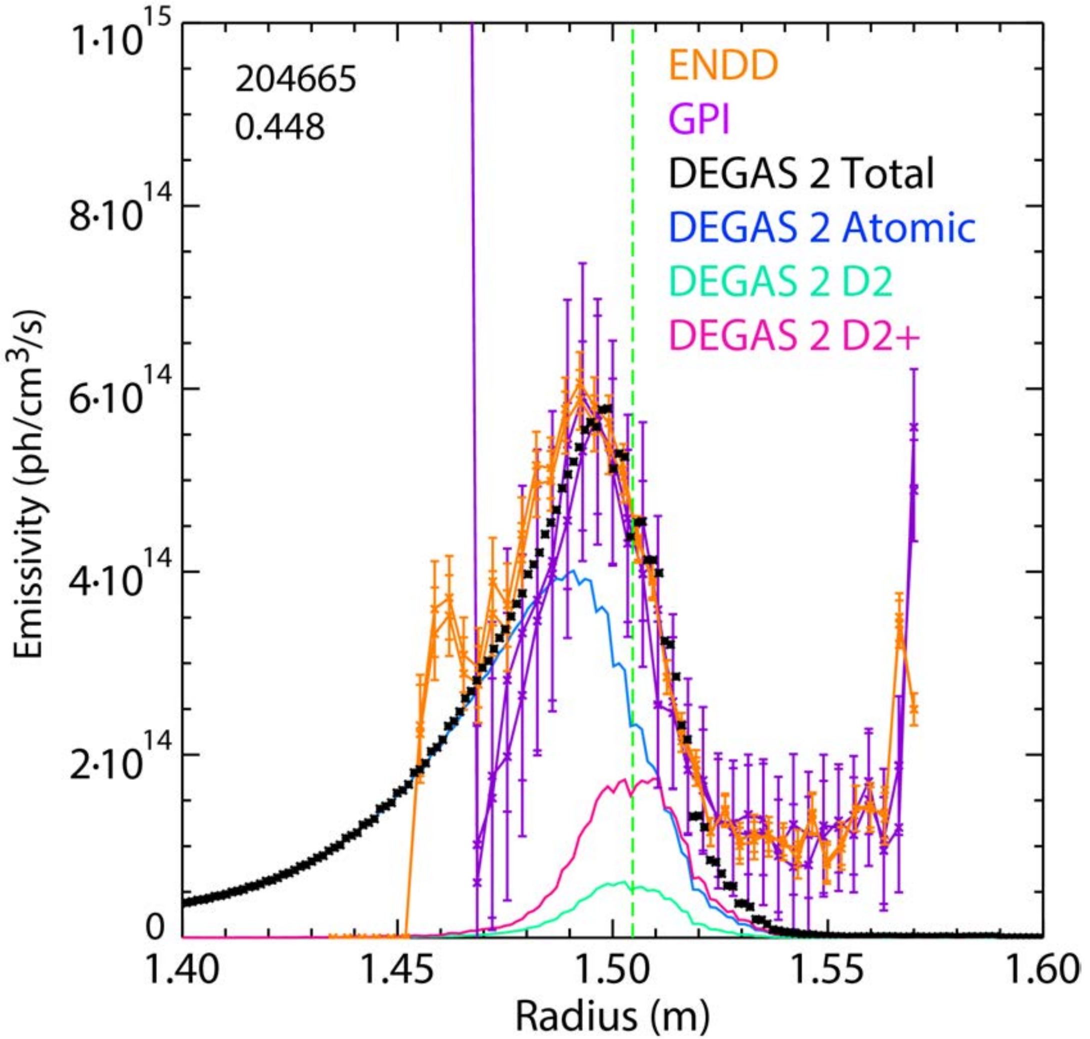
- DEGAS 2 profiles normalized to either peak ENDD emissivity or ENDD emissivity inside separatrix
- After normalization, n_D and ionization source inferred from ENDD and DEGAS 2 have good agreement inside separatrix
  - — Indicating most emission from neutrals excited by electron impact
  - — Peak emissivity can vary, especially in H-mode, due to extra molecular emission predicted





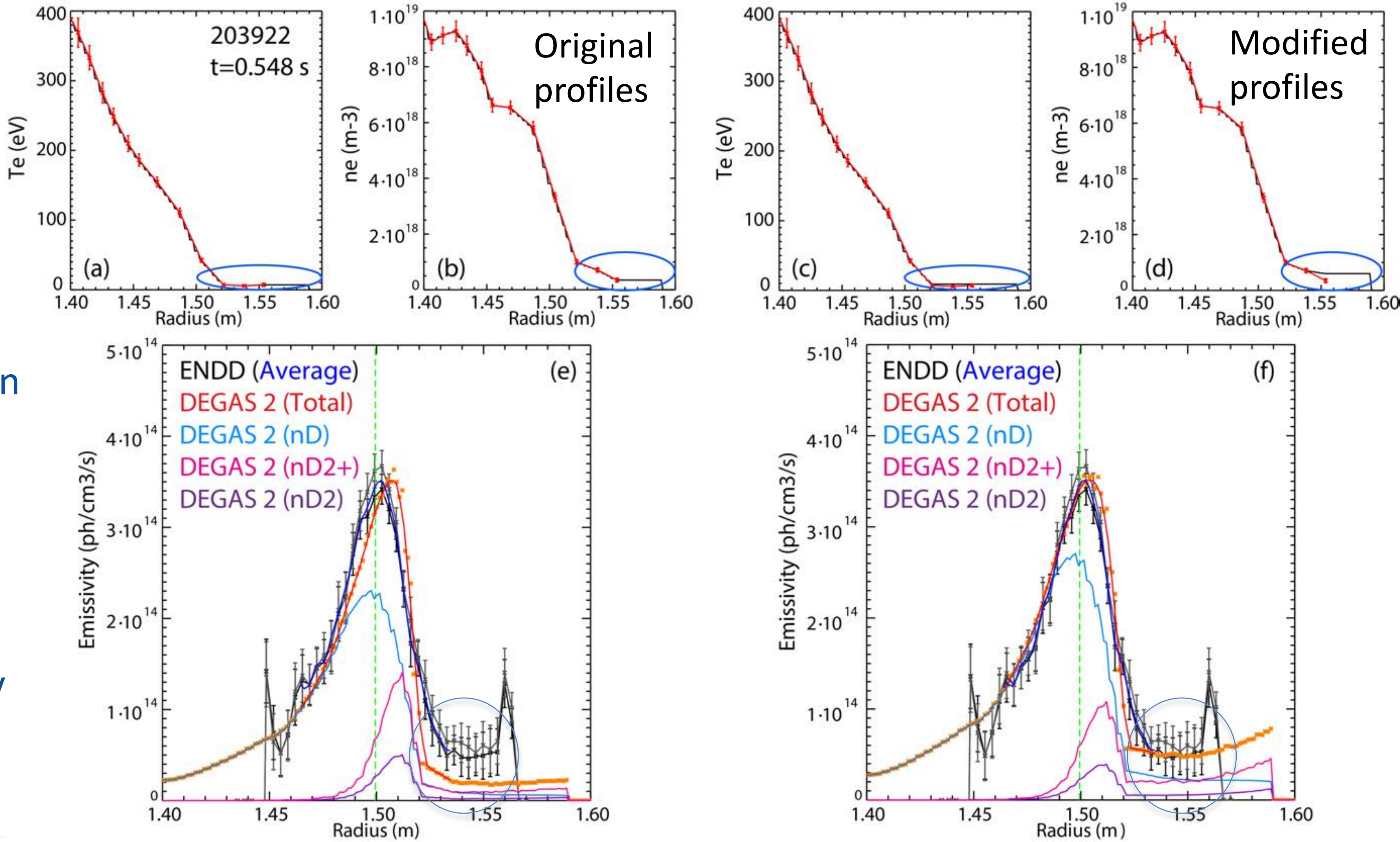
Emissivity profile shape in agreement between ENDD and GPI, molecular emission dominant outside LCFS

- ENDD and GPI normalized profiles compared to exclude diagnostic issues from discrepancies with DEGAS 2 comparison
  - Peak emissivity location and far SOL emission both in agreement between the two diagnostics
- Remaining discrepancies possibly related to inaccuracies in molecular emission model or SOL intermittency
  - Peak emissivity deviation driven by extra molecular emission close to LCFS
  - Far SOL emissivity deviation due to underpredicted molecular emission



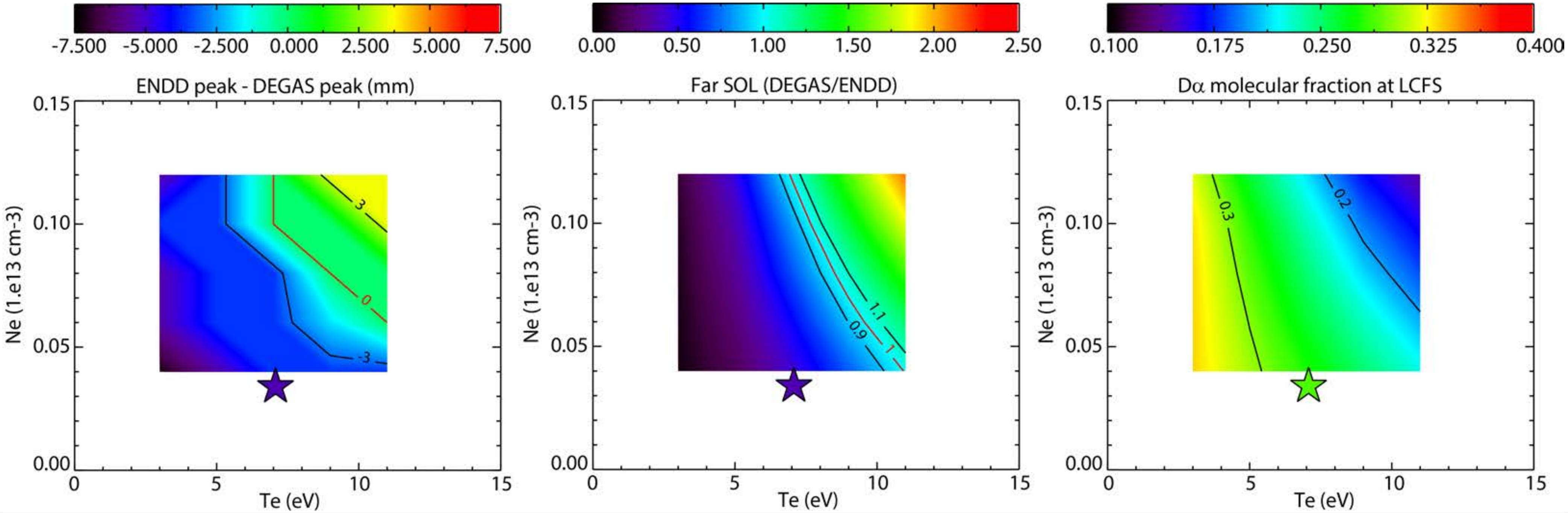
Increase in far SOL T_e, n_e in DEGAS 2 simulations improved agreement with ENDD emissivity in L-mode

- Scan in far SOL T_e, n_e performed to test possible role of intermittent convective transport on simulated emissivity
  - Increase in far SOL T_e, n_e increase molecular dissociation in far SOL, increasing far SOL emissivity and reducing molecular contribution near LCFS
  - Improved agreement in peak location and far SOL emissivity



Peak shift, far SOL emissivity agreement improves for similar far SOL T_e, n_e

- Peak shift, far SOL emissivity agreement improves for similar far SOL T_e, n_e
  - Only minor changes in inferred neutral densities inside separatrix
  - Justifies single MPTS profile use as DEGAS 2 input
- Improvements observed also for H-mode cases but not enough to reconcile profile shape differences
- Uncertainties in molecular emission model also likely to play a role



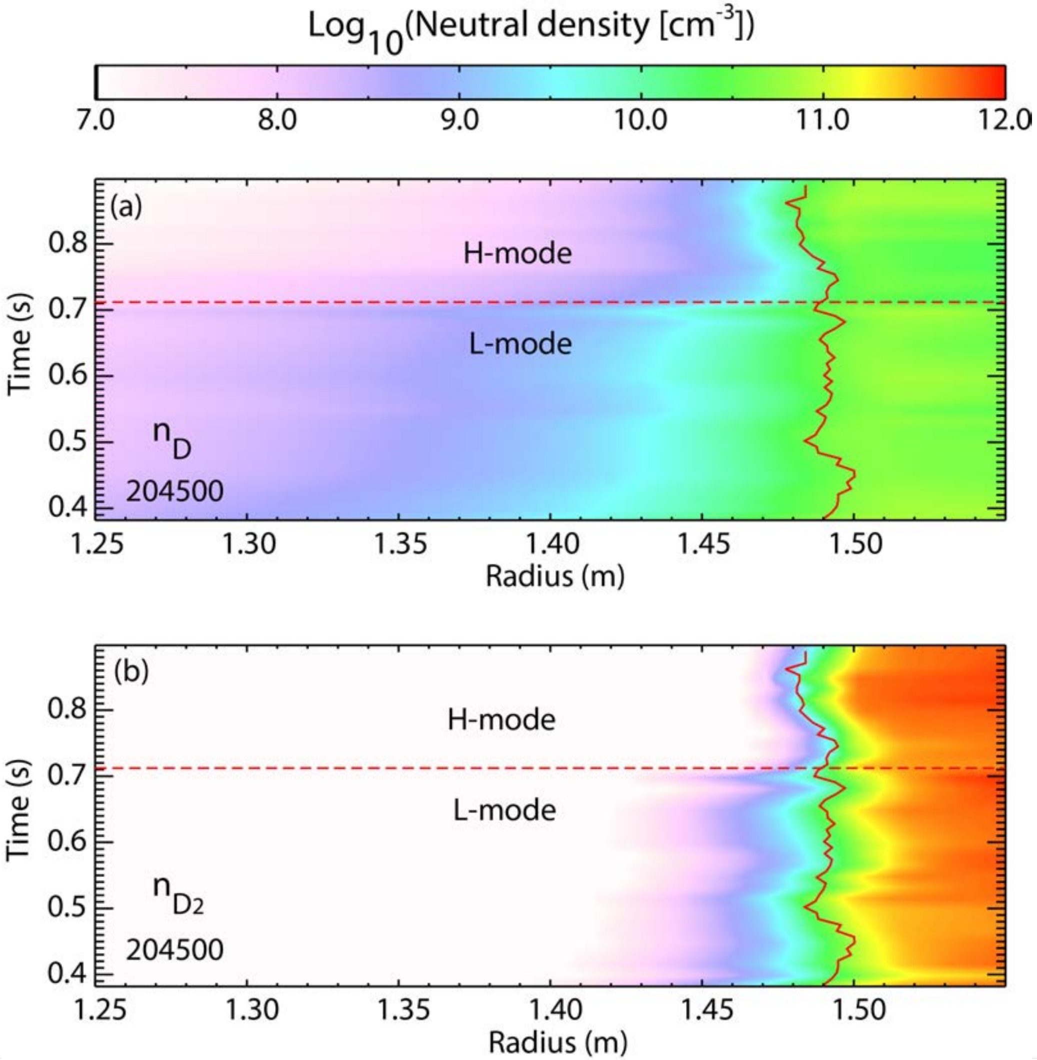
Conclusions from ENDD measurements and assumptions validation via DEGAS 2 simulations

- Measured (ENDD) and simulated (DEGAS 2) emissivity show good agreement
  - Some deviations in peak emissivity location and far SOL emissivity
  - Both point to uncertainties in molecular emissivity contribution
- After emissivity normalization, ENDD n_D and DEGAS 2 n_D are in great agreement
  - Direct ENDD measurement is enough to infer neutral densities and ionization rate profiles inside separatrix over the ENDD field of view
    - This can become a routine n_D measurement
    - Outside LCFS emission is dominated by contributions from atoms excited by molecular processes
  - In the DEGAS 2 simulations, T_e, n_e profiles are entirely sufficient to accurately predict the n_D profile shape
    - Simulations need some absolute emission measurement to also obtain magnitude
  - Combined ENDD/DEGAS 2 analysis can provide n_D, n_{D2} radial profiles, further extending direct ENDD measurements and coverage

Validated ENDD/DEGAS 2 analysis enables derivation of midplane radial profiles of atomic and molecular density

- At each MPTS time, ENDD/DEGAS 2 analysis normalized to ENDD emissivity
  - Time evolution of n_D and n_{D2} densities as a function of time and radius
  - n_D and ionization rate profile at outer midplane inside separatrix are already well approximated by the direct ENDD measurements
  - Interpolating through MPTS times, temporal resolution could be reduced to camera frame rate

- An example is shown for an L-H transition:
  - SOL n_D, n_{D2} relatively constant during discharge
  - Large decrease and steeper gradients for n_D, n_{D2} after L-H transition due to n_e pedestal formation

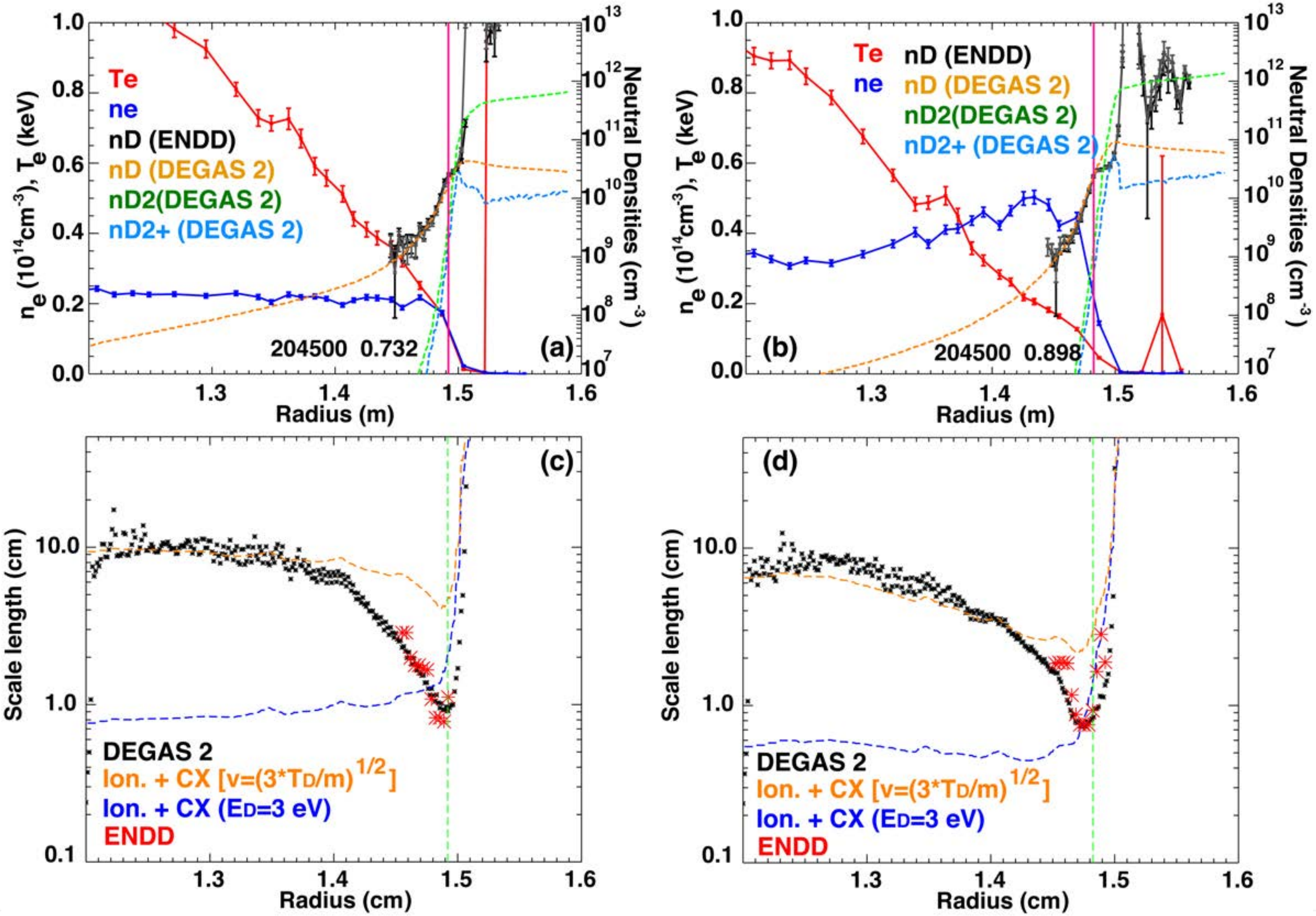


Neutral density profile shape shows importance of kinetic effects in steep gradient region

- DEGAS 2/ENDD n_D scale length compared with ionization + CX λ_{mfp}
  - — As discussed in [Stotler, PoP 2015]

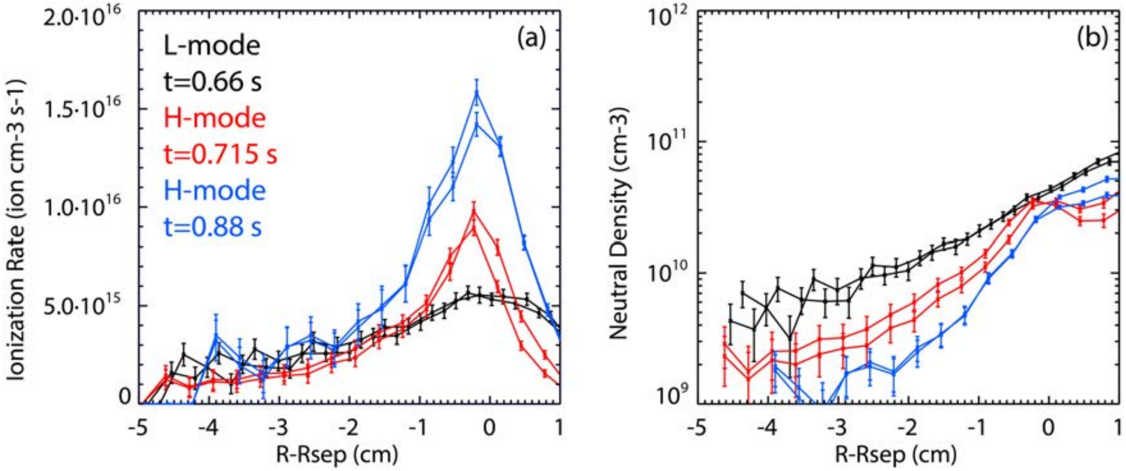
$$\lambda_{mfp} = \frac{v_{th,D}}{n_i S_{CX}(T_i, E_D) + n_e S_i(T_e, n_e)},$$

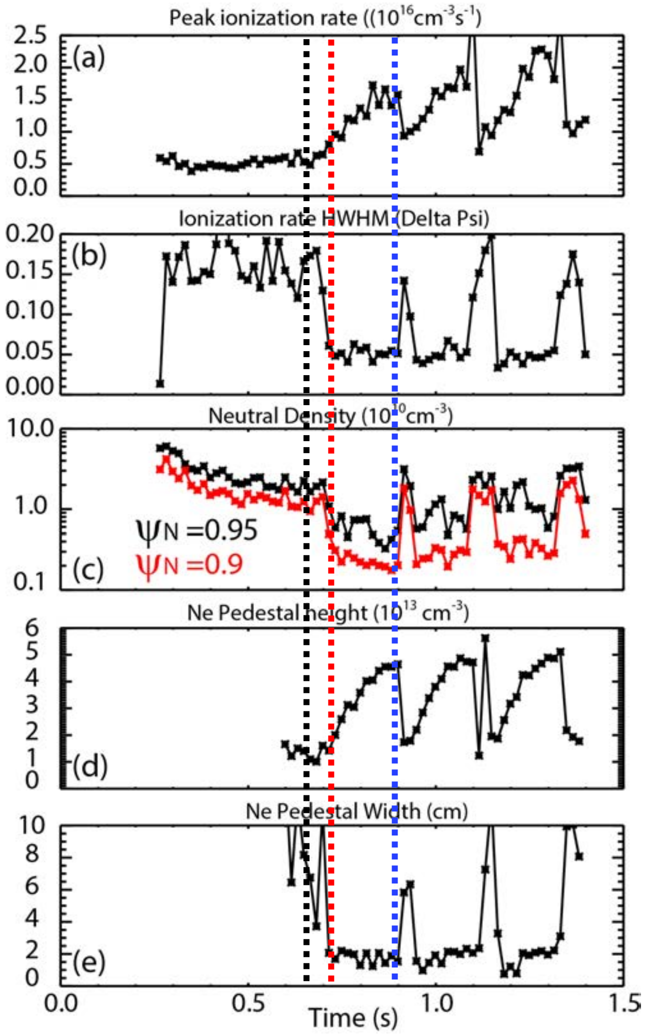
- Agreement with ionization + CX λ_{mfp} of thermalized neutrals inside pedestal top
- Deviations in steep gradient region shows role of non thermalized 3eV neutrals from dissociation
- Extent of region showing deviation from ionization + CX λ_{mfp} reduces with increasing density



ENDD/DEGAS 2 analysis validated direct use of ENDD data for ionization profile derivation inside LCFS

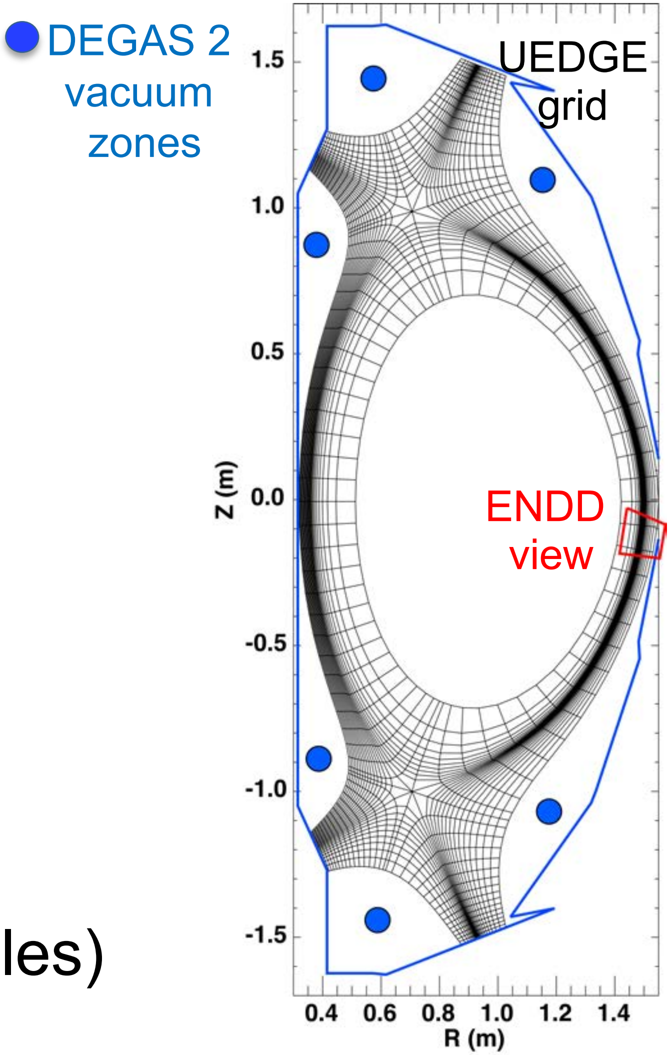
- Inside separatrix emission is dominated by e- impact excitation enables direct use of ENDD for ionization profiles
- With transition in H-mode, increase in peak ionization rate and large decrease in core n_D
- Increase in peak ionization rate with increasing n_e in H-mode





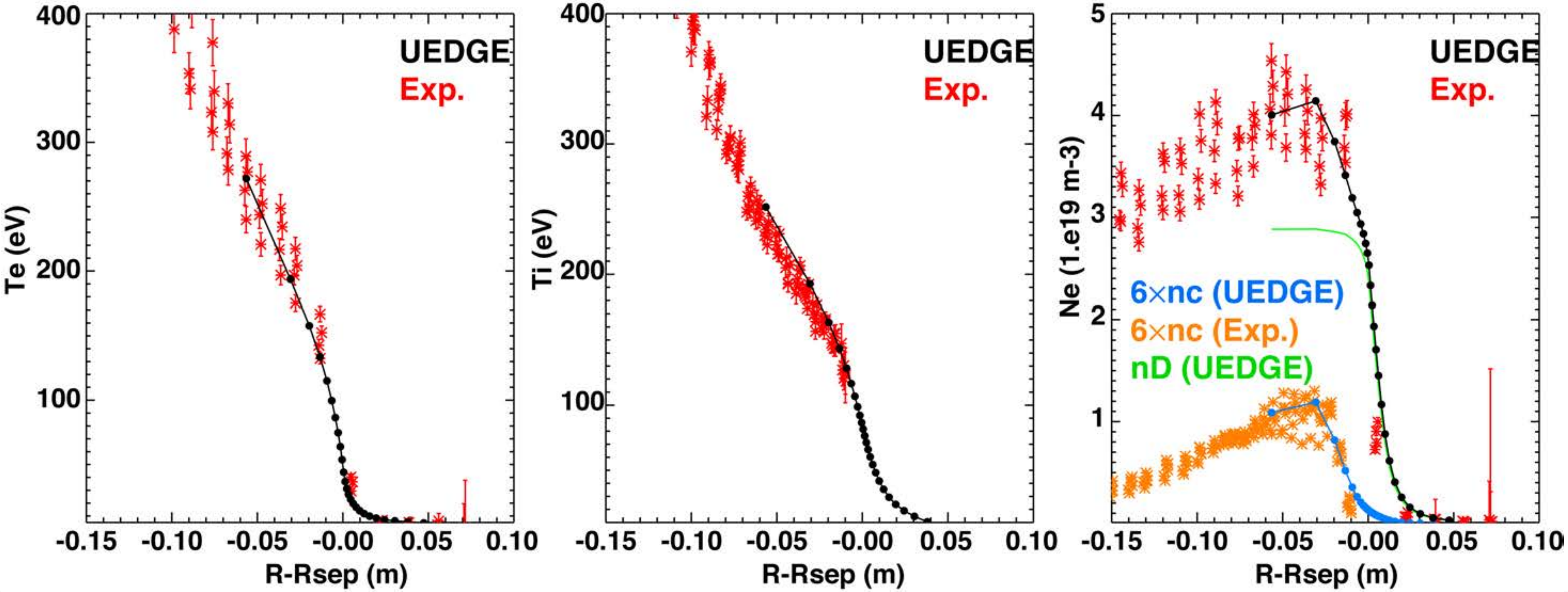
One way coupling of DEGAS 2 to UEDGE code used to study neutral distribution and core fueling

- UEDGE, 2D multi-fluid edge transport code:
  - Fluid model for D^0, D^+, C^0, $C^{1+\text{-}6+}$, e^-
  - No cross-field drifts
  - Same D atomic physics data as DEGAS 2
  - Provides background plasma for DEGAS 2 simulations
- Balanced double null UEDGE grid from EFIT02:
  - 126 poloidal x 25 radial cells
  - Norm. Poloidal Flux 0.7-1.2 - Full ENDD radial coverage
    - Grid extends until LFS limiter
    - Core boundary at ψ_N=0.7 to satisfy zero neutral flux BC
- DEGAS 2 mesh extended to vessel wall with DG
  - Polygons between UEDGE grid and limiter treated as vacuum zones
- Goal: Interpret direct diagnostic results (n_D and ionization profiles) in terms of overall fueling patterns



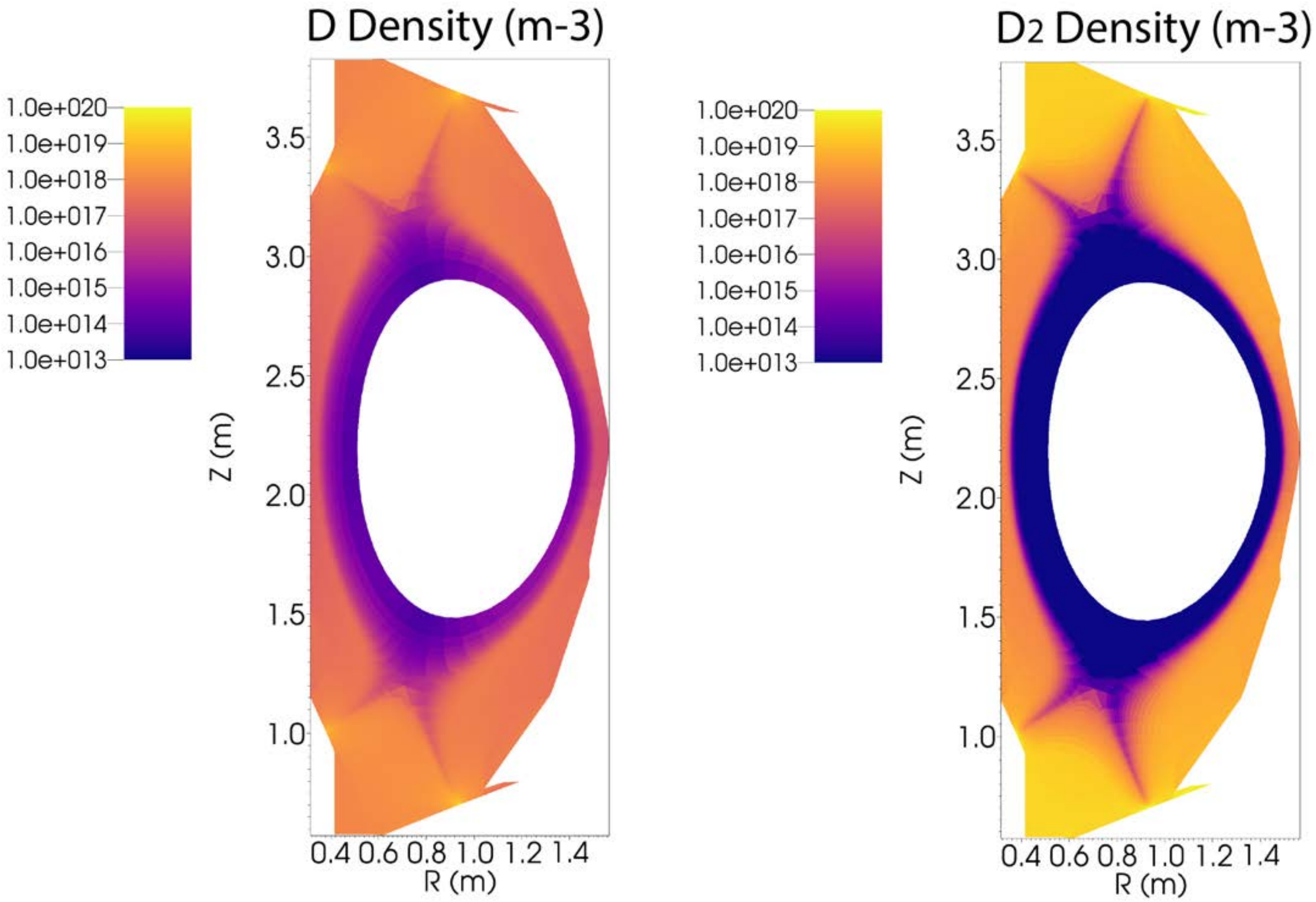
Multi-fluid edge transport code UEDGE generate background plasma for neutral transport simulations

- Boundary conditions from experimental parameters for H-mode 204500:
  - Power B.C. on core boundary: P_{sep} ~1 MW (equally split)
  - χ_e, χ_i, D_{perp}, v_C to match exp. midplane profiles
  - 99% recycling at divertor and walls, 100% albedo , 165 A LFS gas injection, 100 A HFS gas injection



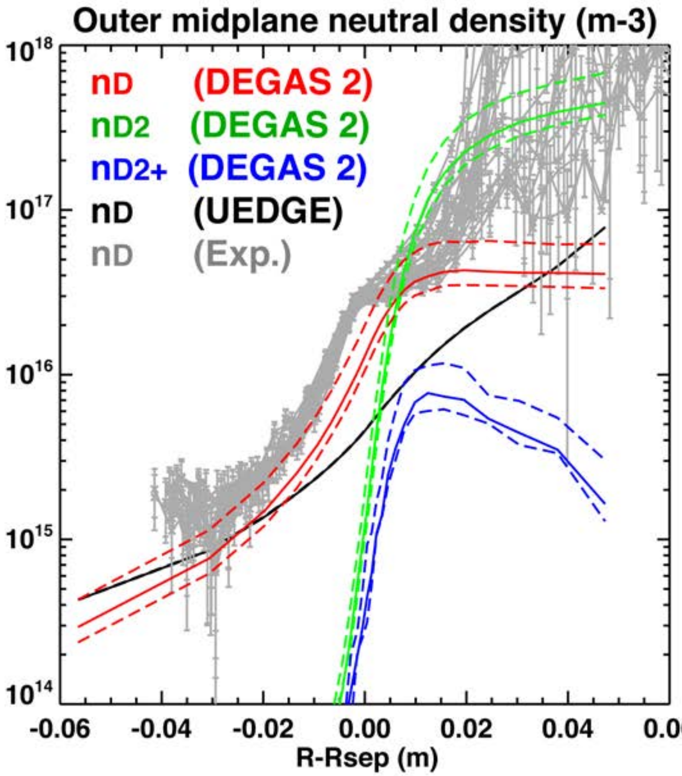
DEGAS 2 coupled "one-way" to UEDGE background plasma to calculate neutral density, core fueling

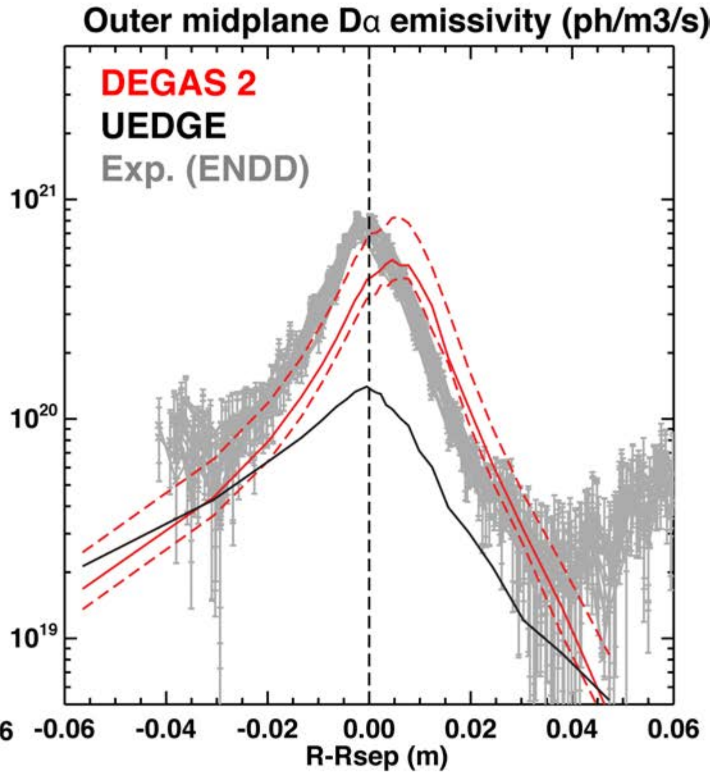
- Wall neutral sources from UEDGE:
  - Recycled fluxes at 4 divertor targets
  - HFS and LFS gas puff
  - Wall and PFR fluxes from UEDGE redistributed to DEGAS 2 wall and sourced as gas puff
- DEGAS 2 coupled "one-way" on static UEDGE background
  - n_D, n_{D2} distribution, fueling, D_α emissivity
  - Similar to what done in past for NSTX, DIII-D (e.g., [Fenstermacher 1995, Allen 1999, Groth 2005] but with addition of wall sources



DEGAS 2 simulations indicate larger midplane neutral densities, higher penetration of divertor sources

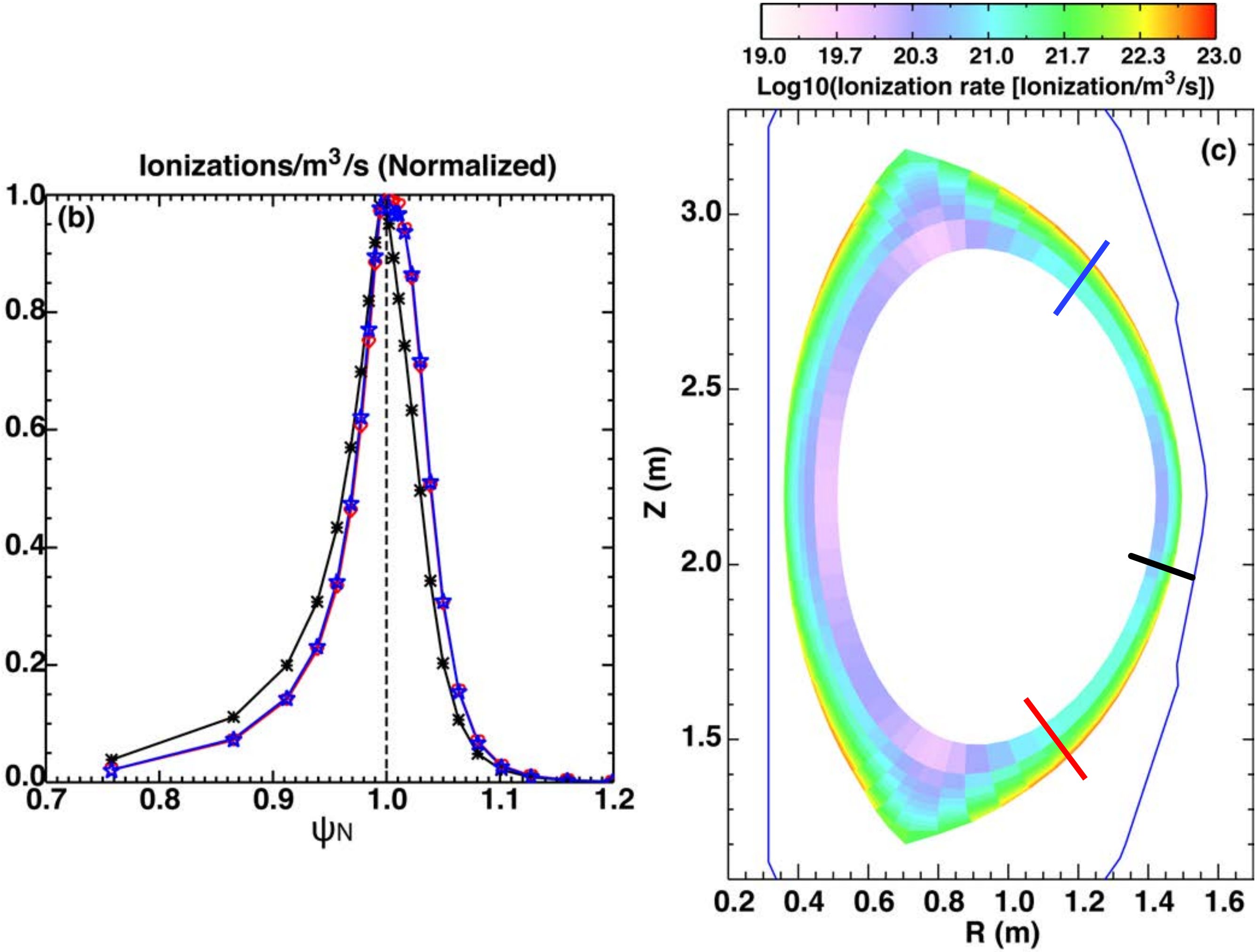
- Better agreement (both in D-α emissivity value and profile shape) between experiment and DEGAS 2 with respect to UEDGE solution
  - — Small neutral bypass in outer divertor legs to help agreement with divertor D-α without changing midplane quantities
- Larger midplane n_D in DEGAS 2 simulations compared to UEDGE:
  - — Higher midplane penetration of divertor neutral sources when compared to UEDGE solution
  - — Possibly due to artificial divertor ’closure’ created by the UEDGE grid





DEGAS 2 one-way coupling used to determine radial and poloidal fueling profiles

- Edge fueling is ~up-down symmetric, dominated by fueling in the region just upstream of the X-point and by sources on the low field side
- Radial ionization profiles are peaked just inside the separatrix
- Shallower neutral penetration in normalized flux coordinates observed at every location away from the outer midplane



DEGAS 2 indicates edge fueling largely dominated by divertor recycling in low triangularity configuration

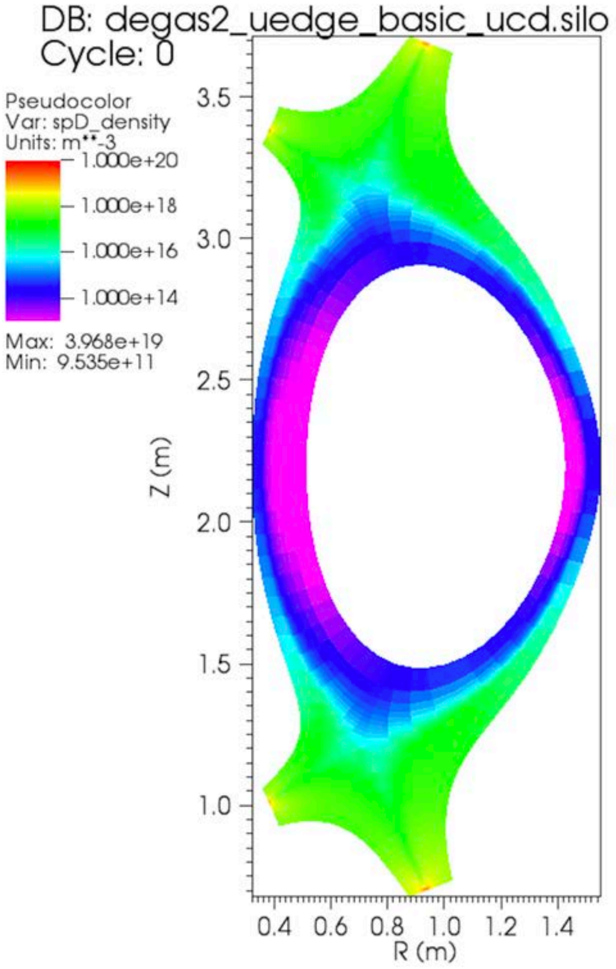
- Scan in DEGAS 2 neutral sources to determine effect on edge fueling and measured n_D
- Edge fueling dominated by recycling at outer strike points
- Outer midplane n_D due to outer strike points and outer wall recycling
- Understanding how fueling and midplane n_D can be determined by different sources is critical to correctly interpret the ENDD data
  - Importance of increased poloidal coverage for radial neutral density measurements

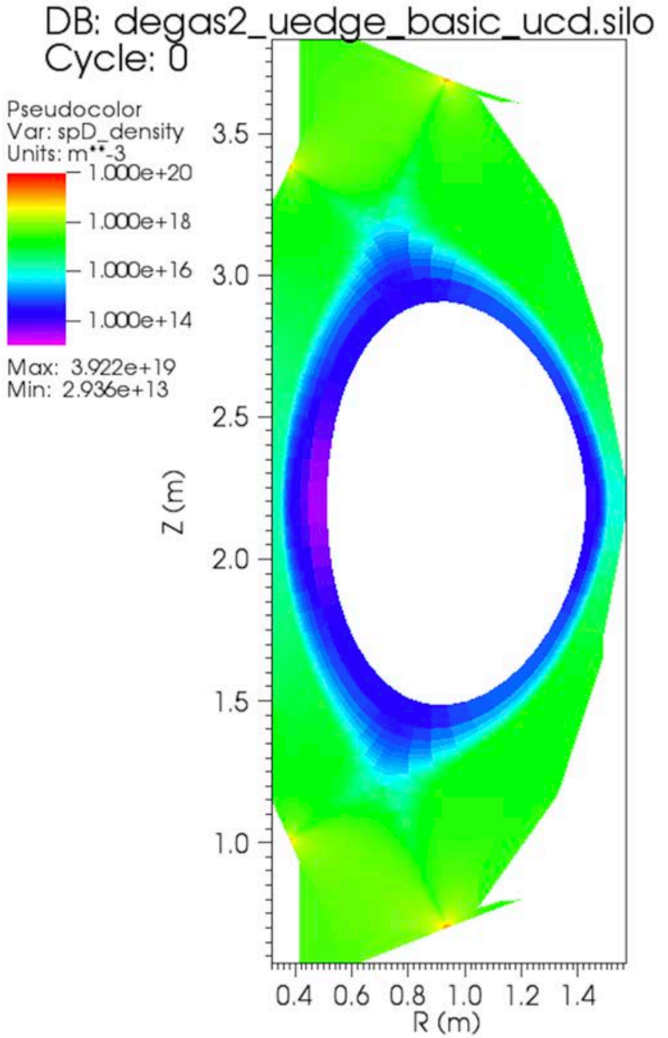
	Fueling fraction	Neutral density fraction at ENDD
Lower inner strike point	8%	2%
Upper inner strike point	8%	0%
Upper outer strike pint	32%	8%
Lower outer strike point	37%	52%
Outer wall	9%	36%
Inner wall and PFR	6%	2%

Fueling picture can change with addition of drifts, which are expected to change in/out fueling balance from divertor strike points

Higher midplane penetration of divertor neutrals observed in DEGAS 2 simulations compared to UEDGE

- To evaluate change in midplane neutral penetration of divertor sources:
  - Re-converge with zero wall recycling and gas puff
  - Use only divertor targets neutral sources
  - Run DEGAS 2 on UEDGE grid
  - Run DEGAS 2 on DG-extended mesh
- Running DEGAS 2 with UEDGE walls, midplane neutral density only slightly higher in DEGAS 2:
  - Up to a factor of 2 at points
  - Likely due to molecules “walking on the walls”
- Running DEGAS 2 on DG-extended grid, midplane n_D several times higher than UEDGE:
  - Due to artificial “closure” generated by UEDGE grid
  - Effect enhanced in these long-legged configurations
  - Can be mitigated with wider grid, neutral bypass





Considerations and recommendations for future neutral density measurements in NSTX-U

- Current view is looking at neutral beam armor with a non-purely toroidal view
  - View should be moved to a different Bay to avoid possible toroidal asymmetries in measured neutral densities due to armor
  - View should be moved to midplane with toroidal view to enable faster inversion

- Add additional poloidal locations on LFS and HFS
  - Enable measurements where ionization source is supposed to be higher and additional constraints for edge modeling

- Fix mirror in current view

- Eventually replace glass bundle with optical relay and camera with radiation hardened detector

Summary

- Radial profiles of outboard midplane neutral density n_D are derived from D_α emissivity measured by midplane tangential cameras in NSTX-U
- Assumptions used to derive n_D measurements were validated via DEGAS 2 Monte Carlo neutral transport simulations
  - Good agreement between simulated and measured D_α emissivity
  - Emission inside separatrix is dominated by e^- impact excitation
  - Deviations in emission profile shape possibly due to intermittency, uncertainty in molecular processes
- “One-way” coupling of DEGAS 2 Monte Carlo simulations to UEDGE background plasmas to study edge plasma fueling
  - Improved agreement with measured neutral densities and D_α emissivity if compared with UEDGE solution
  - Core fueling dominated by divertor recycling