Neutral Beam Analysis Codes Used on the NSTX-U and DIII-D Tokamaks

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IAEA 1. RCM on Data for Atomic Processes of Neutral Beams in Fusion Plasmas

19 – 21 June 2017

Outline

- Background & Introduction
  - Experiments
  - Relevant expertise of Chief & Secondary SI
- Project Codes & Diagnostics
  - TRANSP / NUBEAM
  - FIDAsim
  - CHERS
  - MSE
- NUBEAM – FIDAsim Benchmark
- FIDAsim Validation
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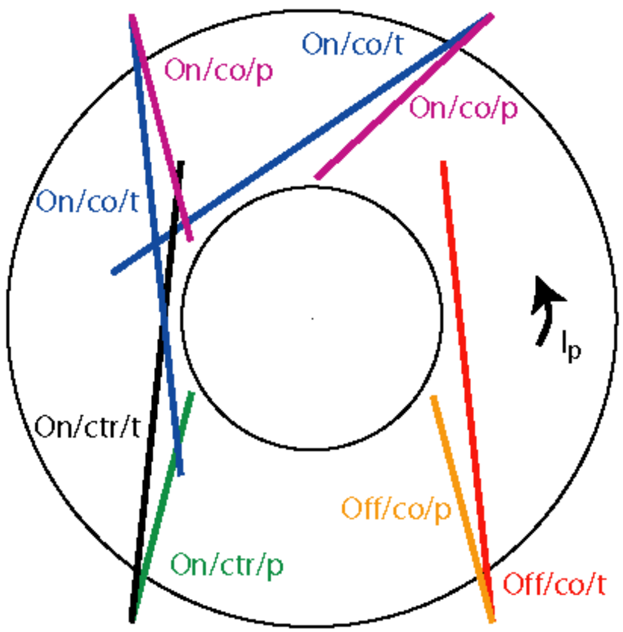
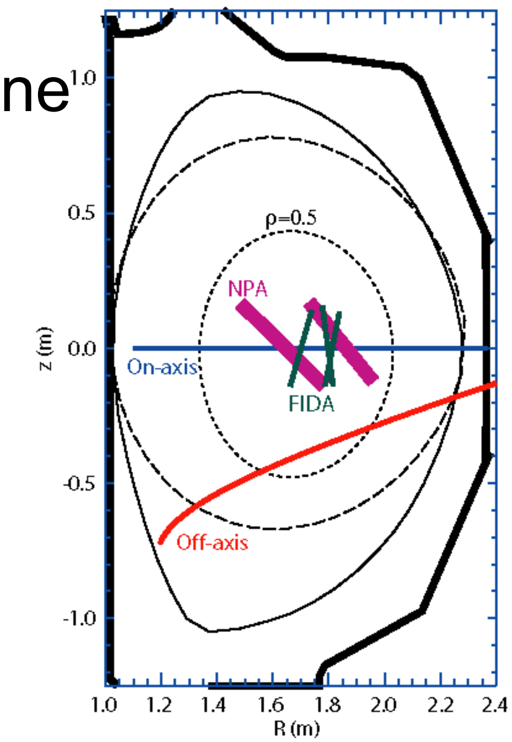
DIII-D Tokamak & NBI Systems

- $R = 1.67$ m, $a = 0.67$ m
  - $B_T = 2.2$ T
  - $I_p \sim 1$ MA
- $T_{e,}$ T_i: 1 – 10 keV,
- n_e up to 10^{20} m^{-3}.



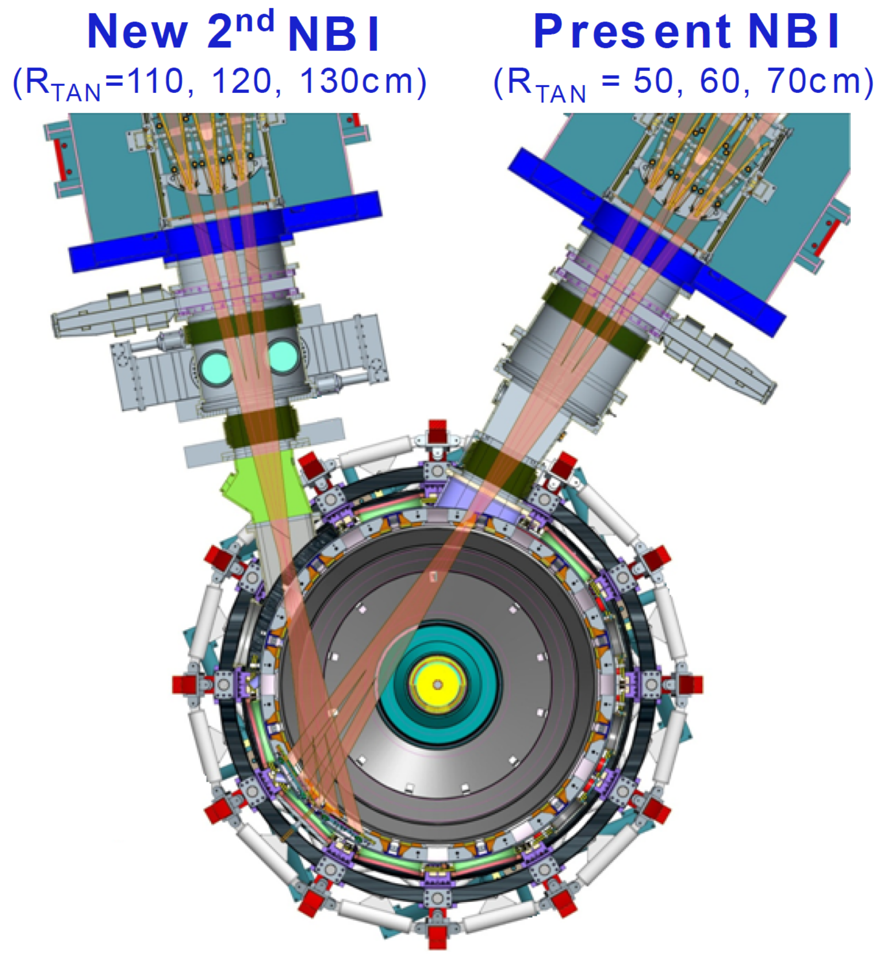
- Four beam boxes, two sources each:
  - 45 – 93 kV, up to 34 MW total.
  - Three co-I_p, one counter.



[W. Heidbrink, et al., Nucl. Fusion 52, 094005 (2012)]

National Spherical Torus Experiment – Upgrade (NSTX-U)

- With the upgrade:
  - R = 0.86 → 0.94 m,
  - a = 0.6 m
  - B_T = 0.5 → 1 T
  - I_p = 1 → 2 MA
- Plasma: T_e ~1 keV,
- n_e up to 10^{20} m^{-3}.
- Two beam lines, three sources each,
  - Energy up to 90 keV,
  - Up to 15 MW total.



[J. Menard et al., Nucl. Fusion 52, 083015 (2012)]

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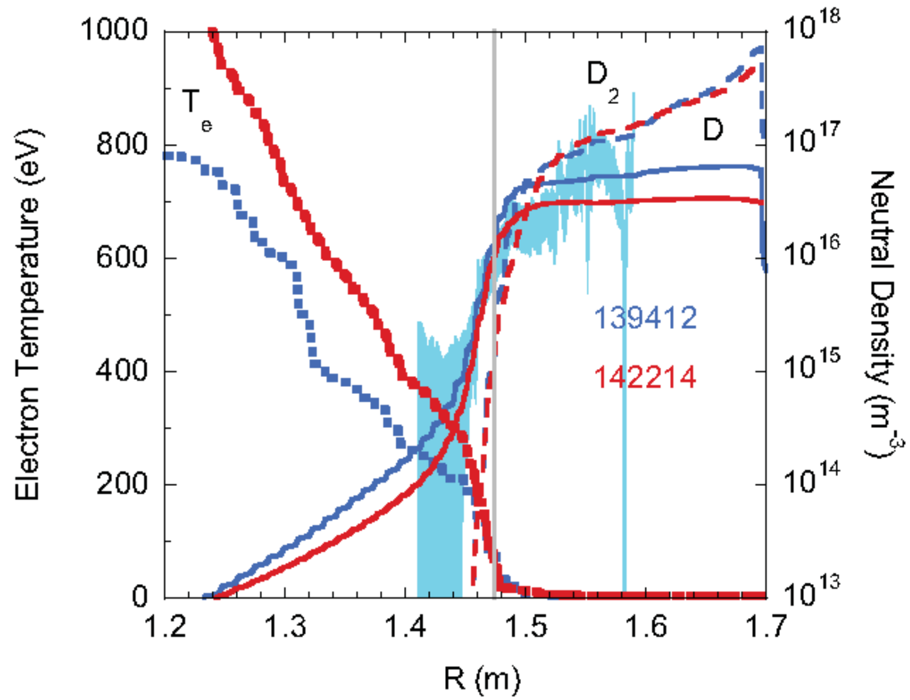
CSI: Neutral Transport & CR Model Data

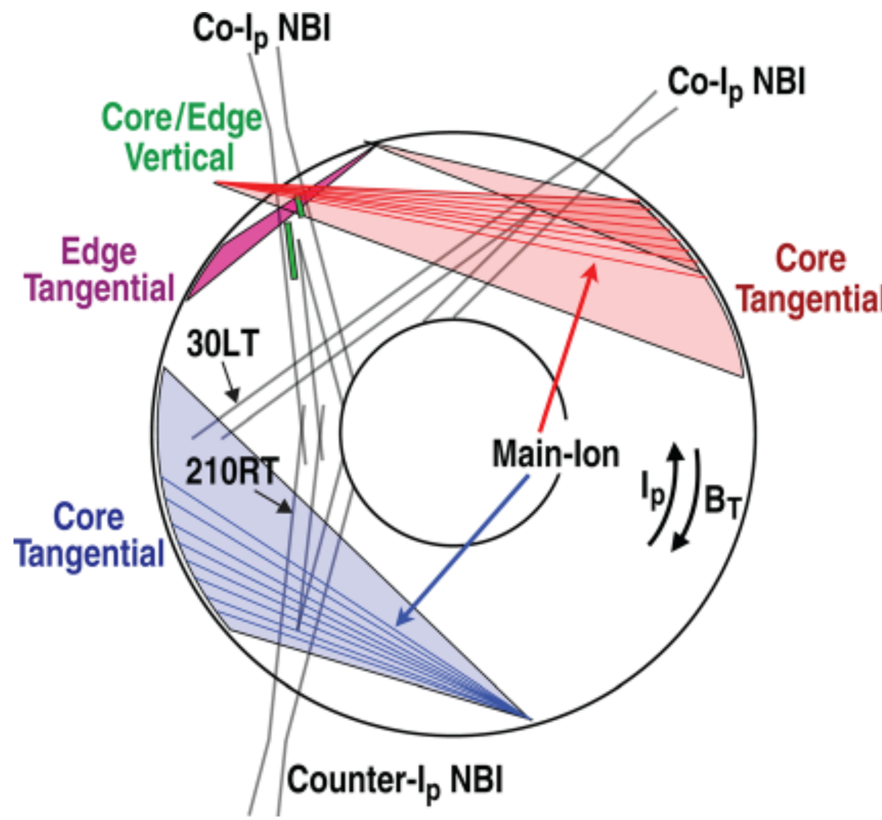
- DEGAS 2: Monte Carlo neutral transport code:
  - Input material surfaces, geometry, plasma, neutral sources,
  - Specify plasma-neutral reactions, material interactions.
  - Output: neutral density, line emission.
- Principal reactions:
  - H effective ionization & recombination rates from CR model,
    - Up to 50 keV.
  - H_2 dissociation, ionization, etc.
  - H^+ + H CX, elastic scattering.



DEGAS 2 inferred ambient neutral density profiles [D. Stotler, et al., Phys. Plasmas 22, 082506 (2015)].

Secondary CSI: Responsible for DIII-D CER Spectroscopy

- & DIII-D Neutral Beam Physics Leader
- 2014 DoE Early Career Research Program winner ⇒develop D^+ charge exchange recombination (CER) diagnostic for DIII-D pedestal.
- Yields D^+ temperature & velocity profiles.
- CER analysis utilizes multiple codes from project.



[B. Grierson et al., Phys. Plasmas 19, 056107 (2012)]

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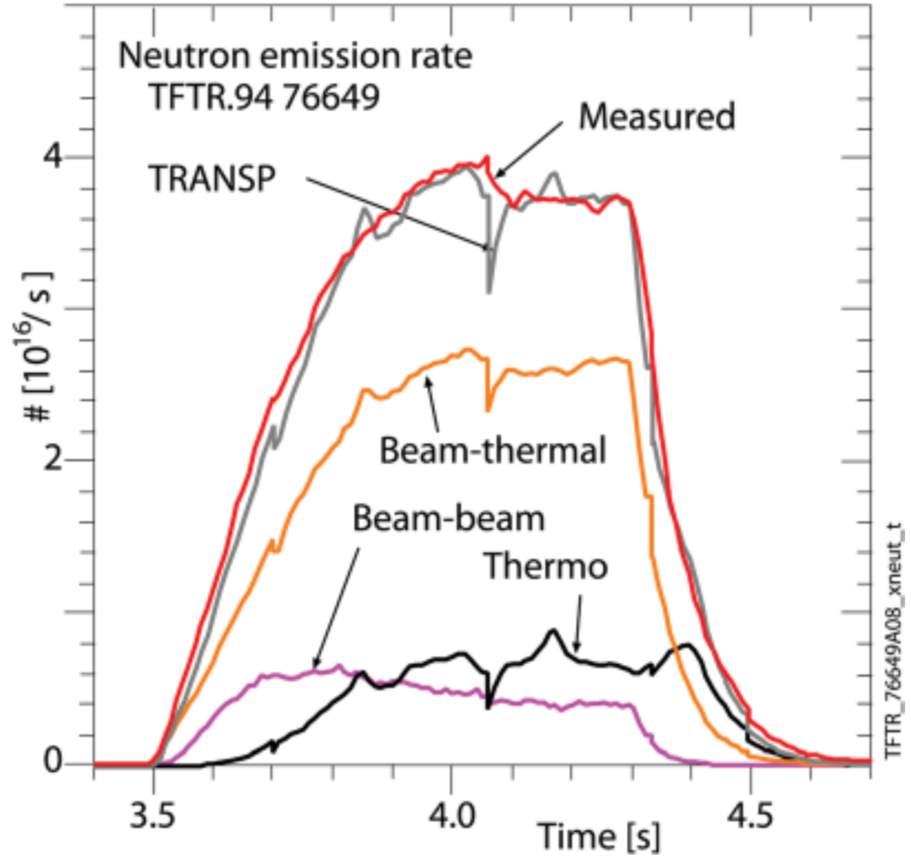
TRANSP: Time Dependent Interpretive & Predictive Transport Analysis Code

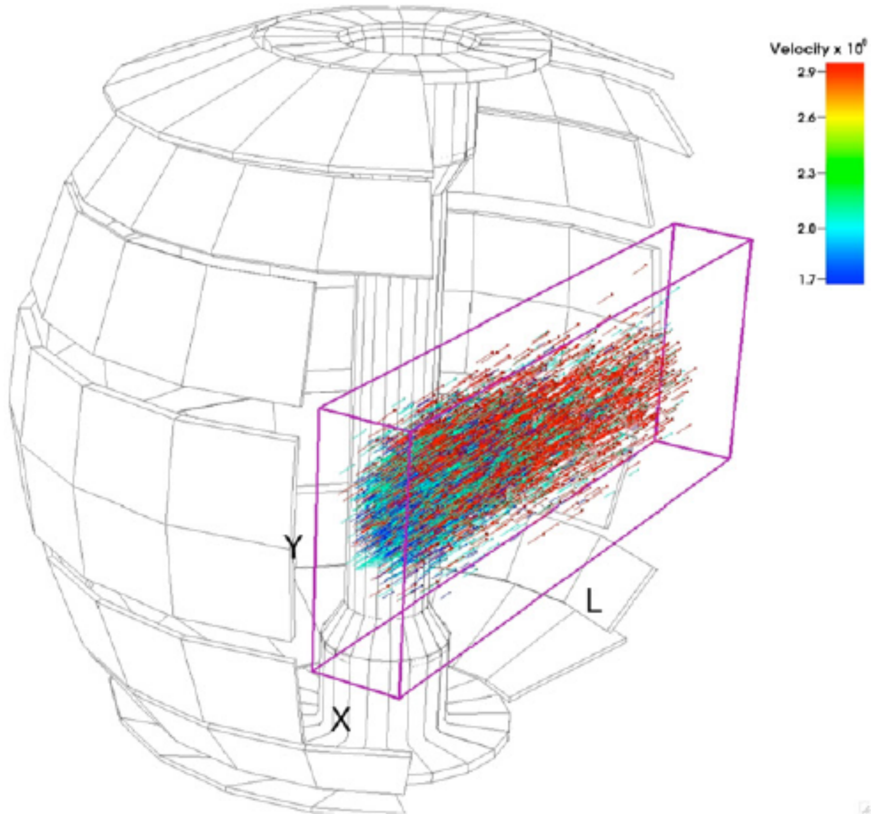
- Dates back to TFTR & earlier.
- Used to analyze data on many tokamaks:
  - NSTX, DIII-D, JET, ASDEX-U, KSTAR, MAST, …
- Connected to IMAS (ITER Modeling & Analysis Suite).
- NUBEAM is a central routine.



[R. Budny, Phys. Plasmas 18, 092506 (2011)]

NUBEAM: Monte Carlo Beam Injection & Slowing Down Module in TRANSP

- [A. Pankin et al., Comput. Phys. Comm. 159, 157 (2004)].
- Includes:
  - Beam deposition,
  - Fast ion orbits & slowing down,
  - Beam driven current,
  - Fusion reactions.
- 3-D, multiple generation, halo neutral population.
- Multiple atomic physics options,
  - Focus here on newest, ADAS based models.



3-D "box" used for a beam [S. Medley et al., Plasma Phys. Control. Fusion 58, 025007 (2016)].

FIDAsim Supports Multiple Fast Ion D_α Diagnostics on DIII-D & NSTX-U

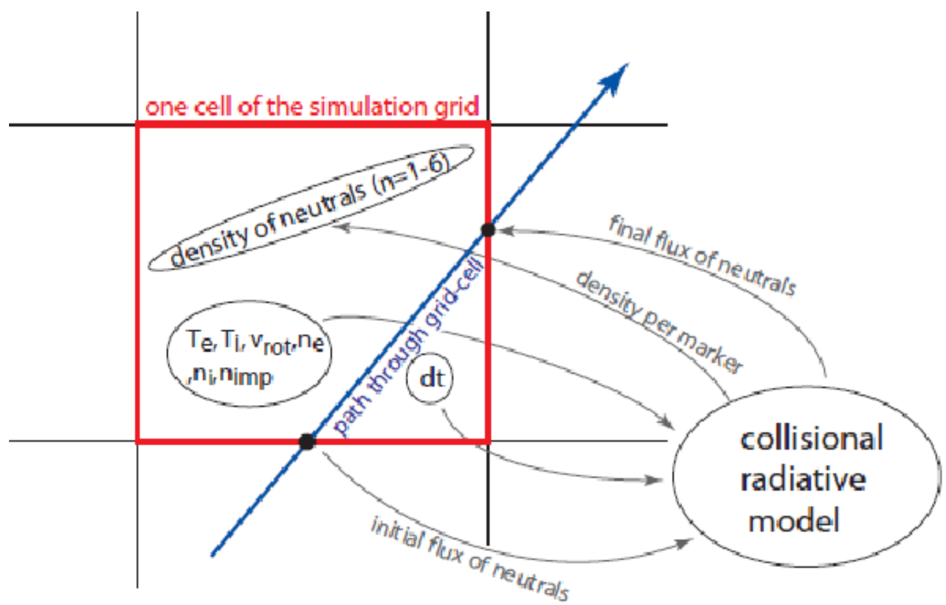
- Supports FIDA, Neutral Particle Analyzer (NPA), CER, ⋯
  - FIDA: Fast Ion D_α, result of CX between fast ions & beam atoms.
- Similar to, but independent of NUBEAM.
  - Monte Carlo beam penetration & halo calculation.
- Includes beam attenuation by electrons, main & impurity ions.
- Time dependent collisional radiative model, up to n=6.
- Charge exchange with main and fast ions,
  - Fast ion distribution obtained from NUBEAM.
- [W. Heidbrink et al., Commun. Comput. Physics 10, 716 (2011)],
  - But see: https://github.com/D3DEnergetic/FIDASIM/

$$D^+_{fast} + D^0_{NB} \rightarrow D^0_{fast} + D^+_{NB}$$

$$D^+_{bulk} + D^0_{NB} \rightarrow D^0_{halo} + D^+_{NB}$$

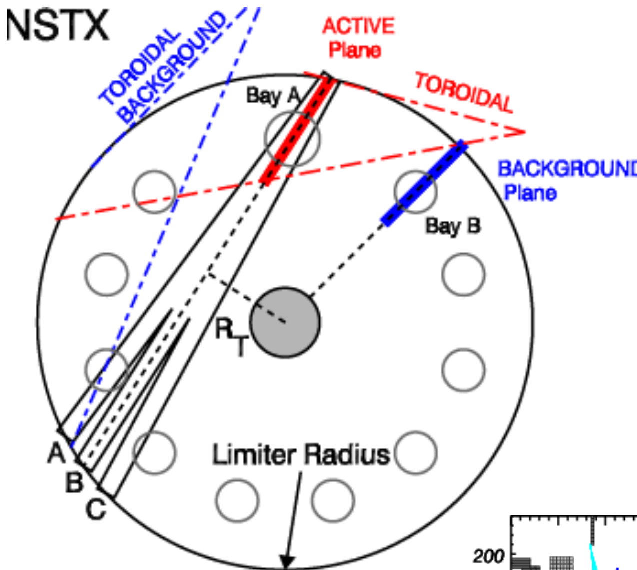
$$D^+_{fast} + D^0_{halo} \rightarrow D^0_{fast} + D^+_{bulk}$$

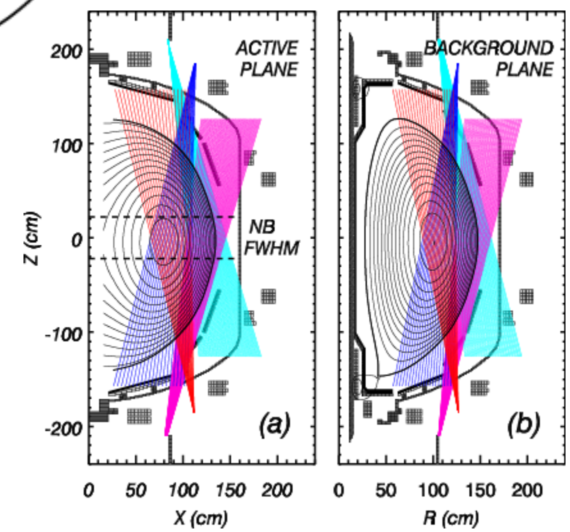
$$D^+_{bulk} + D^0_{halo} \rightarrow D^0_{halo\_high\_generation} + D^+$$



NSTX-U Charge Exchange Recombination Spectroscopy: CHERS

- Determine C^{+6} density, temperature, toroidal & poloidal velocity.
- V_{pol} Measurement sensitive to atomic physics details & gyro-orbit.
  - Presently, all via ADAS.
- $D^0(n_D)+C^{6+} \rightarrow D^{+}+C^{5+}(n)$,
  - View $n = 8 \rightarrow 7$,
  - $n \approx n_D Z^{3/4} \Rightarrow n_D = 2$,
  - But, need data for n_D = 3, 4, 5 also.



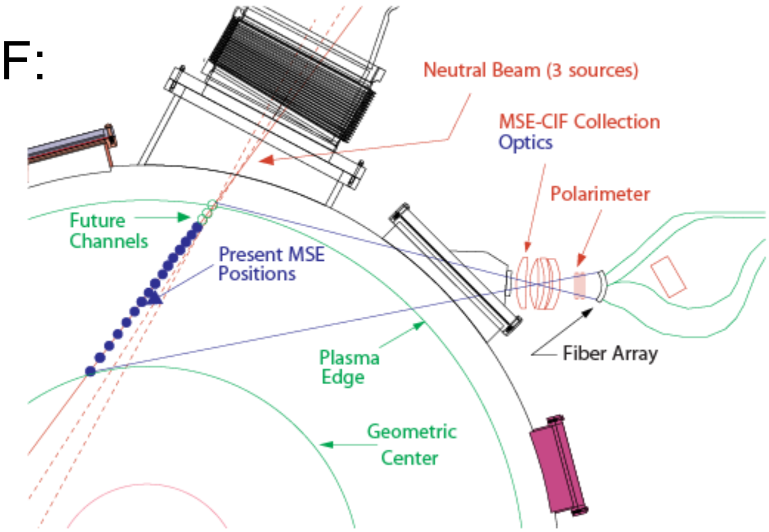


[R. Bell and R. Feder, Rev. Sci. Instrum. 81, 10D724 (2010), R. Bell et al., Phys. Plasmas 17, 082507 (2010)]

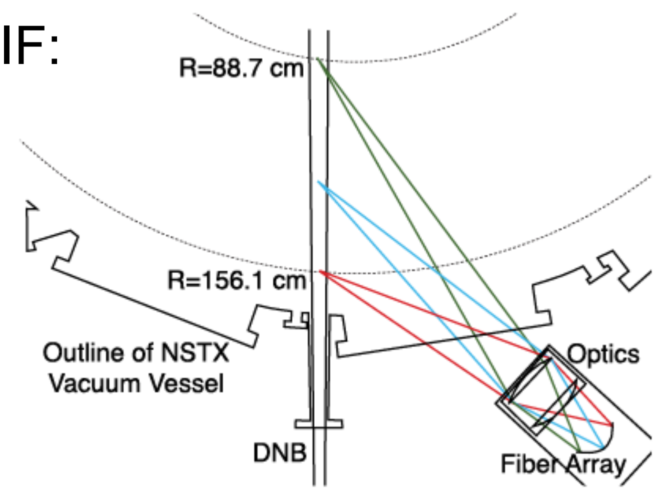
Motional Stark Effect for NSTX-U & ITER

- Measures B_{pol}.
- Initial NSTX system: Collisionally Induced Fluorescence (CIF) [F. Levinton and H. Yuh, Rev. Sci. Instrum. 79, 10F522 (2008)],
  - Collisional excitation of beam atoms ⇒Stark effect polarized D_{α}.
- Laser Induced Fluorescence (LIF) now on NSTX-U [E. Foley and F. Levinton, Rev. Sci. Instrum. 84, 043110 (2013)],
  - Provides radial resolution.
- MSE for ITER will use “line shift” approach [E. Foley et al., Rev. Sci. Instrum. 79, 10F521 (2008)].
  - To minimize effect of mirror coatings.
- CR model used for analysis requires *nl* resolved cross sections [E. Foley and F. Levinton, J. Phys. B 39, 443 (2006)].

CIF:



LIF:



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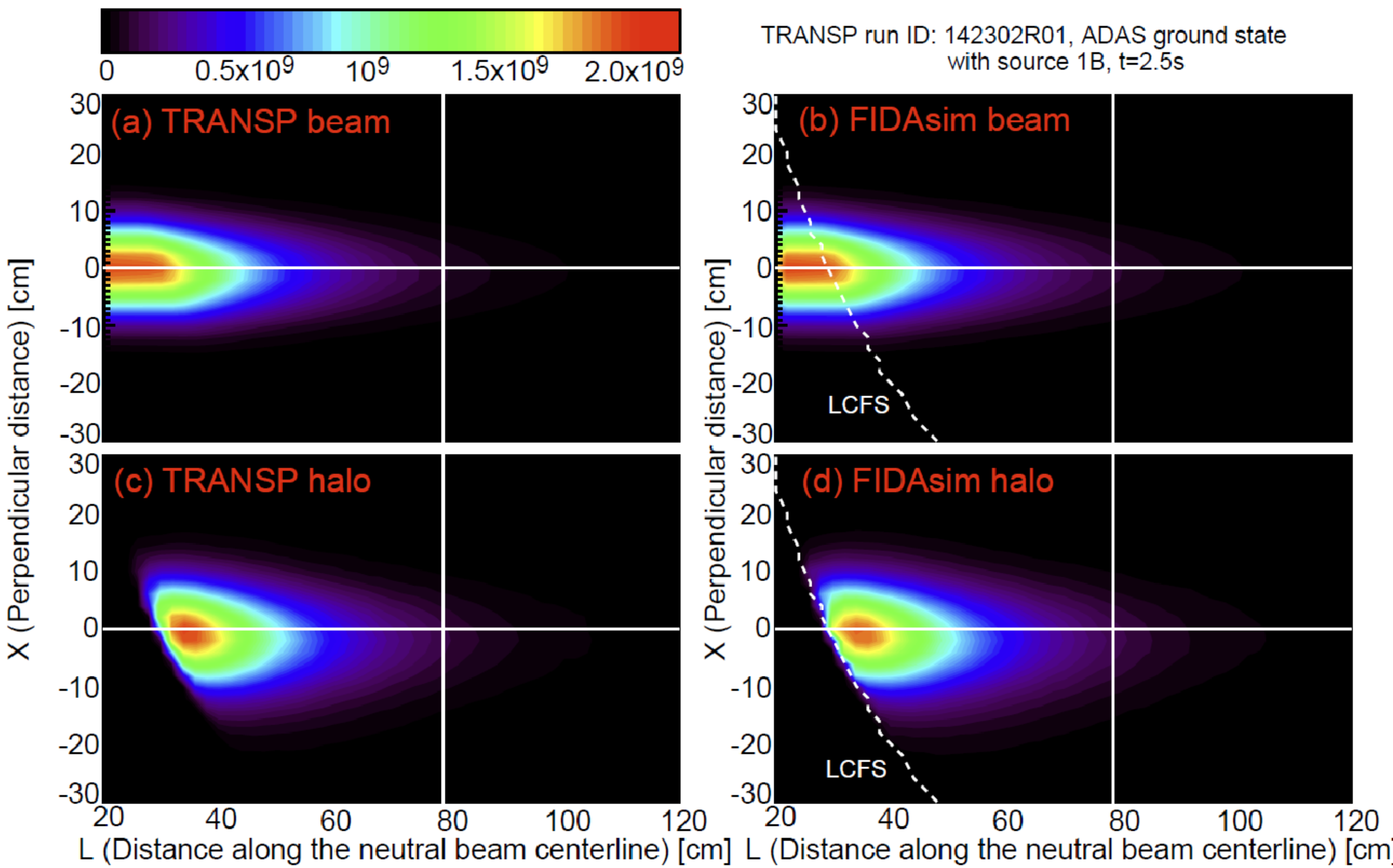
NUBEAM - FIDAsim Benchmark

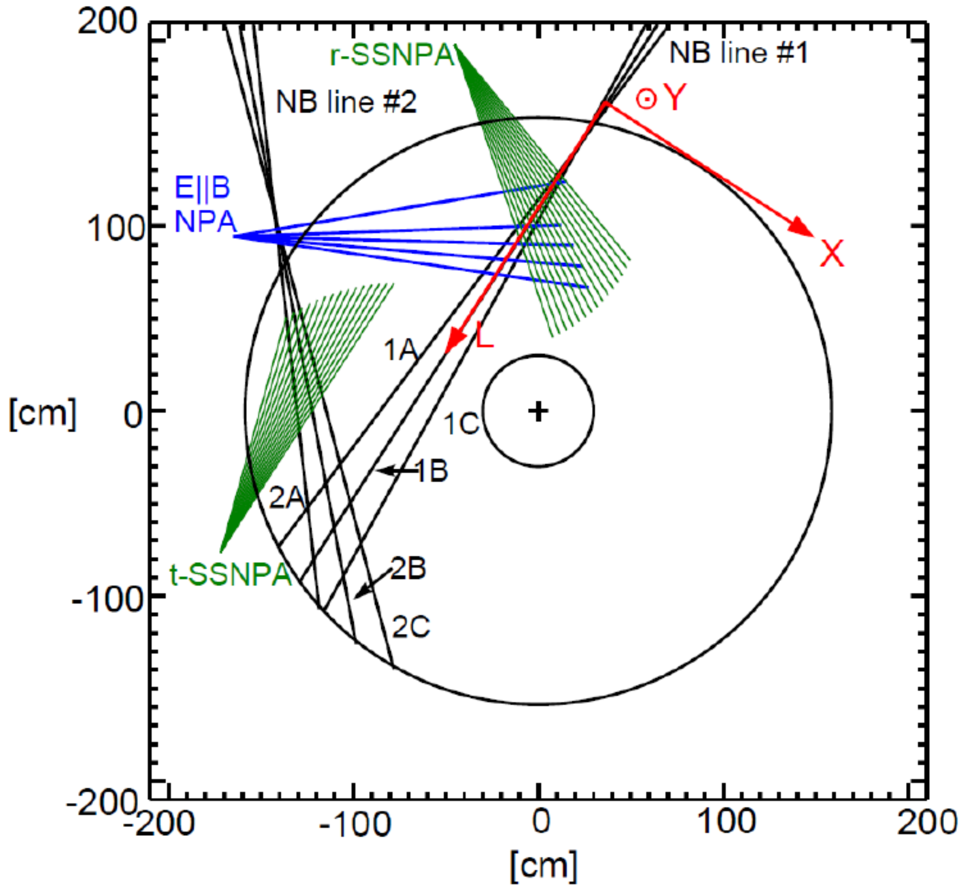
- Focused primarily on verifying NUBEAM's halo model [S. Medley et al., Plasma Phys. Control. Fusion 58, 025007 (2016)].
- Halo density comparable to beam density ⇒cannot be ignored.
- For comparison, use ground state ADAS cross sections only.
  - & no "fast" halo neutrals in TRANSP.
- One NSTX beam source with 3 energy components, focus & divergence,
  - Realistic plasma profiles, including toroidal rotation.

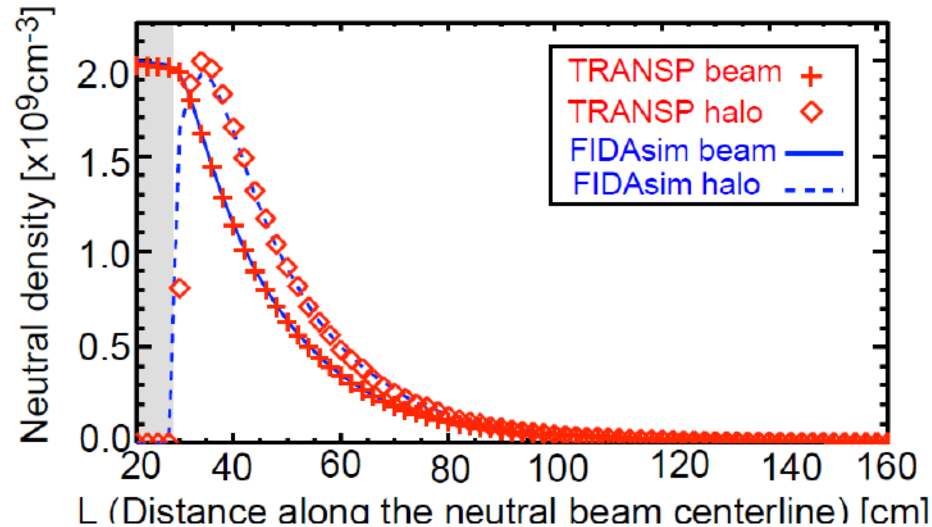
NUBEAM-FIDAsim: Comparison of Beam & Halo Densities

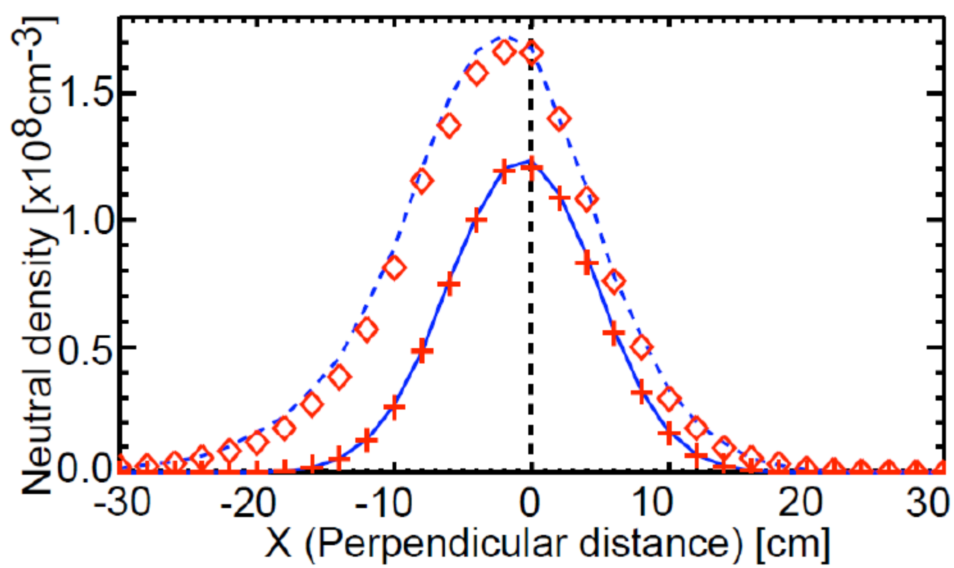


NUBEAM-FIDAsim: Density Profile Comparison

Define local coordinate system:

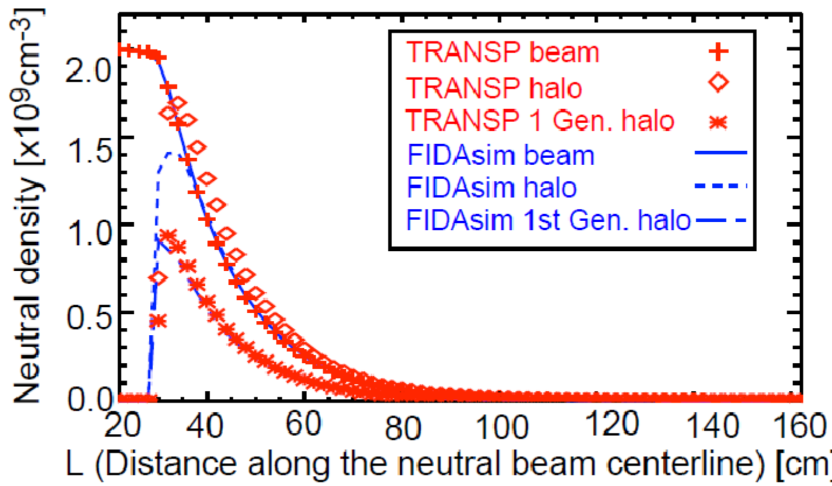


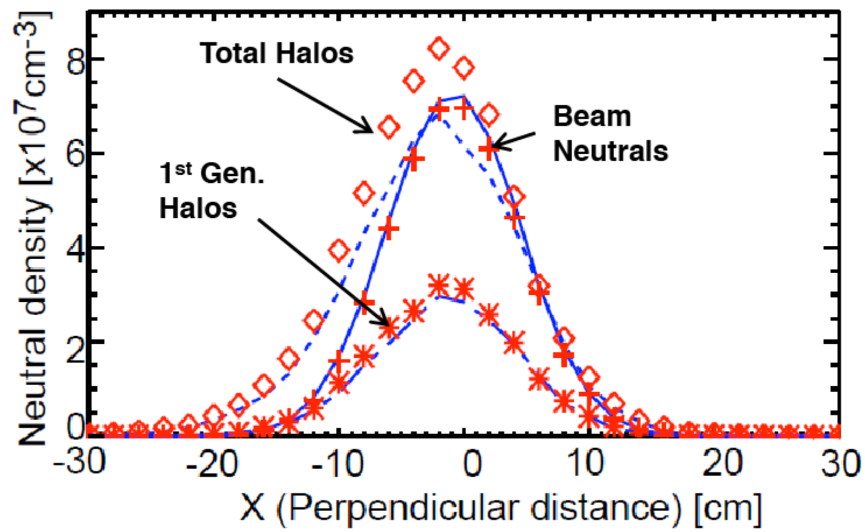




NUBEAM & FIDAsimHalo Densities Sensitive to Cross Sections

- Now use default sets of cross sections for both codes:
  - NUBEAM: ADAS310.
  - FIDAsim: excited states n ≤ 6 from ADAS & [Janev, Reiter, Samm, Juel-4105 (2004)].
- Beam densities match,
- But, NUBEAM halo density ~20% larger than FIDAsim.





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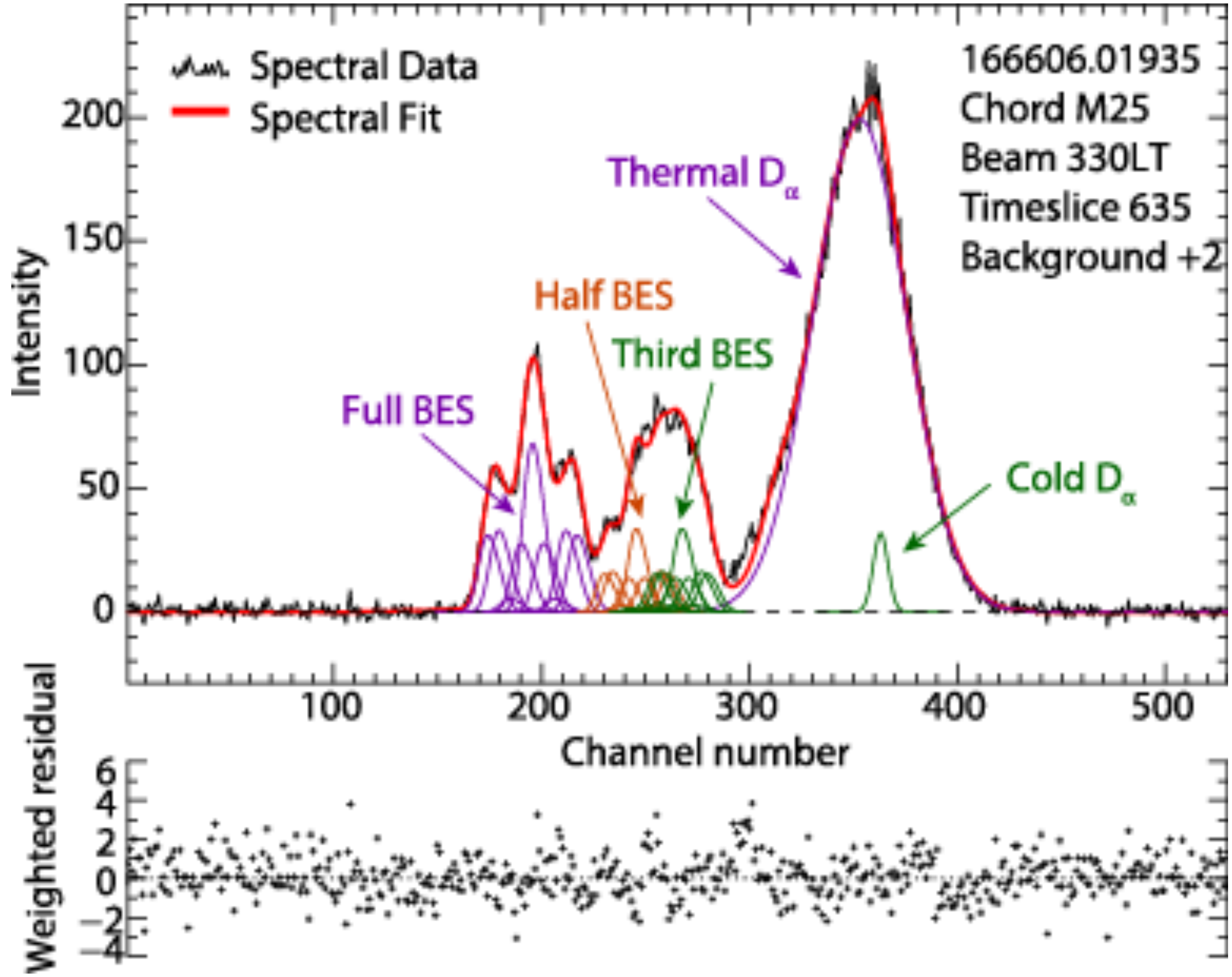
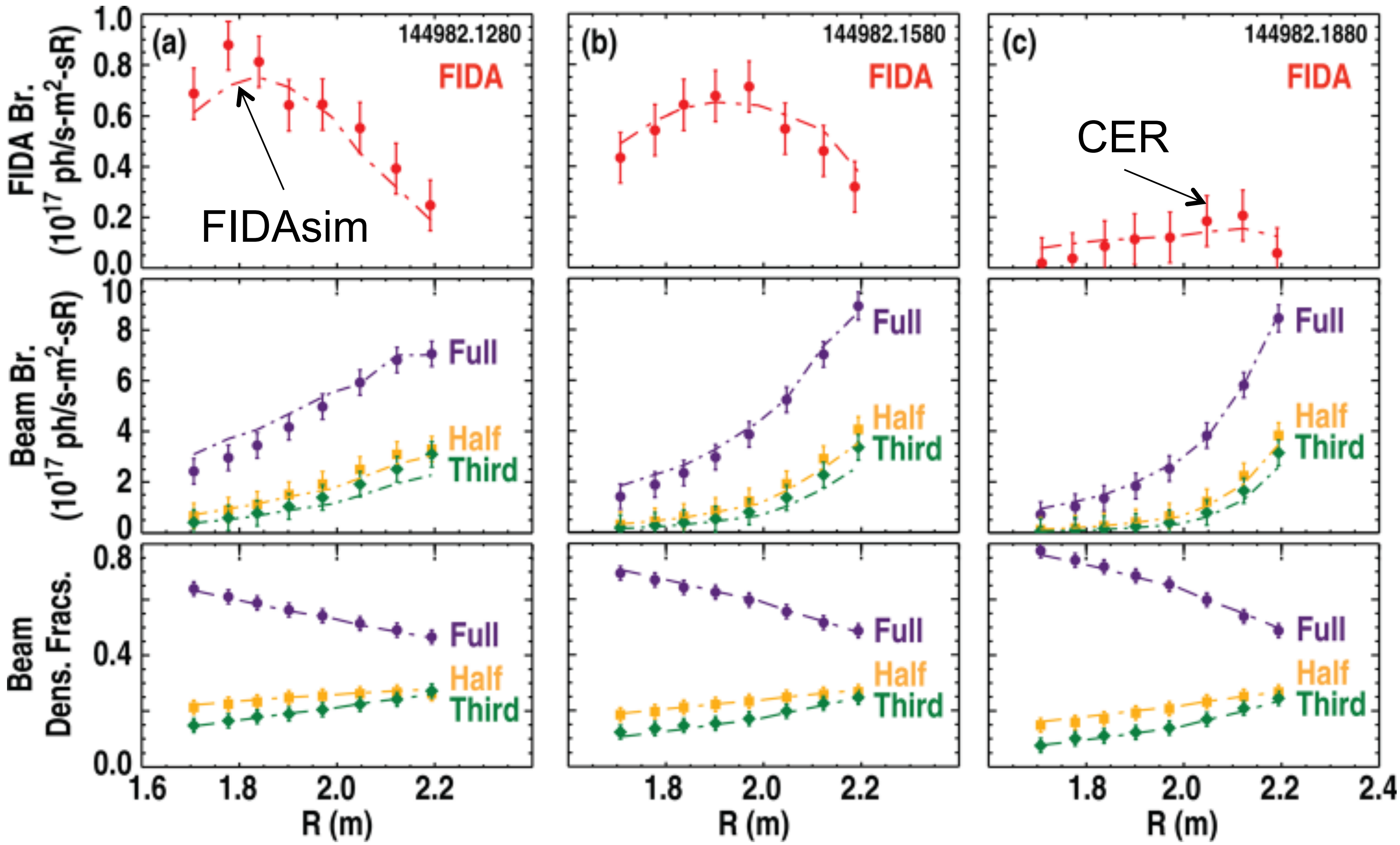
CX Spectrum Gives DIII-D Beam Density Components & FIDA



[B. Grierson et al., Rev. Sci. Instrum. 87, 11E545 (2016)].

DIII-D CER FIDA & Beam Densities Match FIDAsim



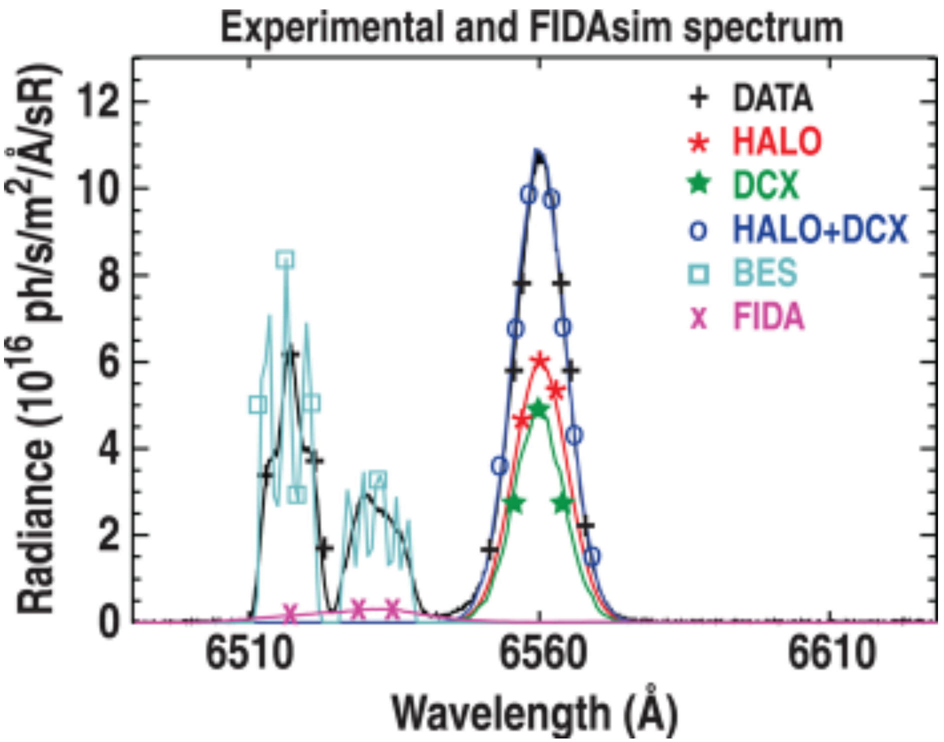
$n_e = 2.5 \times 10^{19}\ m^{-3}$ $n_e = 4.5 \times 10^{19}\ m^{-3}$ $n_e = 6.7 \times 10^{19}\ m^{-3}$

[B. Grierson et al., Phys. Plasmas 19, 056107 (2012)]

FIDAsim Spectrum & Halo Also Match DIII-D CER Data

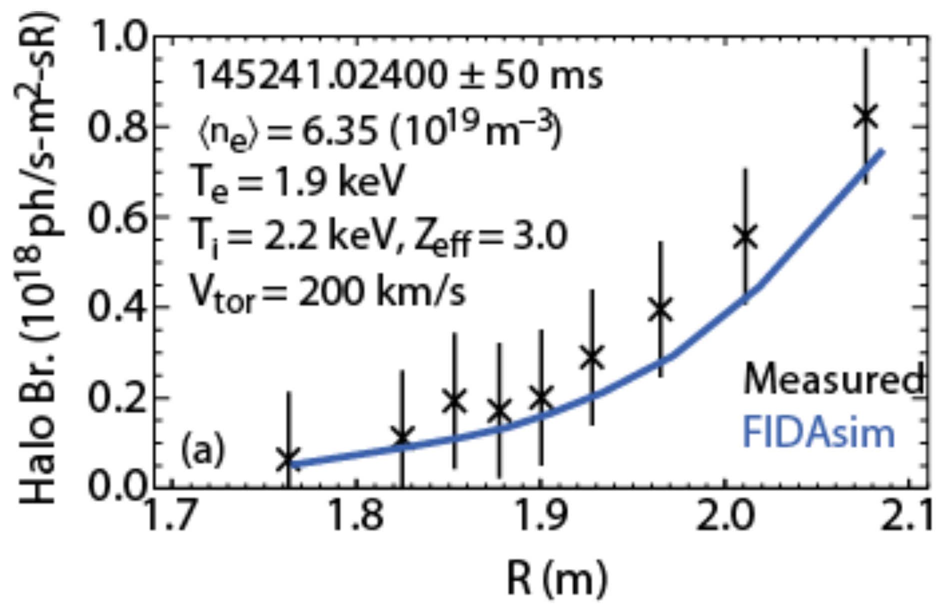
FIDAsim matches CER spectrum:

144982, R = 1.84 m @ 1.58 s



[B. Grierson et al., Phys. Plasmas 19, 056107 (2012)]

Comparison of direct halo emission:



[B. Grierson et al., Rev. Sci. Instrum. 83, 10D529 (2012)]

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Project Scope

- Limited to codes run for DIII-D & NSTX-U,
  - Beam energy up to ~90 keV, T ~ 1-10 keV.
- Carbon plasma facing components ⇒ principal impurity is carbon,
  - NSTX-U will use extensive Li conditioning,
  - Both seed impurities for radiative divertor studies.
- Primary lines for diagnostics: D_α and C^{5+} ($n=8 \rightarrow 7$).
- NUBEAM developers working on He beam model.

Project Plan: Year One

- List atomic physics processes in these codes,
  - Identify sources of cross sections & rates.
- Assess data consistency where processes overlap.
  - Are any data obsolete?
- Determine status of data for CHERS: $D(n > 2) + C^{6+}$ charge exchange.

Project Plan: Year Two

- Compare collisional radiative rates in overlapping regimes.
- Provide NUBEAM-FIDAsim benchmark details, as needed.
- Document parameters of DIII-D FIDAsim validation tests.
- Report on progress towards understanding inconsistencies in DIII-D impurity injection & beam voltage variation experiments.

Project Plan: Year Three

- Document outstanding data needs, if any.
- Revise atomic physics data according to input from CRP.
- Update progress towards understanding inconsistencies in DIII-D experiments.
- Assess data requirements for NUBEAM simulation of He beams.

Project Status

- FIDAsim extremely well documented,
  - Processes included easily identified,
  - Sources of data have already been established.
- NUBEAM: focusing on processes & data used in FIDAsim benchmark,
  - All NUBEAM data based on ADAS.
- Have for comparison data from H CR model used by DEGAS 2 for low energy neutral modeling.
- Prepared to discuss need for D(n > 2) + C^{6+} charge exchange data.

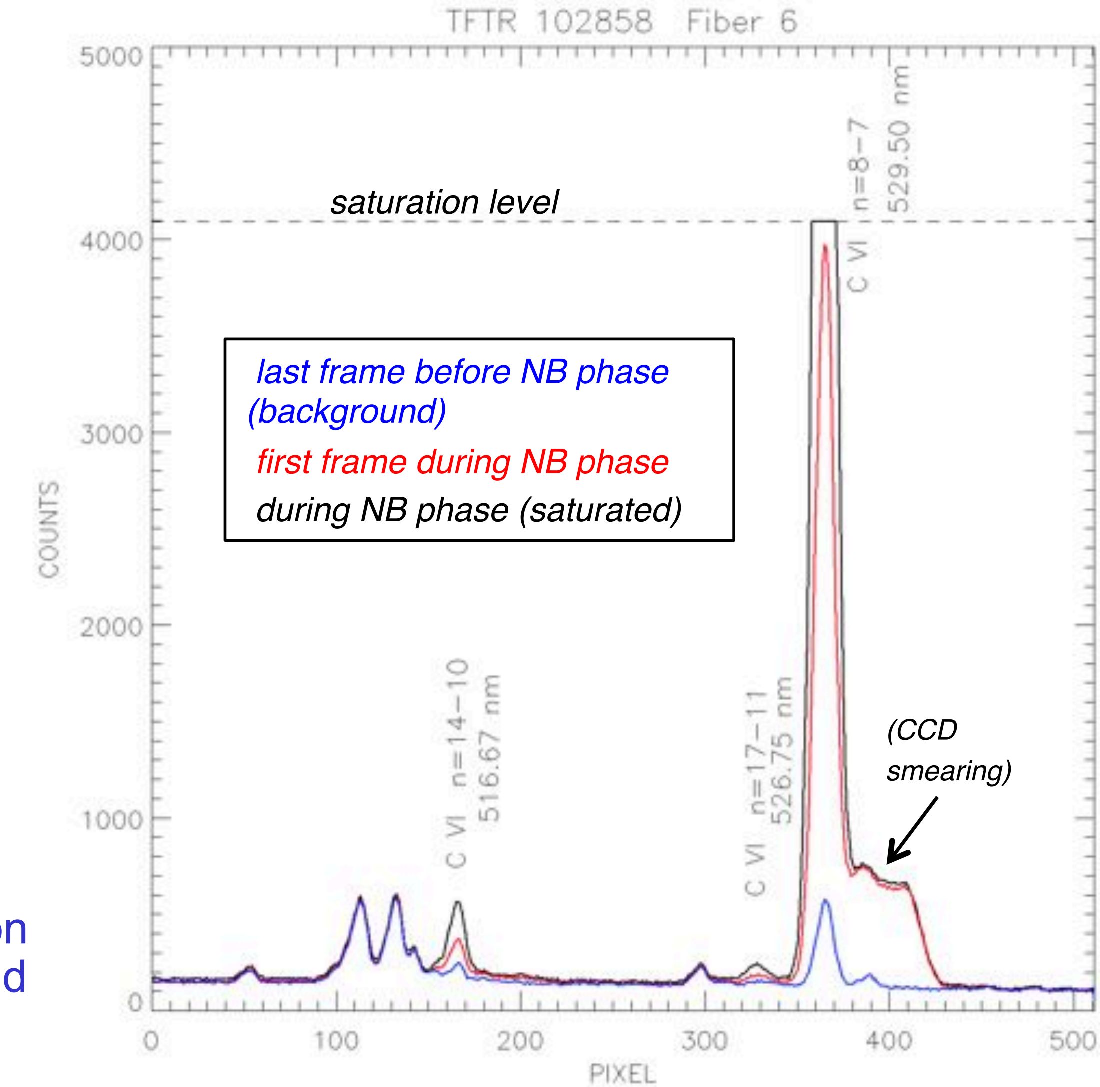
FOR DISCUSSION

Need for C^{+6} + D(n>2) CX Data

- Following slides show CHERS measurements on TFTR of n = 8 → 7, 14 → 10, and 17 → 11 line ratios,
  - Similar ratios have been seen more recently on DIII-D.
- The $n \approx n_D Z^{3/4}$ scaling ⇒ n_D = 2, 3, 4, 5 preferentially populates n = 8, 12, 15, 19.
  - ⇒ $n_D > 2$ data needed to explain these ratios.

TFTR spectra indicate that C VI (n=14-10) to C VI (n=8-7) brightness ratio is ~3.6 %

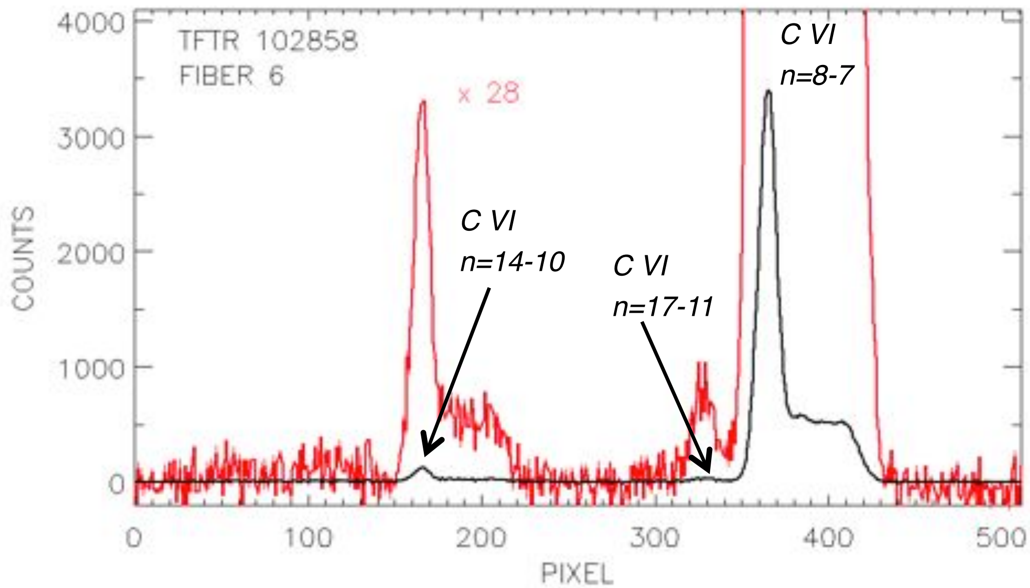
- Data taken during TFTR pCHERS commissioning near beam turn-on
- n_e~1.2 x $10^{19}m^{-3}$, T_i,T_e~ 3 keV
- Measured relative brightness of C VI
  - n=8-7 @ 529.5 nm
  - n=14-10 @ 516.7 nm
  - n=17-11 @ 526.8 nm
- Brightness ratio B_{8-7}:B_{14-10} is 28:1
- Measured ratio provides an estimate for expected C VI (n=14-10) brightness on NSTX
  - Collisional-Radiative (CR) model for CX using n_D=1,2,3 excited donor neutrals under populates upper n levels compared to measurement
  - From CR model, expect little variation between these TFTR parameters and NSTX parameters



About 50% of brightness @516.7nm on NSTX can be due to C VI

Brightness ratios measure n-level population ratios

CX spectra obtained by subtracting pre-beam spectrum from post-beam turn-on spectrum.



- Assuming fully mixed levels, the TFTR measurements imply that the *n*=14 and *n*=17 levels are more populated by charge exchange with the neutral beams that the *n*=8 level
- The CR model using donor neutrals n_D=1,2,3 does not adequately populate the upper levels
- Other populating mechanisms, e.g. n_D=4,5,6 , are required to match measured brightness ratio.

$$B \propto A_{ki} N_k$$

N_k is population of n - level k

A_{ki} coefficients for C VI:

$$A_{8-7} = 2.94 \times 10^{8}$$

$$A_{14-10} = 7.02 \times 10^{6}$$

$$A_{17-11} = 2.08 \times 10^{6}$$

$$\frac{B_{14-10}}{B_{8-7}} = \frac{A_{14-10}}{A_{8-7}} \frac{N_{14}}{N_8} = \frac{1}{28}$$

$$\frac{N_{14}}{N_8} = \frac{B_{14-10}}{B_{8-7}} \frac{A_{8-7}}{A_{14-10}} = 1.5$$

$$\frac{B_{17-11}}{B_{8-7}} \approx \frac{1}{120} \quad \Rightarrow \quad \frac{N_{17}}{N_8} = 1.2$$

O'Mullane Proposed Plan for Assessing Existing Data & Scalings

- ADAS CXRS model needs *nl*-resolved input cross sections,
  - Only have comprehensive data for n = 1 & 2.
  - Some data for n = 3 & 4.
- Janev APID Vol. 4 has scaling for D(n > 3), but needs to be checked.
- More details in his email dated June 24, 2015.

FIDAsim Time Dependent CR Model

- Proton excitation:
  - All n, m from JRS-4105,
  - For n ≥ 4, m >n, this is Lodge-Percival-Richards.
- Proton charge exchange on next slide
- Proton ionization:
  - For n = 1, use JRS-4105,
  - For n = 2 → 5, use adas_c09_01.pdf.
  - Higher n uses scaled n=5 cross section.
- Electron impact excitation:
  - All from JRS-4105 (“Johnson” for n ≥ 2, m ≥ 4).
- Electron impact ionization:
  - All from JRS-4105 (“Johnson” for n ≥ 4).
- Charge exchange on fully stripped impurities:
  - Uses ADAS data where available,
    - For C^{+6}, n = 1 (qcx#h0_old#c6.dat), 2 (h0_ex2), 3 (h0_ex3).
    - Also has fits for B^{+5}.
  - Everything else uses q > 3 fit from APID Vol. 4.
- Excitation by fully stripped impurities:
  - All use general Z expressions in APID Vol. 4.
- Ionization by fully stripped impurities:
  - All from APID Vol. 4,
  - Specific fits for B^{+5}, C^{+6} & n = 1.
  - General fit for everything else.

$$\frac{df_n}{dt} = -\left(\sum_{k=i,Z} f_n d_k X_n^k + \sum_{k=e,i,Z} f_n d_k I_n^k\right)$$
$$+\sum_{m>n}\left(f_m A_{m\to n} + \sum_{k=e,i,Z}(f_m d_k q_{m\to n}^k - f_n d_k q_{n\to m}^k)\right)$$
$$+\sum_{n>m}\left(-f_n A_{n\to m} + \sum_{k=e,i,Z}(f_m d_k q_{m\to n}^k - f_n d_k q_{n\to m}^k)\right)$$

$$\frac{d\mathbf{f}}{dt} = \mathbf{C}\cdot\mathbf{f}$$

$$\mathbf{f}(t) = e^{\mathbf{C}t}\cdot\mathbf{f}(0) = \mathbf{S}\cdot e^{\Lambda t}\cdot\mathbf{S}^{-1}\cdot\mathbf{f}(0)$$

FIDAsim Proton Charge Exchange Data

- Use "equivalence principle" to obtain reverse reactions for data available in ADAS:

$$\sigma(n_f \rightarrow n_i) = \frac{E_i}{E_f}\frac{n_i^2}{n_f^2}\sigma(n_i \rightarrow n_f)$$

- Data from JRS-4105 used to fill out table,
  - But, cross sections summed over m ⇒ "spread" out assuming exponential variation with energy difference.
  - Scaling expressions used for n ≥ 4.

ADAS files used in adf01/qcx#h0:
qcx#h0_old#h1.dat
qcx#h0_e2s#h1.dat
qcx#h0_e2p#h1.dat
qcx#h0_ex3#h1.dat

H-H Charge Exchange Data Source

n \ m	1	2	3	4	5	6	Total
1	ADAS	ADAS	ADAS	ADAS	Spread	Spread	Janev(n=1)
2	Equivalence	ADAS	ADAS	Spread	Spread	Spread	Janev(n=2)
3	Equivalence	ADAS	ADAS	ADAS	ADAS	Spread	ADAS/Janev(n=3)
4	Equivalence	Equivalence	Equivalence	Spread	Spread	Spread	Janev(n=4)
5	Spread	Equivalence	Equivalence	Spread	Spread	Spread	Janev(n=4)
6	Spread	Equivalence	Equivalence	Spread	Spread	Spread	Janev(n=4)

NUBEAM Data

- Many options ⇒ this is a work in progress.
- Focused on three options examined in FIDAsim benchmark, all based on ADAS data:
  1. Ground state beam atoms only,
  2. Incorporate excited state effects through enhanced stopping cross section,
  3. Stopping cross sections from ADAS_310.
     - ADAS code incorporated into the PREACT package compiled into NUBEAM.
- Ground state data used:
  - Ion interactions from adf02/sia#h/sia#h_j99#h.dat files for both D+ & fully stripped impurities.
  - Electron impact data from adf07/szd93#h/szd93#h_h.dat.
- ADAS files referenced by ADAS_310 related routines:
  - From adf18/p310_a17/bndlen_exp#h0.dat
  - And adf01/qcx#h0/qcx#h0_e2p#h1.dat
  - And adf04/hlike/hlike_bn#h91h.dat and l91h.dat.
  - And adf02/sia#h/sia#h_j99#h.dat.