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TCV-X21 modeling with the SOLPS-ITER wide-grid version

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Research Foundation Flanders
Opening new horizons

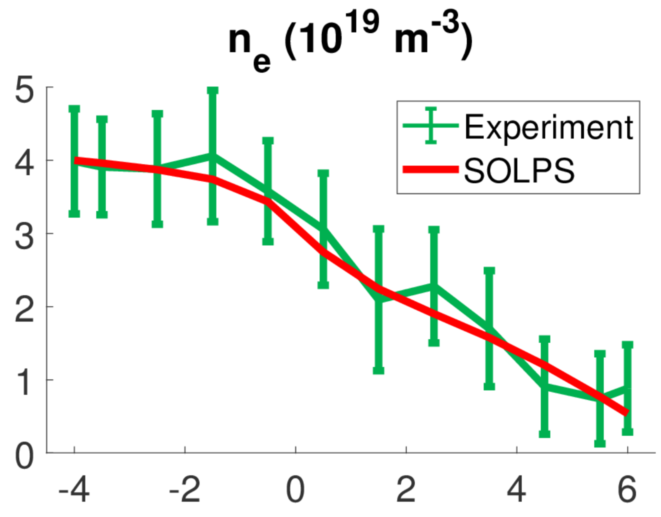
EUROfusion

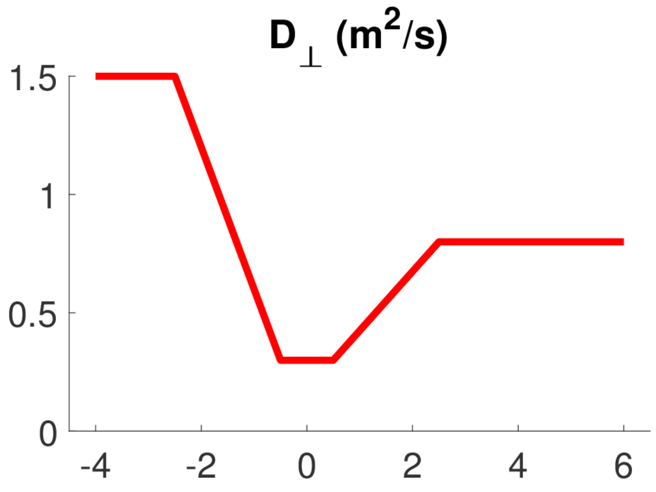
Outline

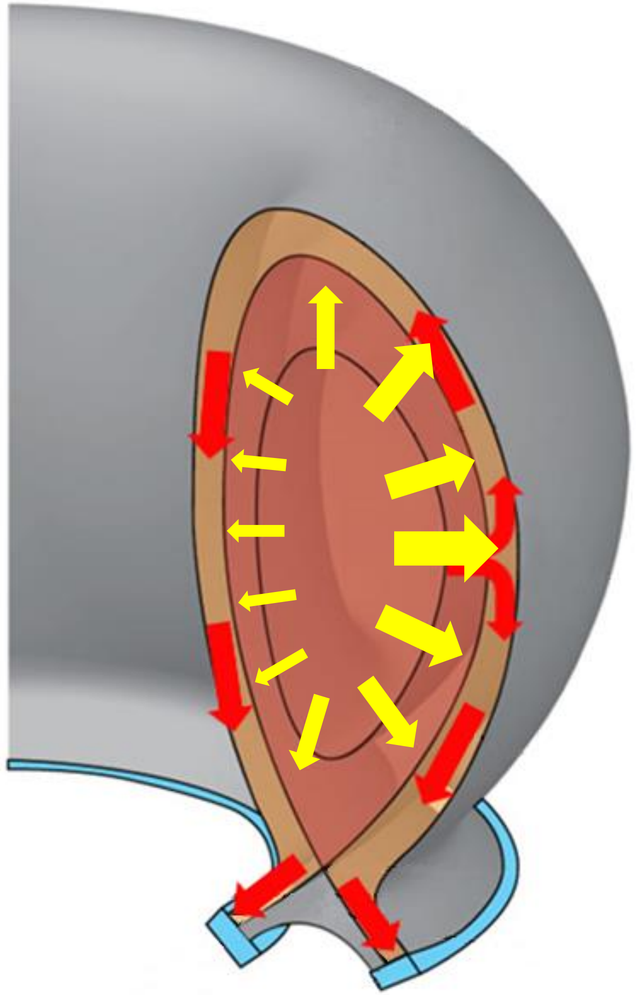
- Intro
- Results
- Conclusions and next steps

Unknown parameters needs calibration

- Perpendicular turbulent transport not resolved in SOLPS-ITER
- Use of ad-hoc diffusion coefficients (reactor, operation and space dependent)
- Estimation based on experimental data







Model calibration through optimization

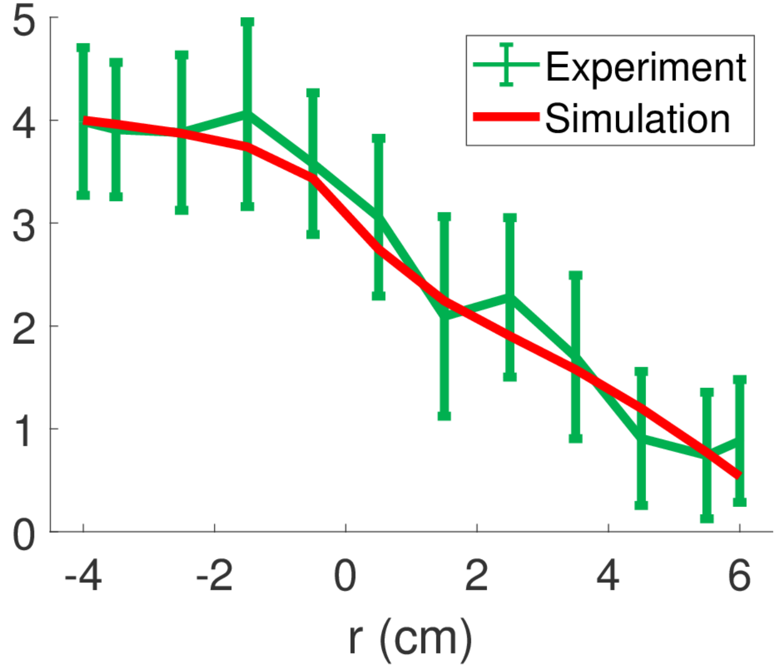
- **Cost function: match to experimental data**

$$\mathcal{J}(\theta, \boldsymbol{q}) = \frac{1}{\Omega} \int_{\Omega} \omega_q \left(\frac{1}{\overline{\mathcal{D}}^2} (q - \mathcal{D})^2 \right) \mathrm{d}\Omega$$

- **PDE-constrained optimization problem**

$$\min_{\theta, \boldsymbol{q}} \mathcal{J}(\theta, \boldsymbol{q})$$

$$s.t.\ \boldsymbol{\mathcal{B}}(\theta, \boldsymbol{q}) = 0$$



θ unknown parameters, e.g. $D_{\perp}$, BC, …

→ Efficiently solved with gradient-based methods

An optimization framework in SOLPS-ITER

1. Evaluate $\mathcal{J}(\theta^k)$,
2. Evaluate $\nabla\mathcal{J}(\theta^k)$
3. Update $\theta^{k+1} = \theta^k - f\left(\nabla\mathcal{J}(\theta^k)\right)$
4. Repeat until tolerance met

Gradient computation using Algorithmic Differentiation[1]

Coupling to optimization tool PETSc/TAO[2]

→ Calibration of complex, non-linear models & large parameter sets now possible!

[1] Carli *et al* 2023 *JCP* 491 112403

[2] Carli *et al* 2022 *CPP* 62 e202100184

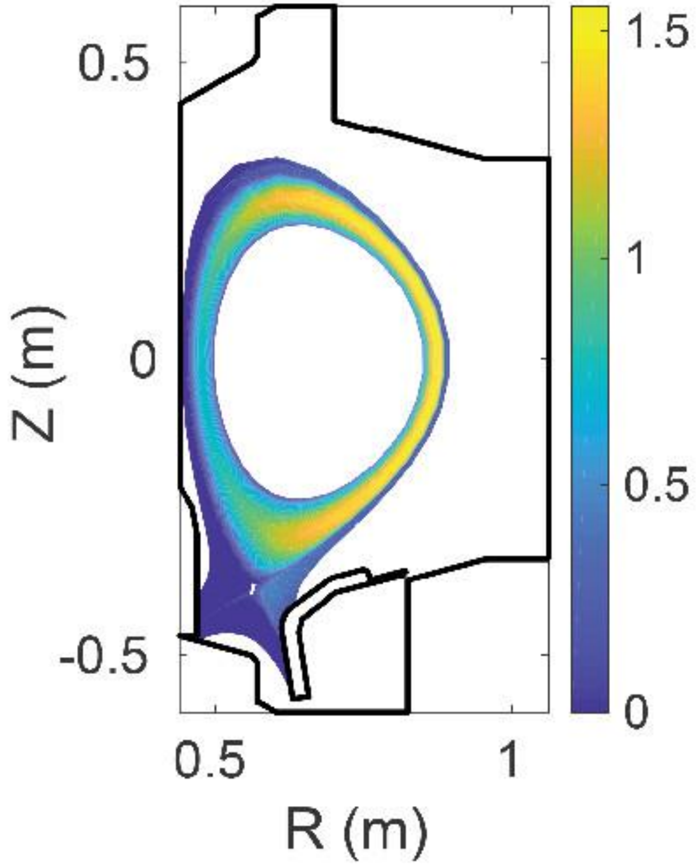
κ-model for the radial turbulent transport[3,4]

New model equation for turbulent kinetic energy κ…

$$\frac{\partial n_i \kappa}{\partial t} + \nabla \cdot (\Gamma \kappa - D_\kappa \nabla \kappa) = S_{\kappa,prod} - S_{\kappa,diss}$$

..and closure for anomalous transport coefficient(s)

$$D_{E\times B} = C_d \frac{\kappa/m}{\sqrt{\kappa/m}/\rho_L + C_S |S_{mean}|}$$



[3] Coosemans *et al* 2022 *CPP* e202100193

[4] Dekeyser *et al* 2022 *CPP* e202100190

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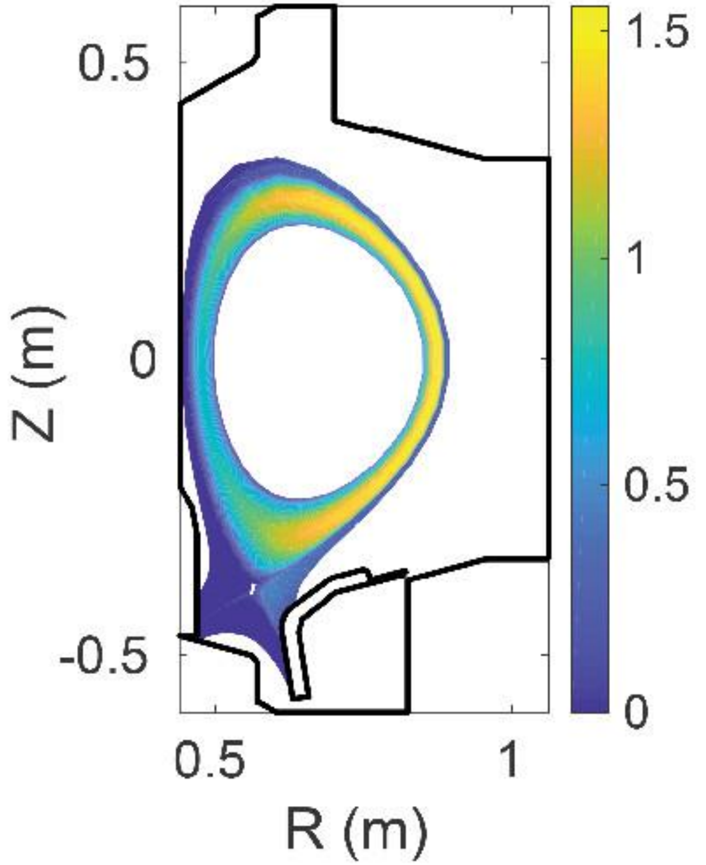
$$\chi_{e,E\times B} = C_{h,e} D_{E\times B}$$

$$\chi_{i,E\times B} = C_{h,i} D_{E\times B}$$



[3] Coosemans *et al* 2022 *CPP* e202100193

[4] Dekeyser *et al* 2022 *CPP* e202100190

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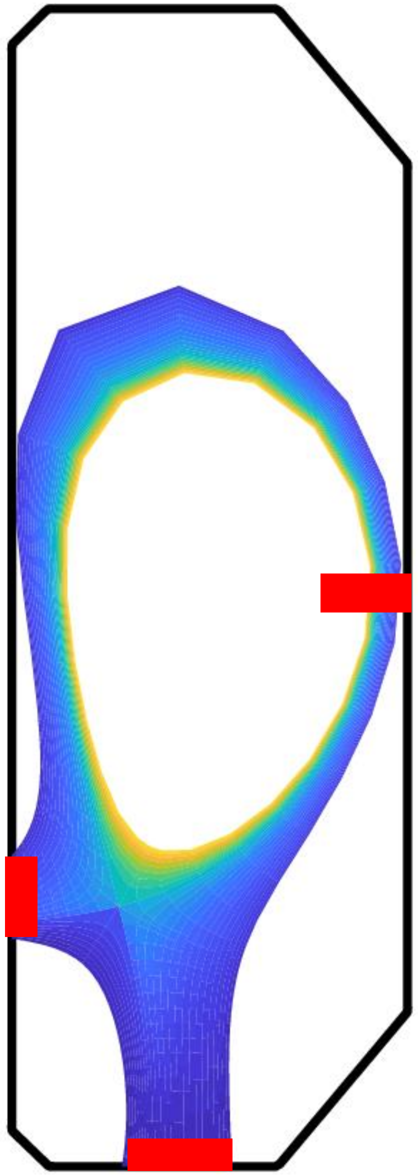
First calibration on real data: TCV-X21[5]

- Use radial profiles of:
  - n_e, T_e at OMP
  - $j_{sat}, T_e, q_{\parallel}$ at OT
  - j_{sat}, T_e at IT



Research questions

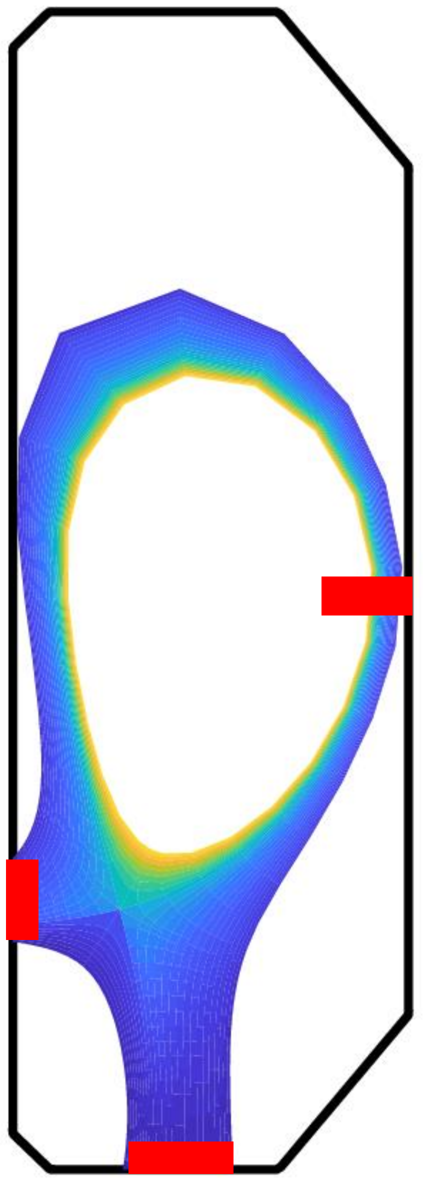
1. **How does κ-model compare to standard models?**
2. **Is the κ-model better at *predictions*?**
3. **How do they compare in a density scan?**

[5] Oliveira and Body *et al* 2022 *NF* 62 096001

DOI 10.5281/zenodo.10841179

Case setup

- SOLPS-ITER wide-grid version
- Forward field
- Pure D plasma
- Drifts ON
- Advanced Fluid Neutral (AFN) models[6,7]
- Core BC: fixed density + $P_{ohm} \sim 125$ kW
- Recycling 0.99
- Relatively coarse grid 60×24



[6] Horsten *et al* 2017 *NF* 57 116043

[7] Van Uytven *et al* 2022 *NF* 62 086023

Results

1. How does κ-model compare to standard models?

2. Is the κ-model better at *predictions*?

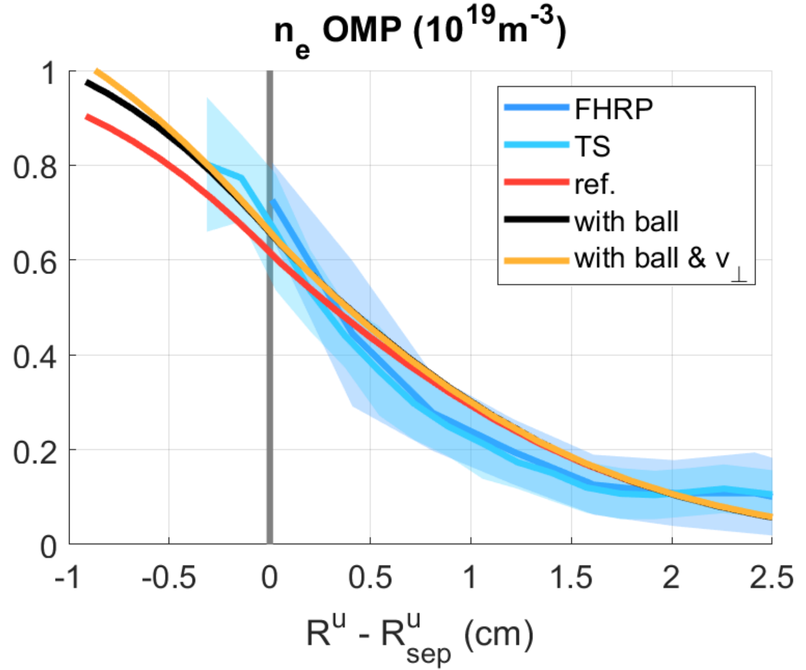
3. How do they compare in a density scan?

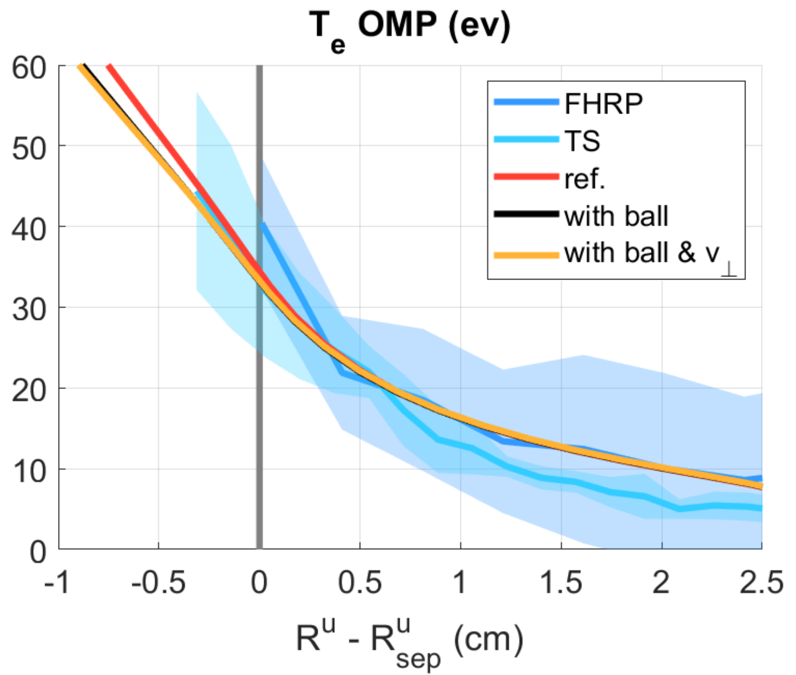
1.1 – Estimation with standard model

- Unknown parameters θ
  - Reference: $\theta = \left(n_{e,core}, \mathrm{D}_{\perp}, \chi_{e,\perp}, \chi_{i,\perp}\right)$
  - With ballooning $\theta = \left(n_{e,core}, \mathrm{D}_{\perp}, \chi_{e,\perp}, \chi_{i,\perp}, n\right)$
  - With ballooning and pinch velocity $\theta = \left(n_{e,core}, \mathrm{D}_{\perp}, \chi_{e,\perp}, \chi_{i,\perp}, n, v_{\perp}\right)$

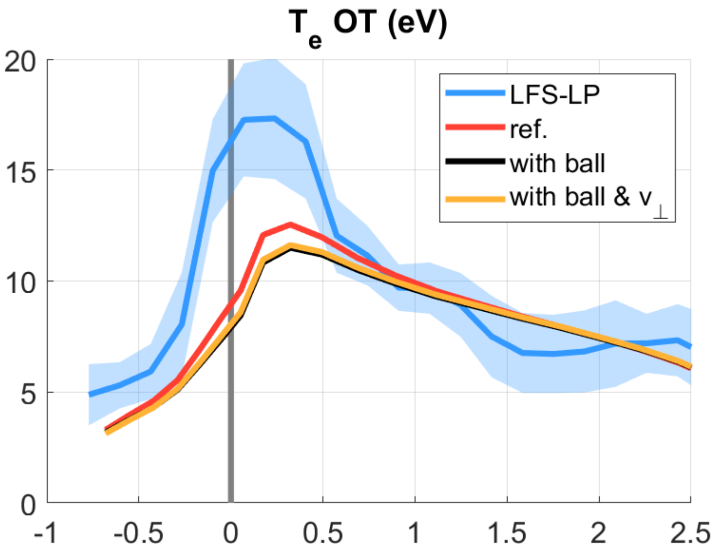
$$\left(\frac{B_{T,ref}}{B_T(r,\theta)}\right)^n$$

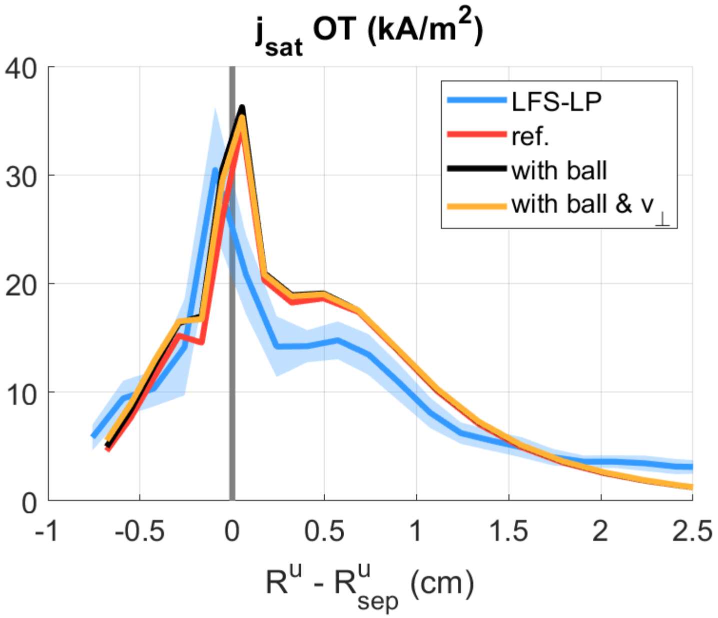
Note: estimation with ballooning gets exponent $n = 0$, i.e. no ballooning



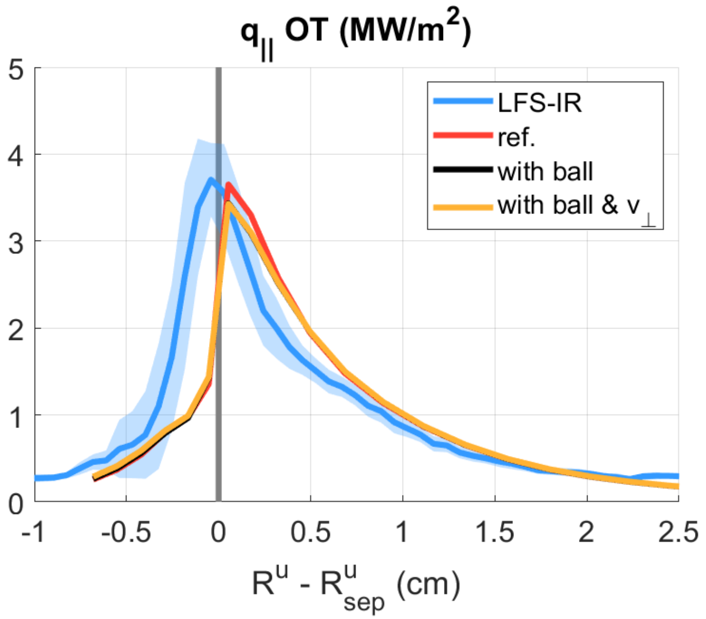


Good agreement at OT, small differences in models





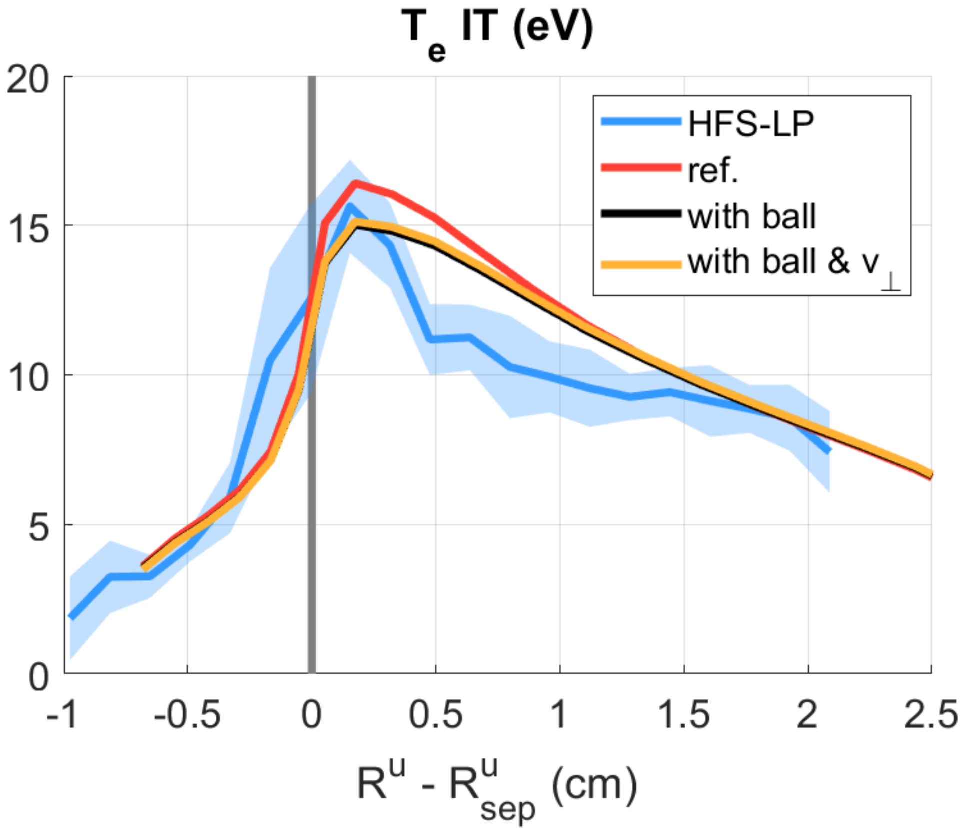
- Underestimation of T_e peak and gradient, far SOL profile less flat than exp.
- j_{sat} profile and peak captured, but shifted outward
- $q_{\|}$ also shifted, inner/outer decay lengths captured

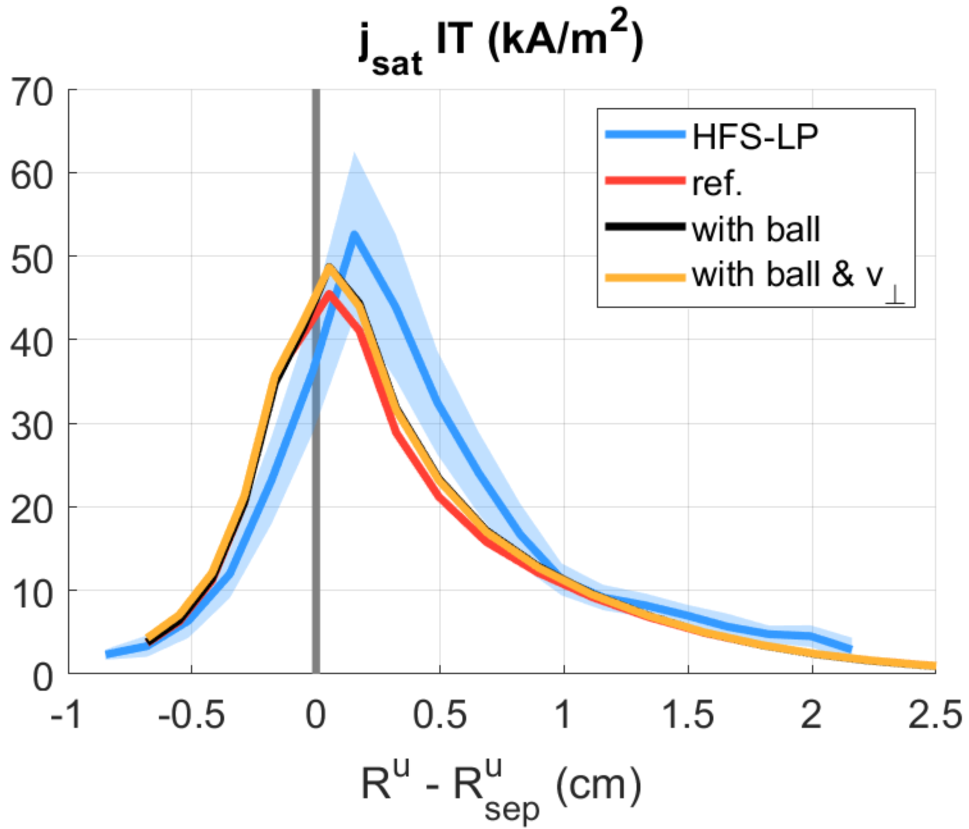


Good agreement at IT, some differences in models

- T_e peak well captured, (far) SOL profile somewhat captured

- j_{sat} profile and peak captured, but slightly shifted inward





1.2 – Estimation with κ-model

κ-model prone to instabilities + use of drifts → very unstable!

→ Adapted BC at PFR enforcing zero-gradient, not leakage

→ Quite smaller step-length in line-search

Several parameters inside κ-model:

- $D_{E\times B} = C_d \frac{\kappa/m}{\sqrt{\kappa/m}/\rho_L + c_S |S_{mean}|}$
- $\chi_{e,E\times B} = C_{h,e} D_{E\times B}$
- $\chi_{i,E\times B} = C_{h,i} D_{E\times B}$
- $\eta_{i,E\times B} = C_\eta D_{E\times B}$
- $D_\kappa = C_{D_\kappa} D_{E\times B}$

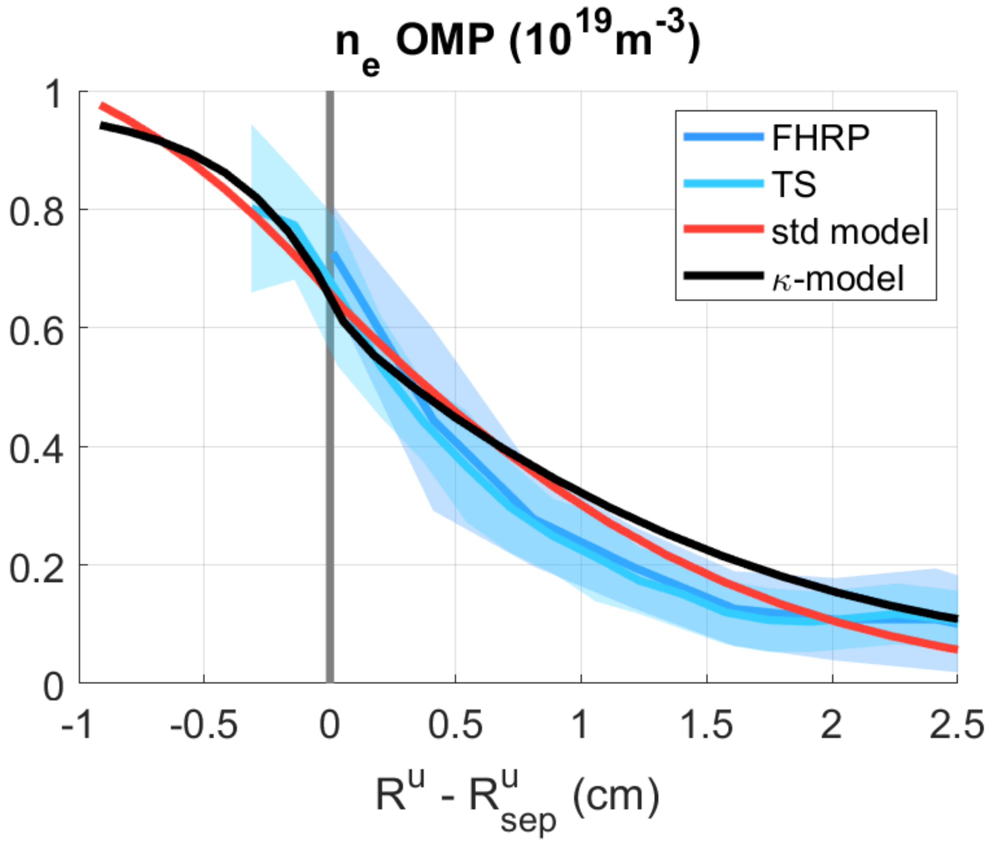
Kept fixed at 0.1, needs additional turbulence data from experiment or turbulence codes

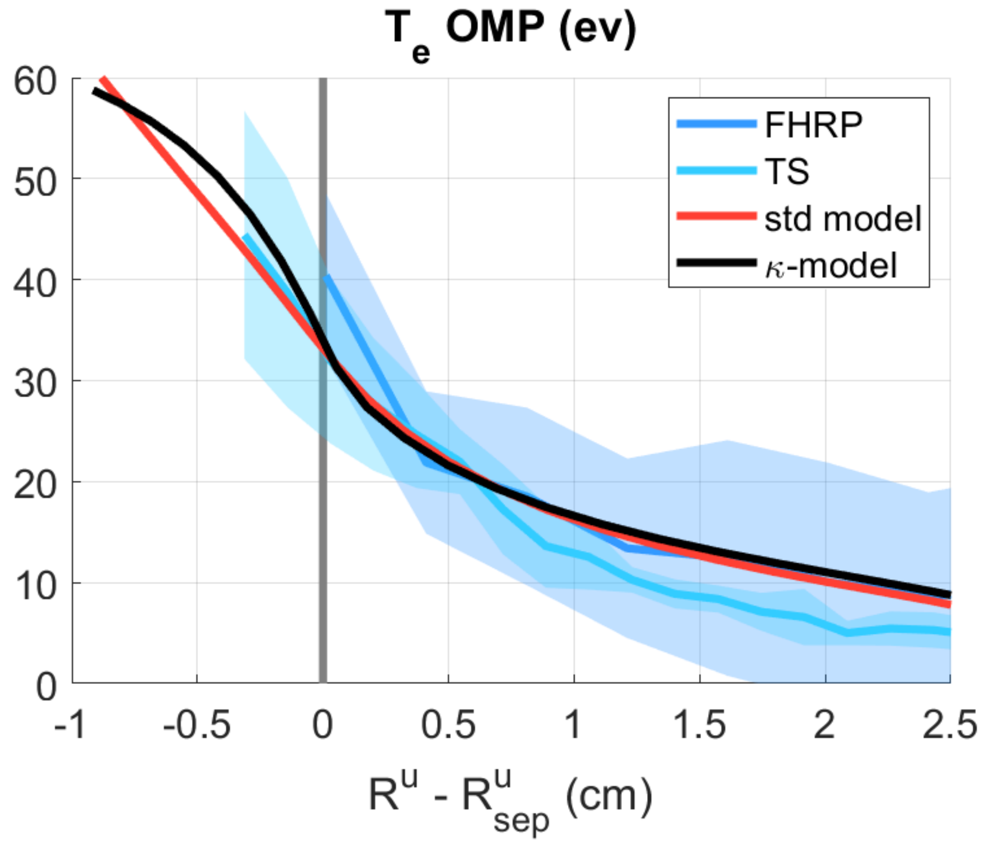
- κ BC at core κ_{core}
- Parallel transport of κ $C_{\sigma_\parallel,1}$
- Dissipation of κ $C_{\sigma_\parallel,2,core}$, $C_{\sigma_\parallel,2,SOL}$

1.2 – Estimation with κ-model

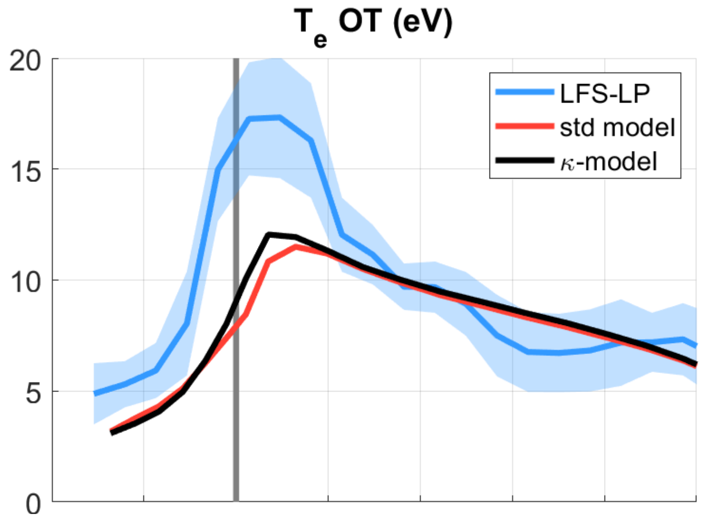
Comparison with standard model on ‘similar’ setup (i.e. ballooning included)

Note n_e and T_e at separatrix are the same as consequence of optimization but no constraint is active there



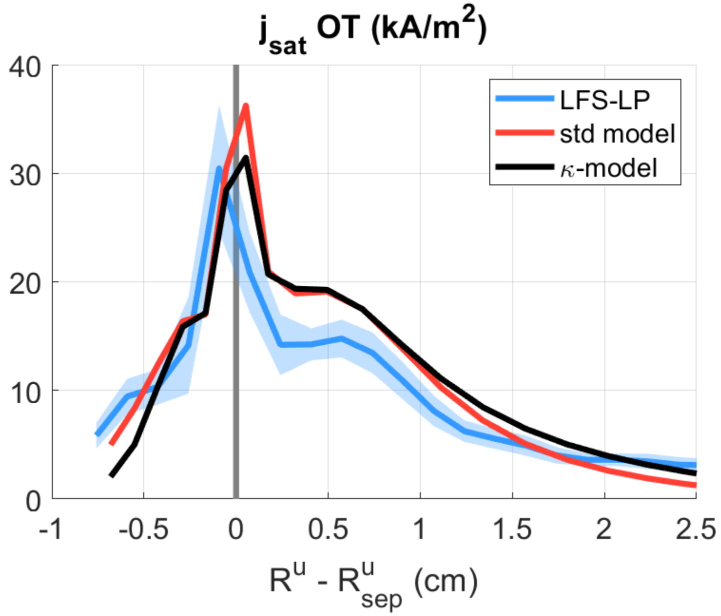


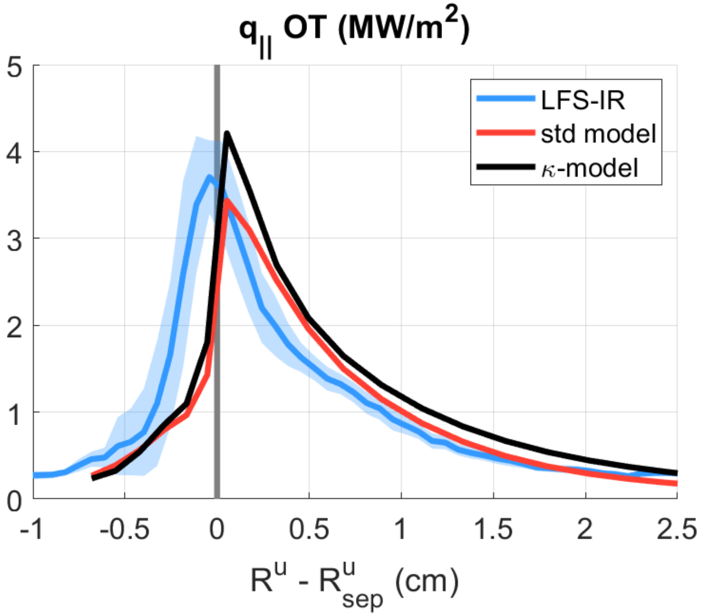
κ-model able to reproduce experimental data at OT



- Further underestimation of T_e, likely linked to small increase in j_{sat} and $q_{\|}$

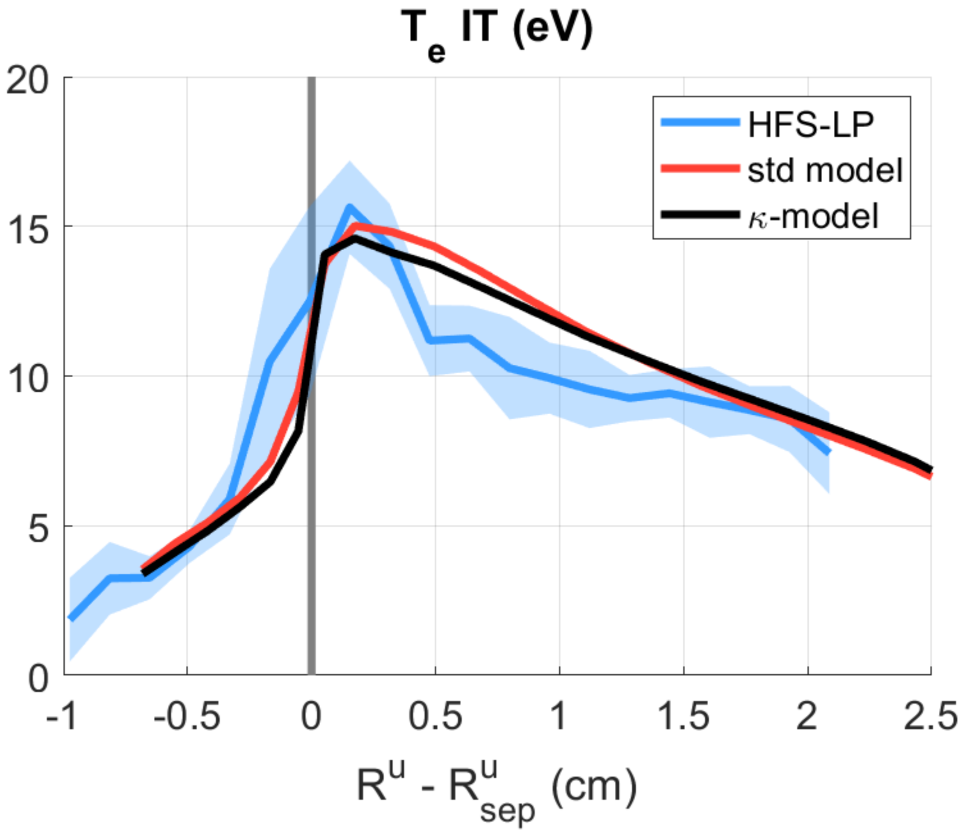
- Same profile shapes obtained as standard model and experiments

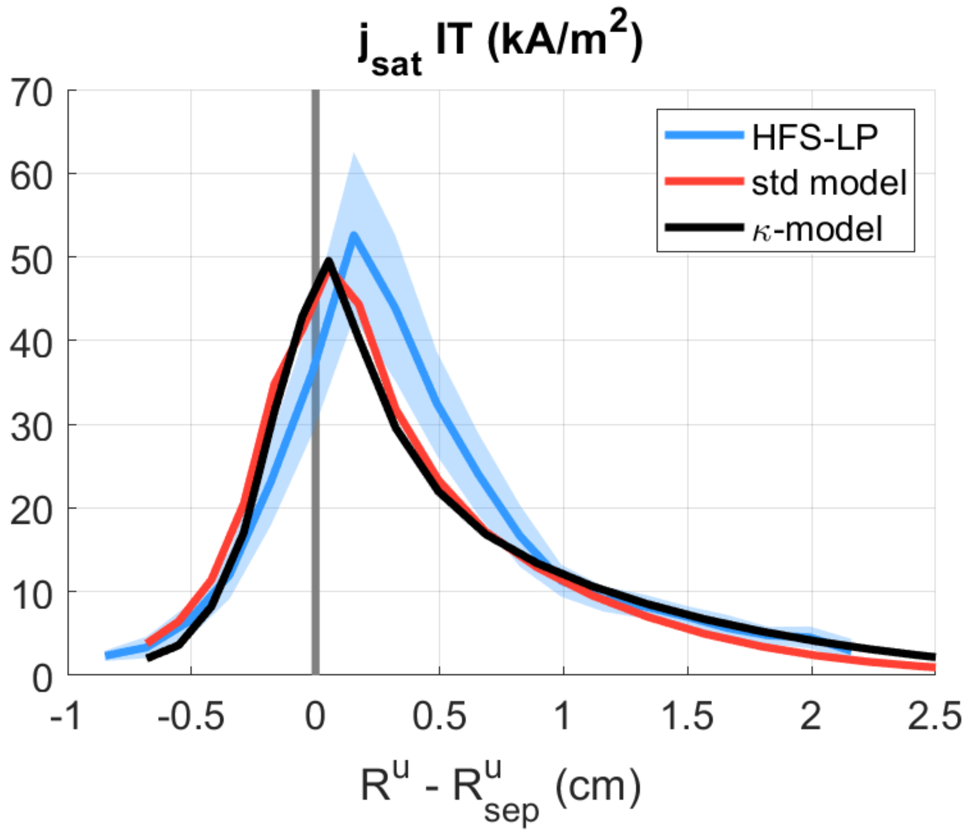




κ-model able to reproduce experimental data at IT

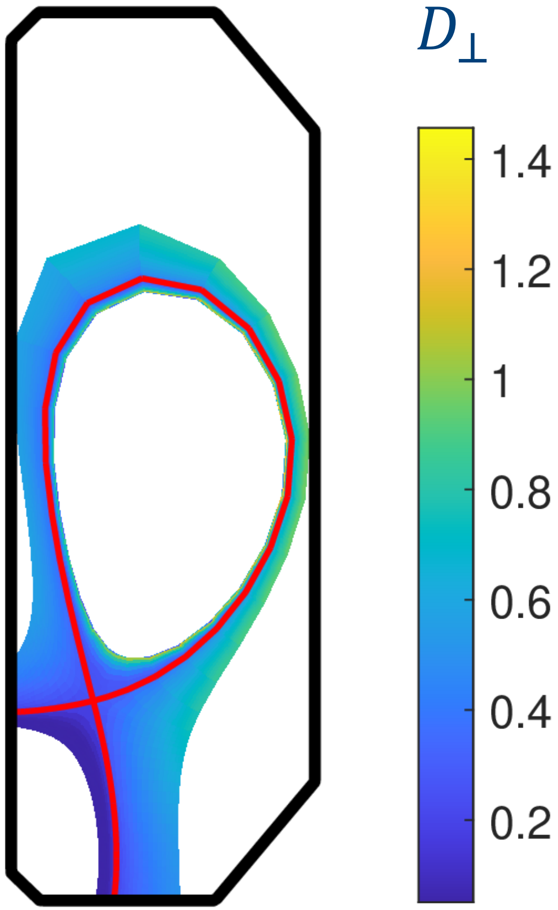
- No significant discrepancies between two models at IT



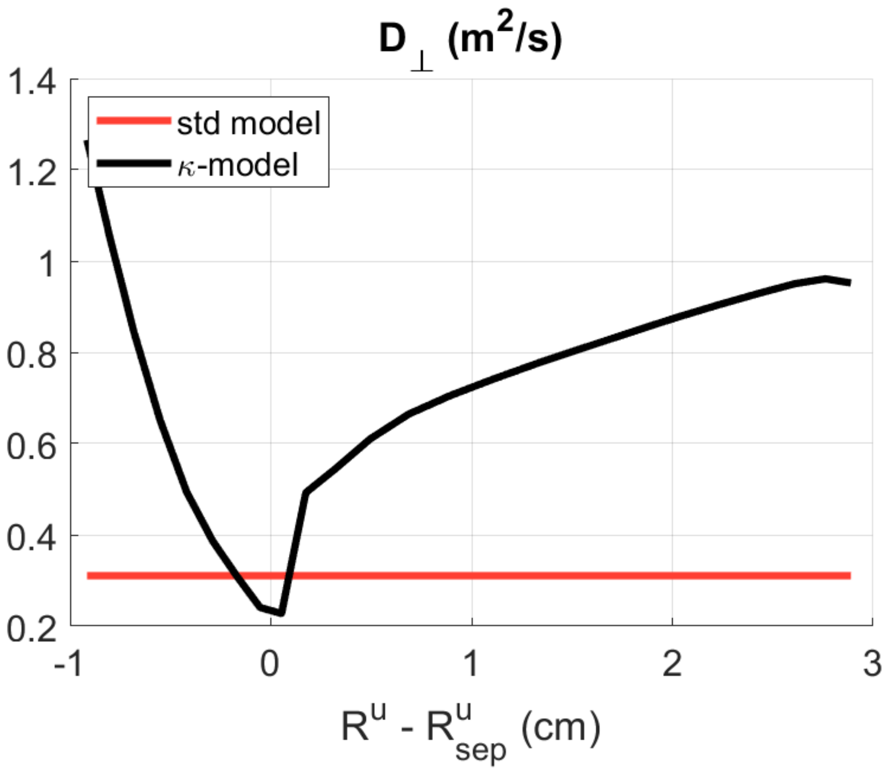


$D_\perp$ with ‘small’ ballooning profile, shear suppression at separatrix

- Standard model & κ-model show that no/negligible ballooning is required to match data
- How can they reproduce results in similar way when $D_\perp$ is so different?



1. They have same separatrix n_e and T_e
2. Larger role of drifts rather than turbulent transport?



Results

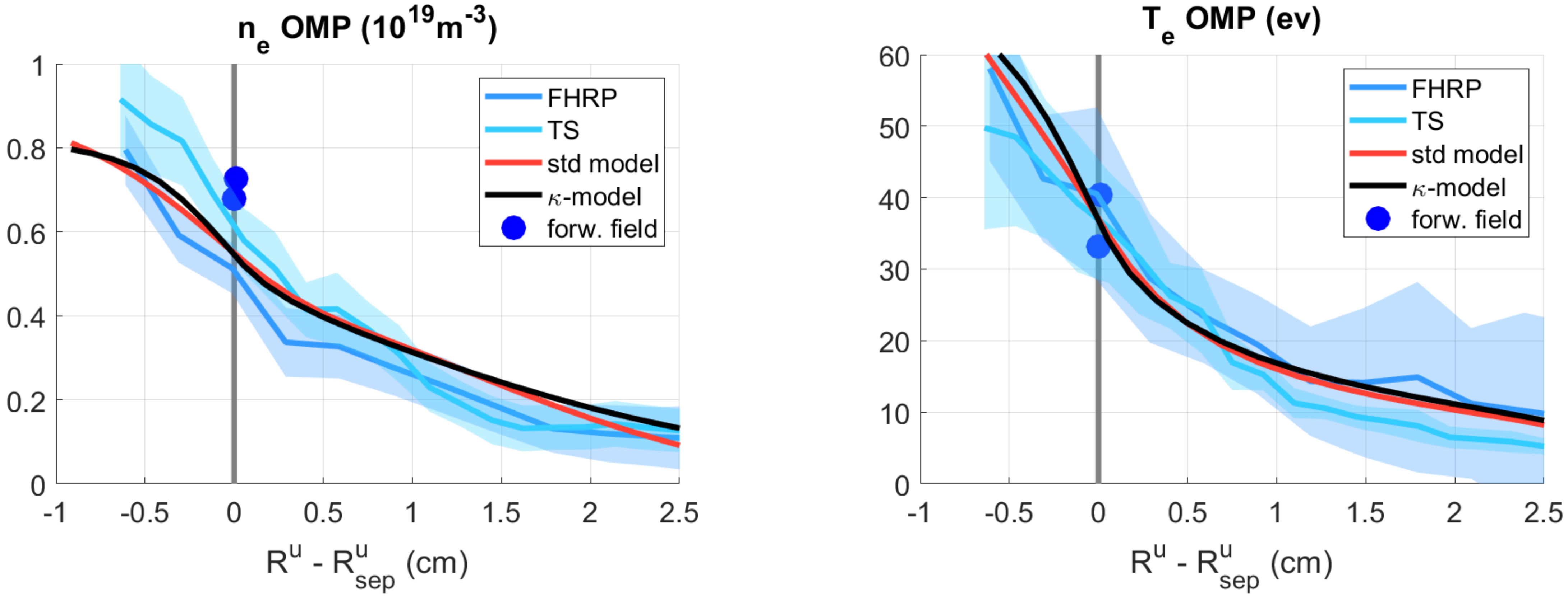
1. How does κ-model compare to standard models?

2. Is the κ-model better at *predictions*?

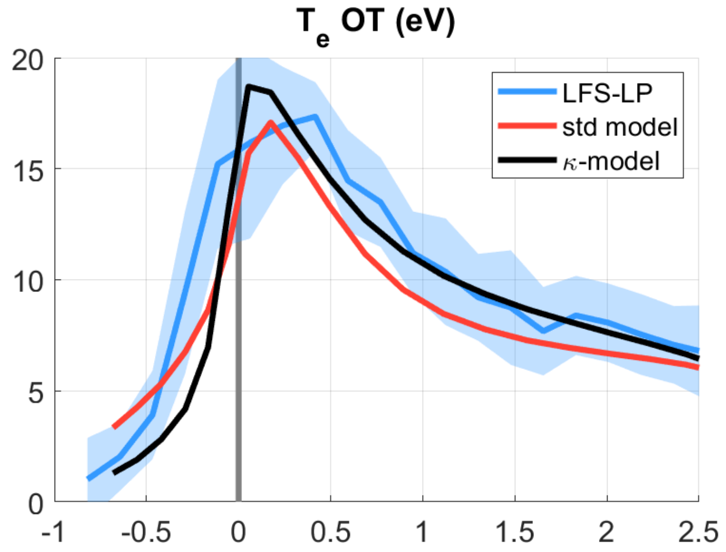
3. How do they compare in a density scan?

Predictions on reversed field

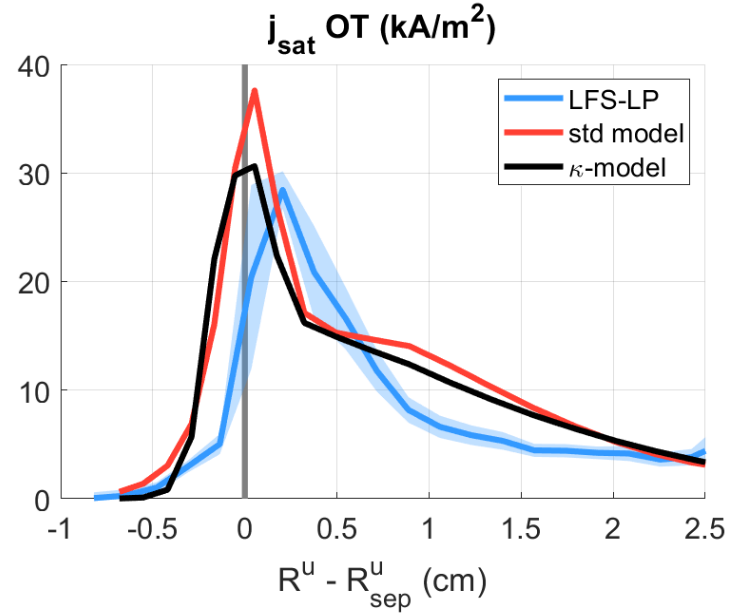
- n_e BC at core adjusted as reverse field $n_{e,sep}$ is lower (need to setup feedback scheme)
- κ BC at core kept constant (does it make sense??)
- Density decay length not fully captured by both models

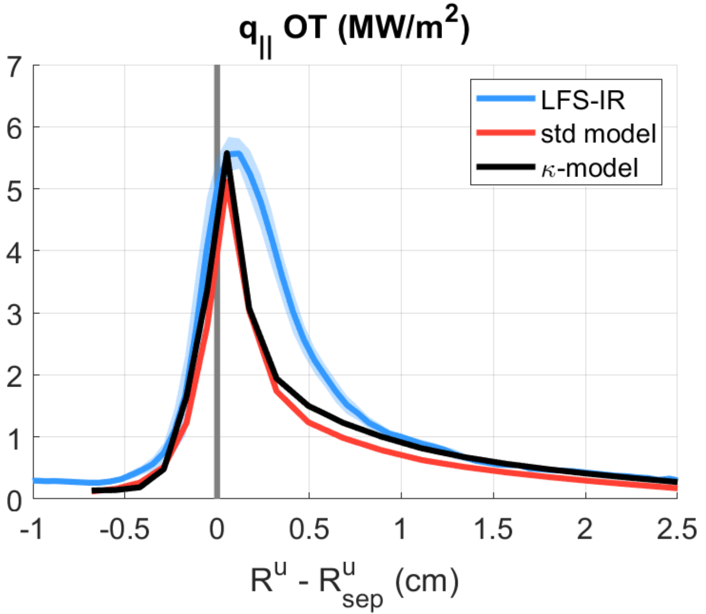


Good T_e and worse j_{sat} prediction at OT



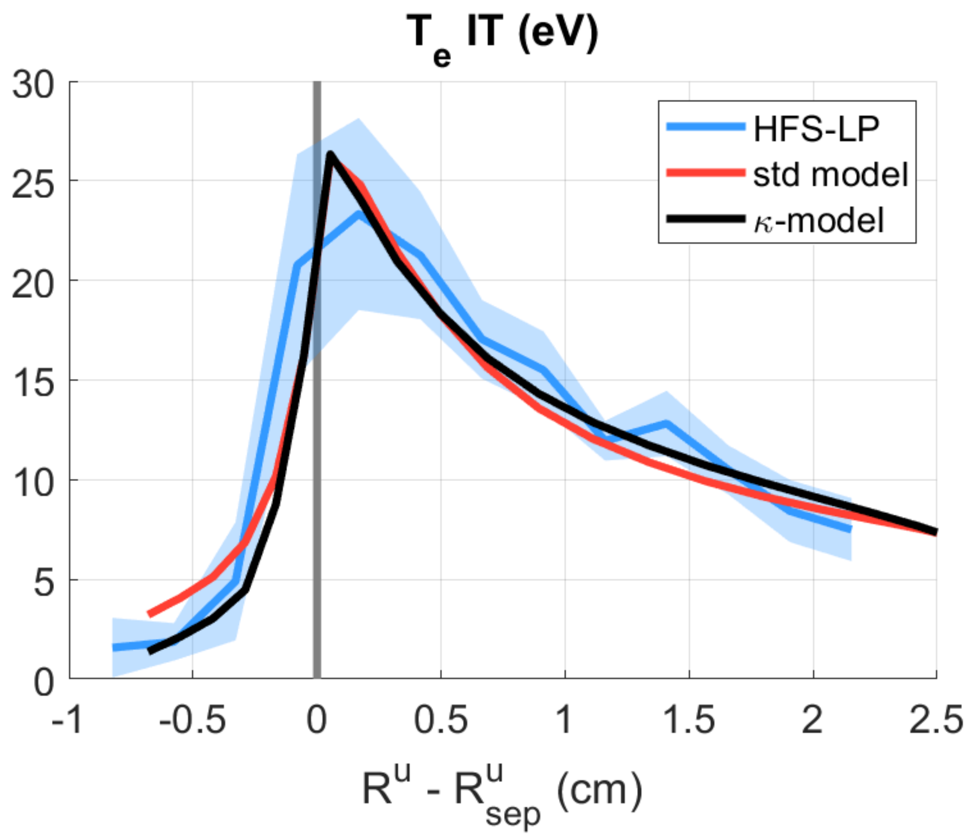
- T_e peak captured, κ-model seems to better predict rise and fall
- j_{sat} profile similar to forward field in simulations, κ-model captures peak, both *shifted left*
- $q_{\|}$ fall-off not that good, but peak captured
- Slight differences among models (small upstream difference?)

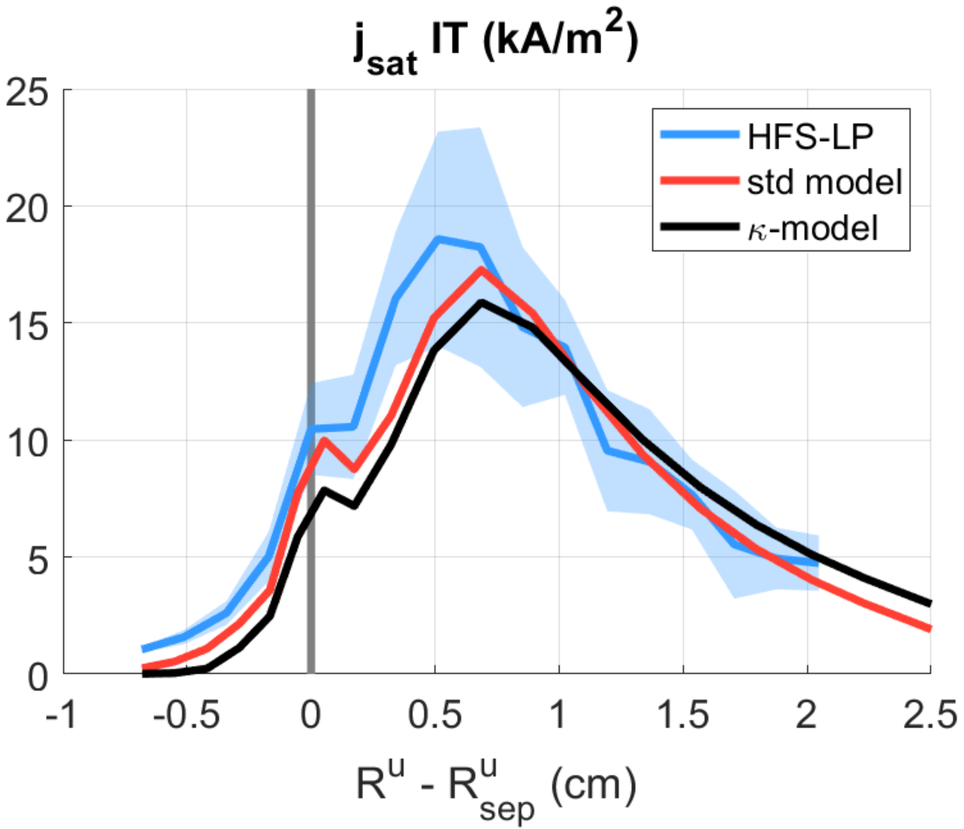




Very good predictions at IT

- T_e well captured, also rise and fall-off profiles
- Very good match with j_{sat}, peak *shifted right*
- Small discrepancies between two models at IT (again, small upstream difference?)





Results

1. How does κ-model compare to standard models?

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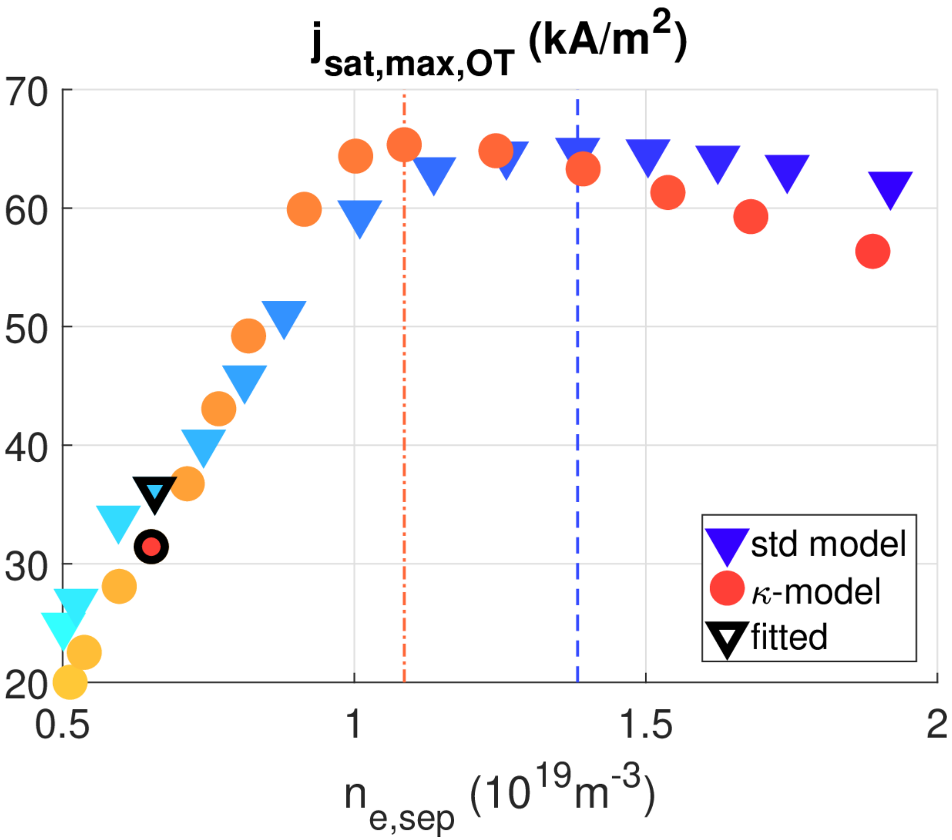
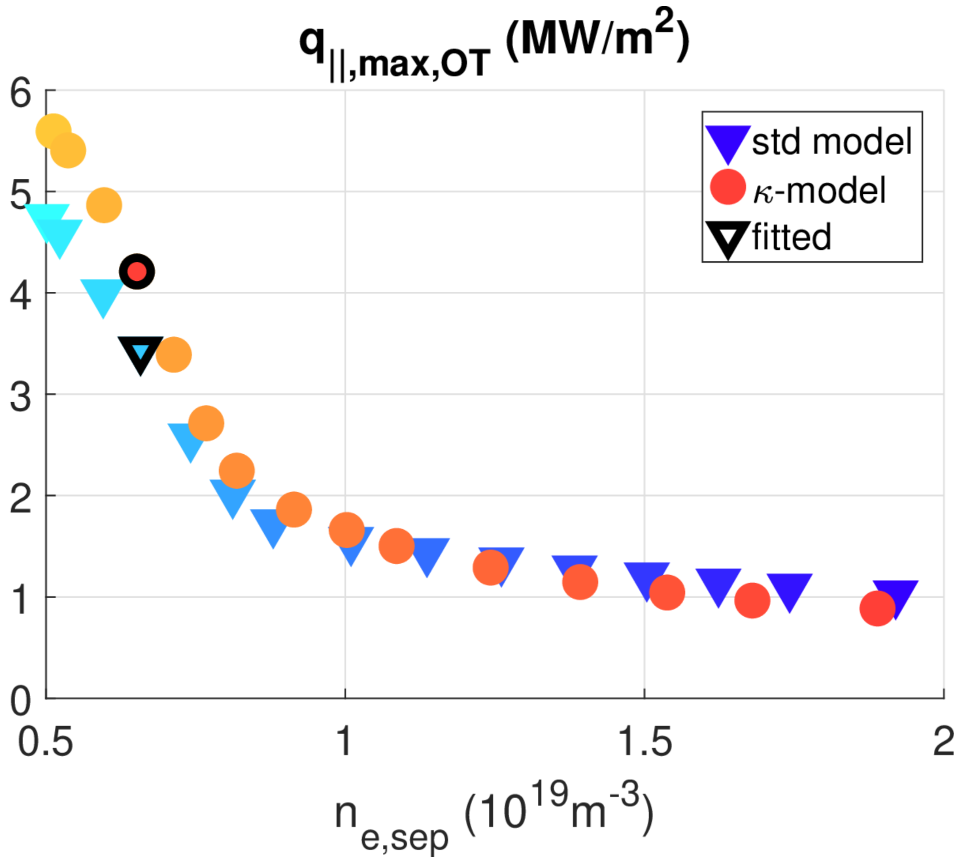
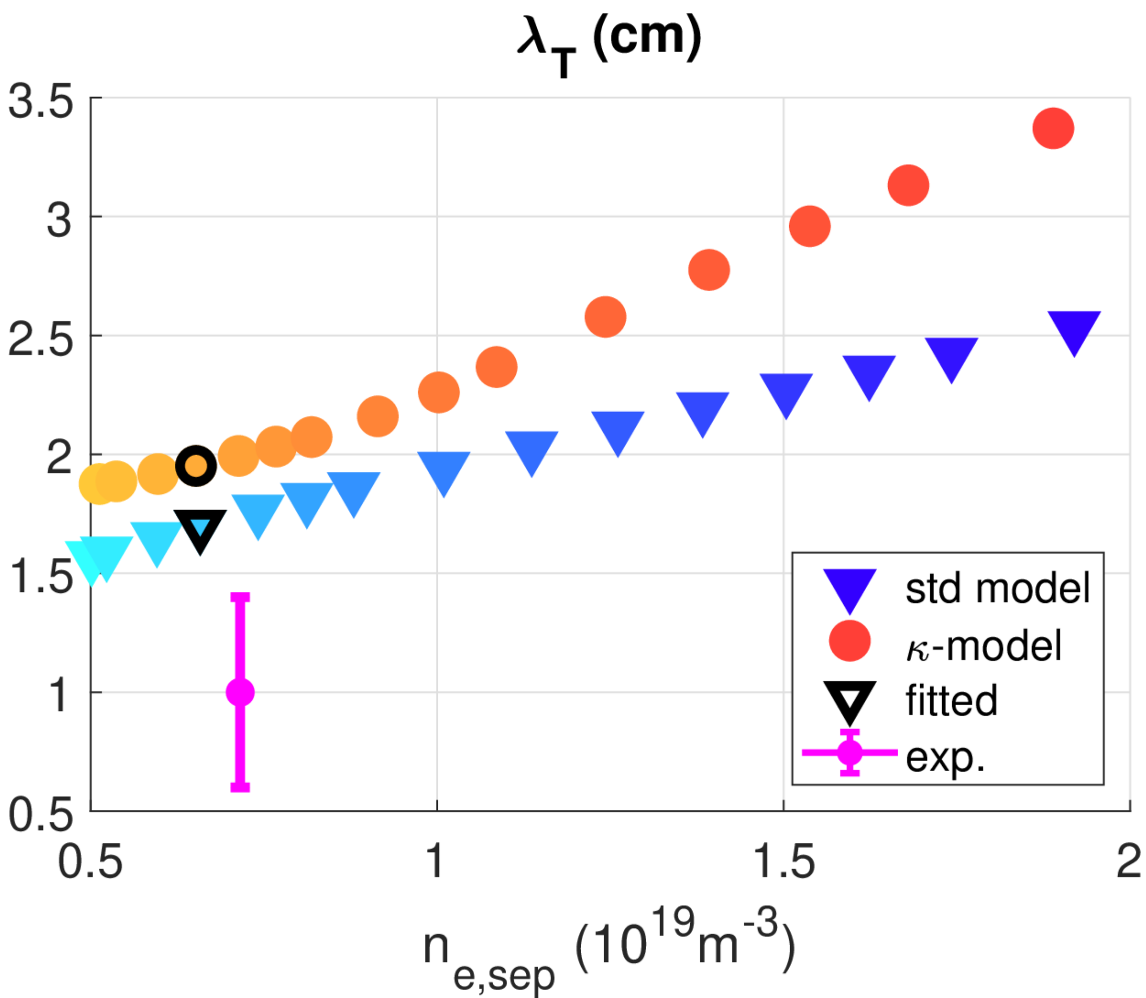
Maximum j_{sat} and $q_{\parallel}$ at OT

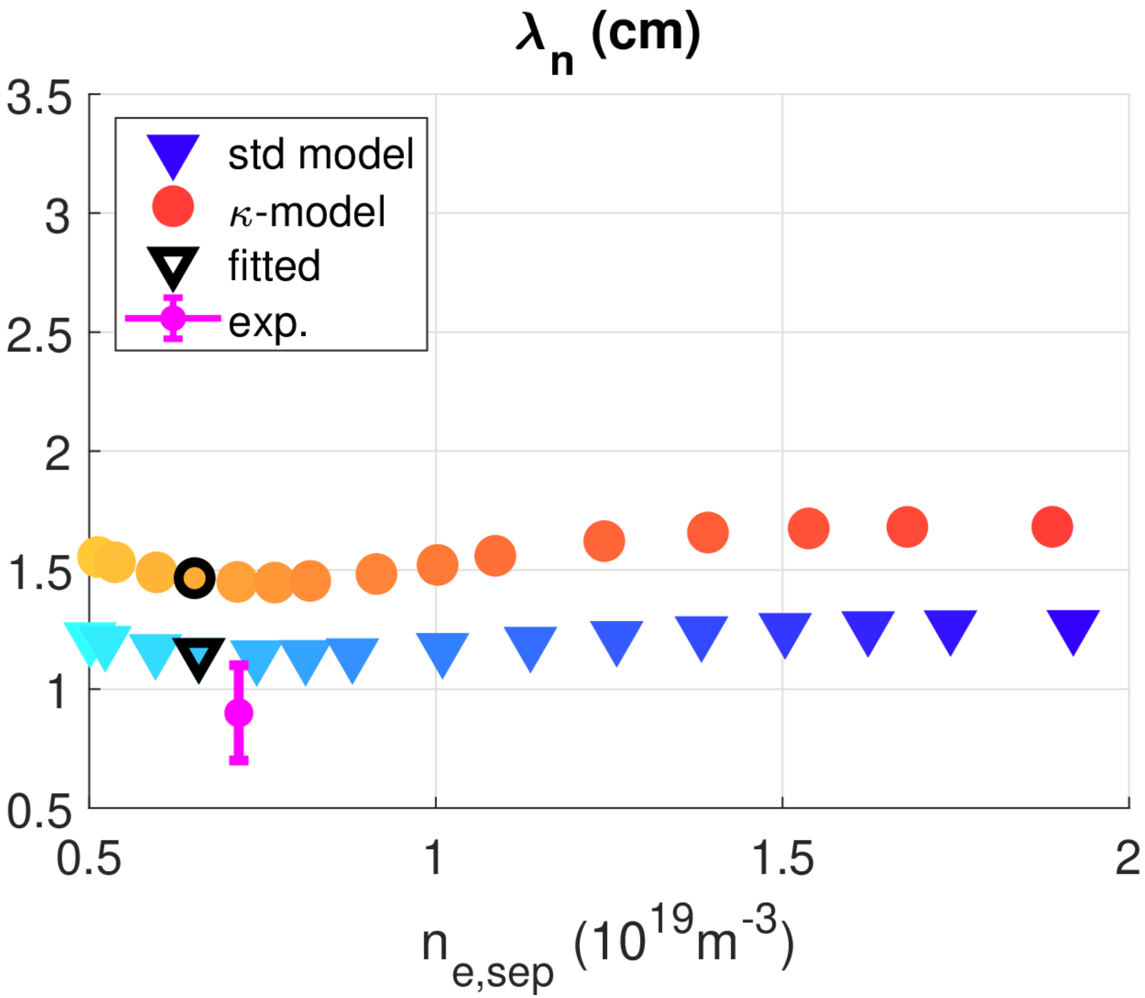
- j_{sat} rollover present, anticipated in κ-model



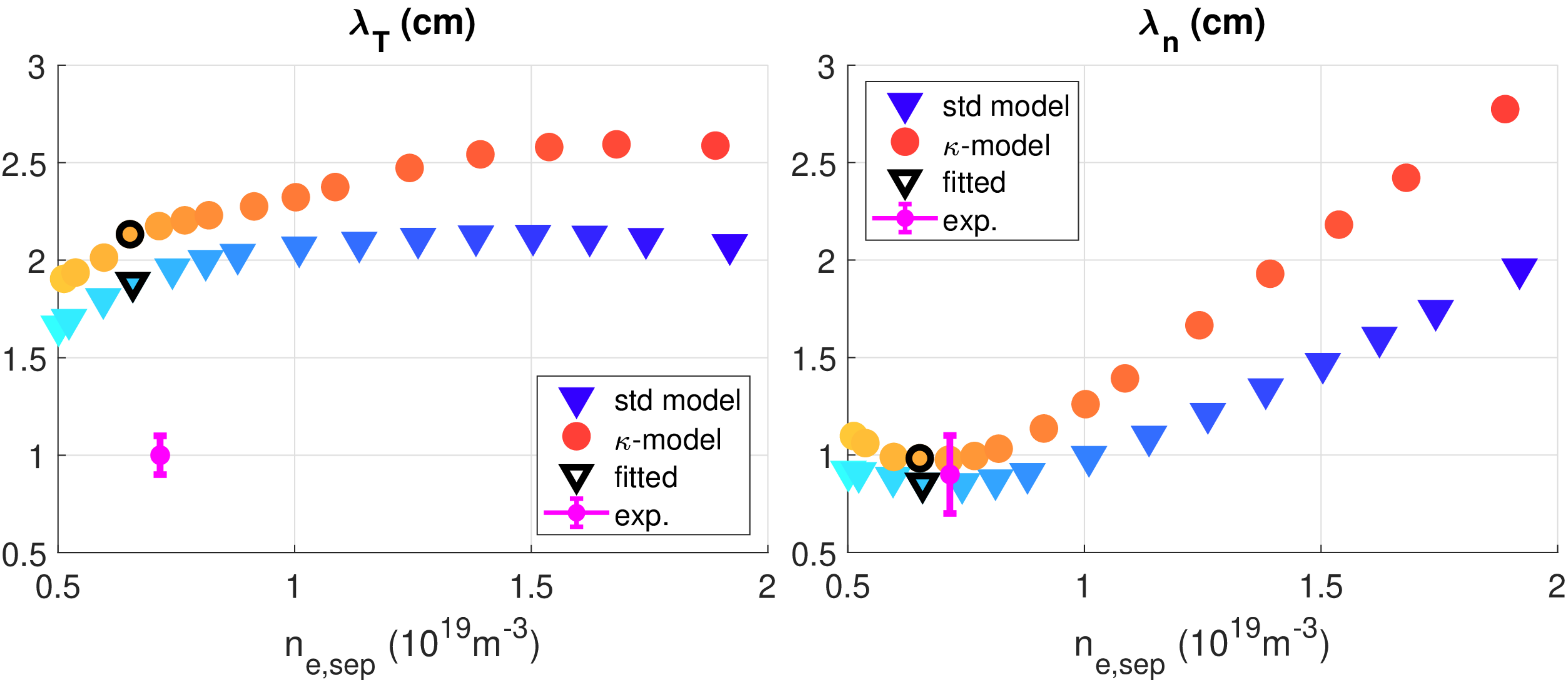


Decay lengths at OMP (Reciprocating probe)





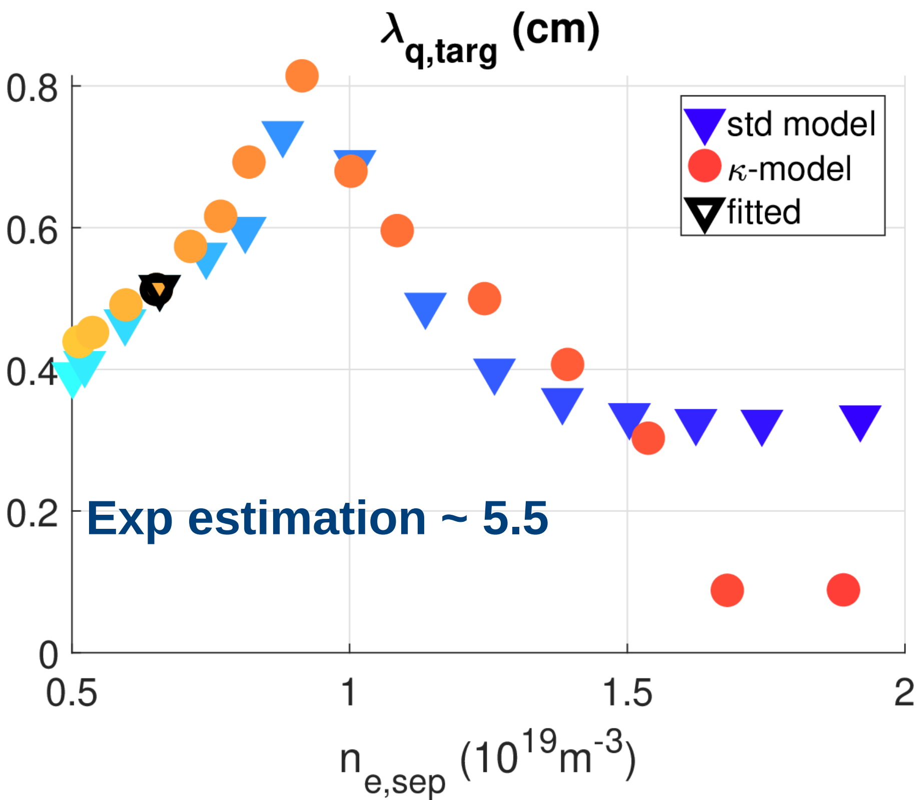
Decay lengths at divertor entrance (Thomson Scatt)

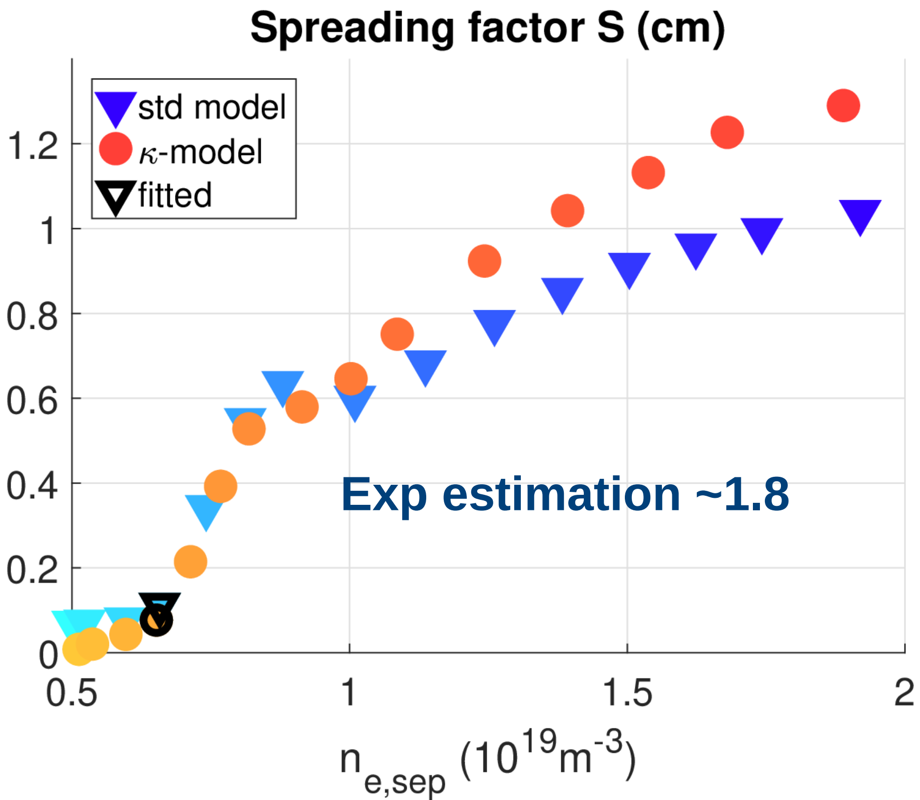


Decay length at target (infrared camera)

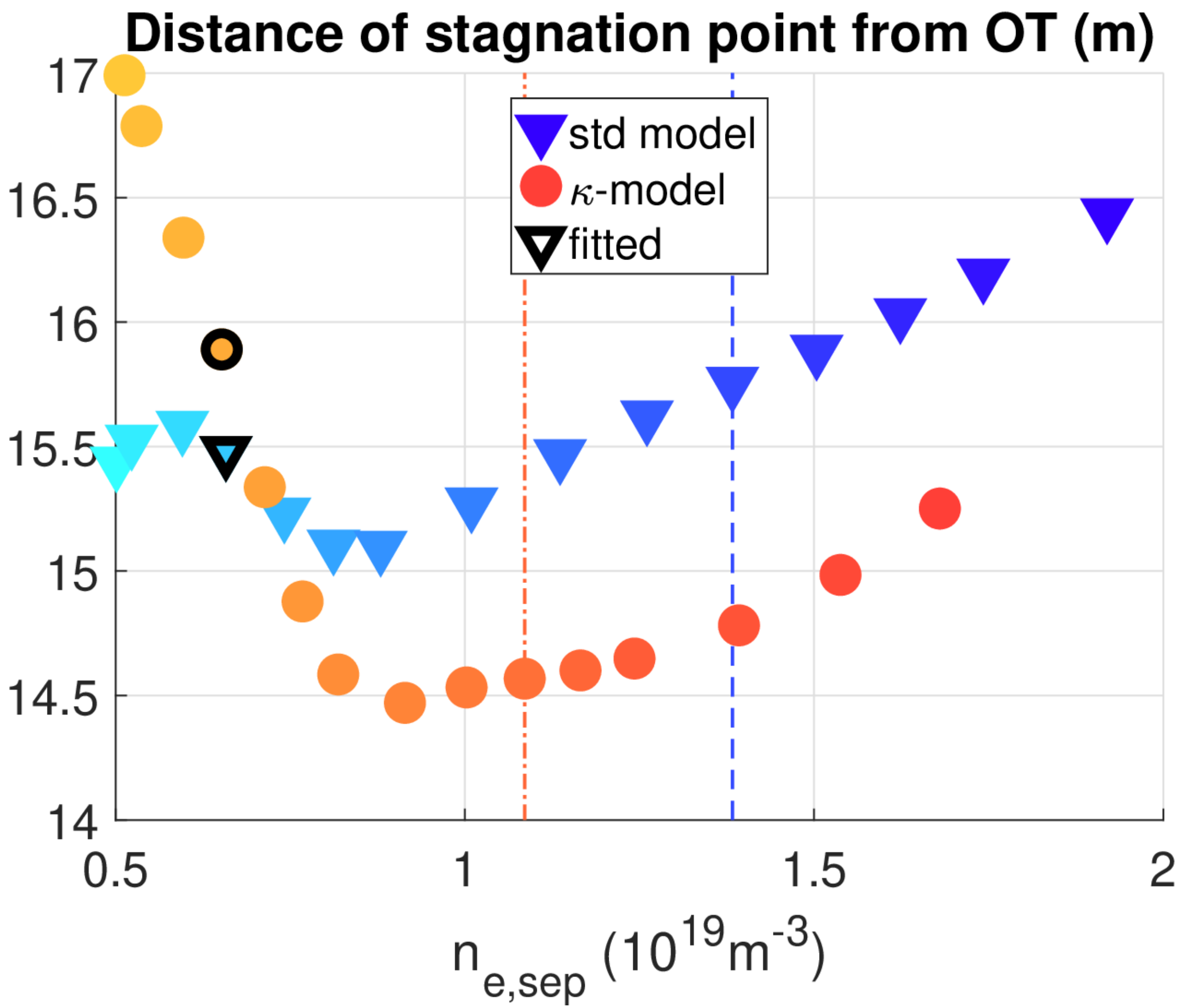
- Fitting curve

$$q_{\parallel}(r) = \frac{q_0}{2}\exp\left[\left(\frac{S}{2\lambda_q}\right)^2 - \frac{r-r_0}{\lambda_q}\right]\operatorname{erfc}\left(\frac{S}{2\lambda_q} - \frac{r-r_0}{S}\right) + q_{bg}$$





Trying to understand the differences…

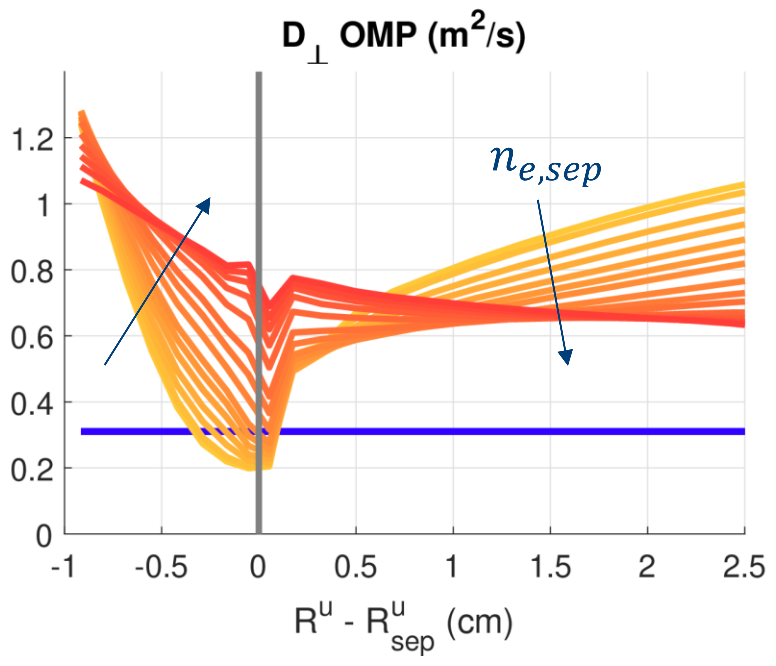


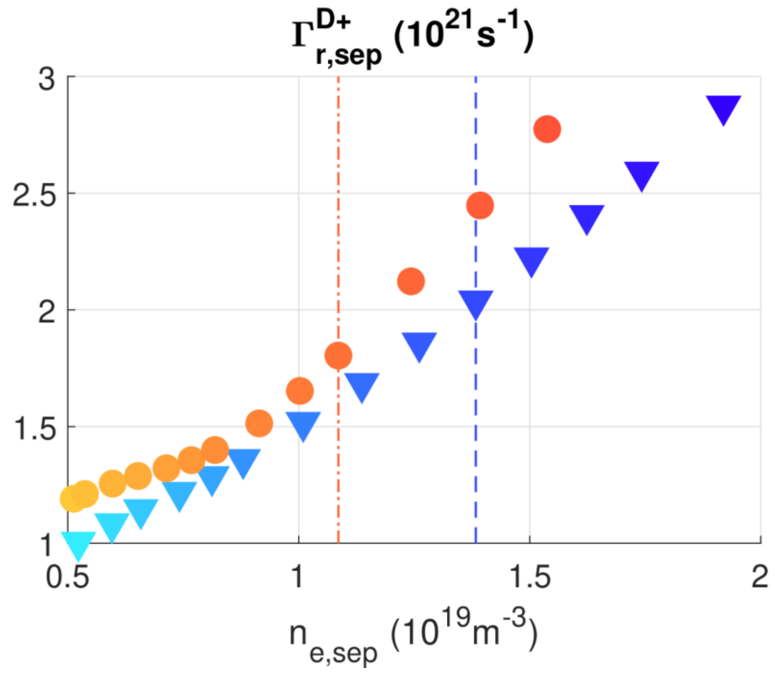
Trying to understand the differences…

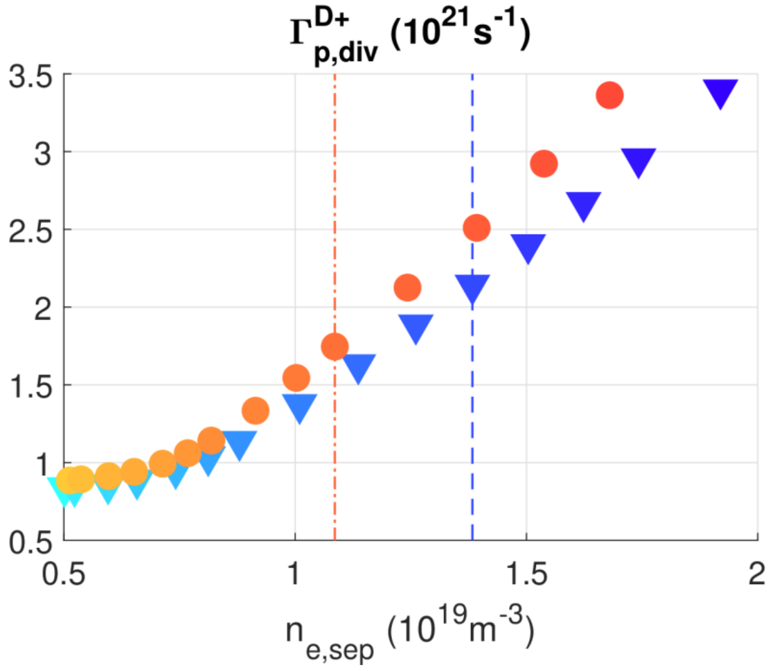
- Larger $D_\perp$ at separatrix for κ-model

→ Somewhat larger particle outflux at same density

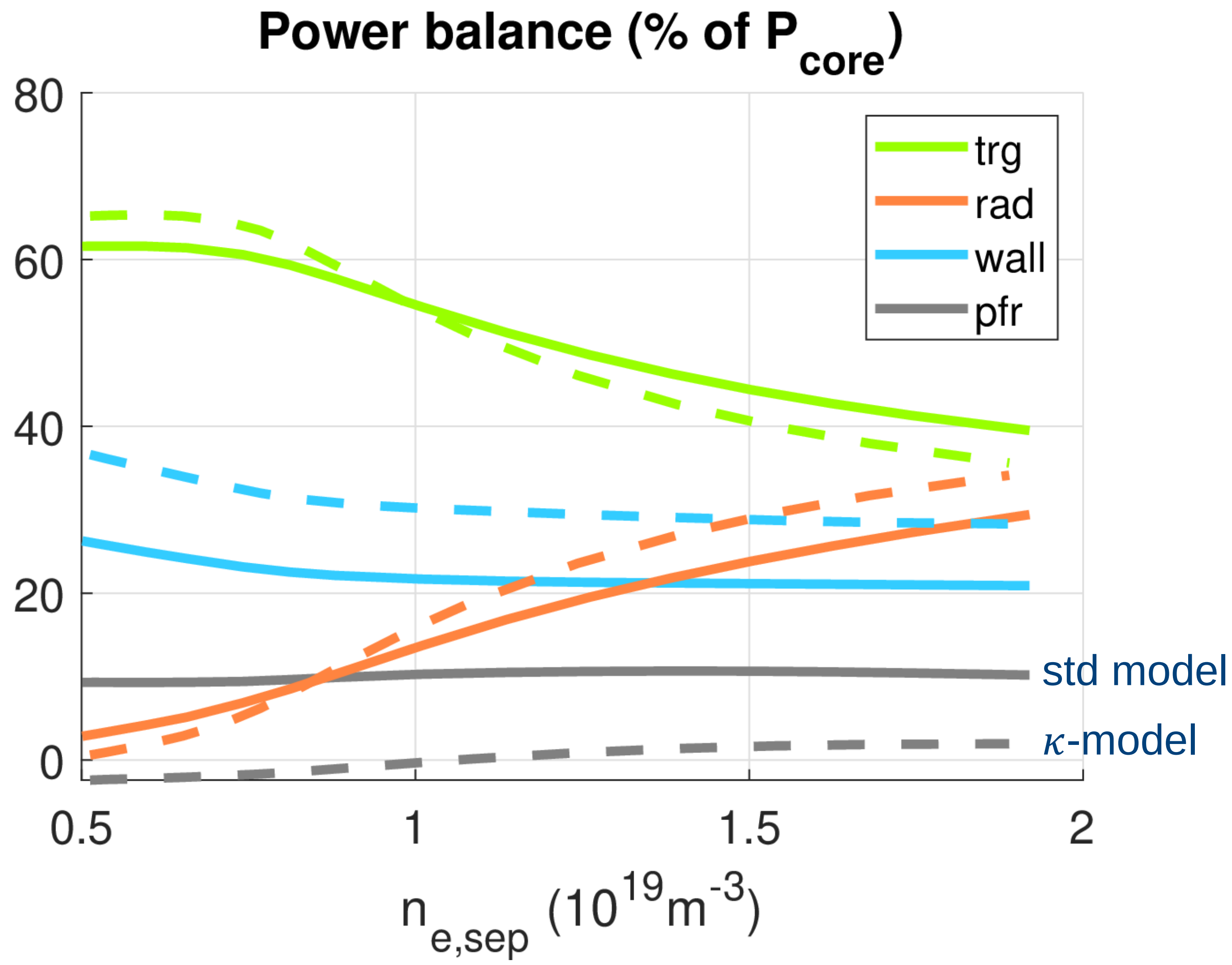
→ somewhat larger total particle flux at outer divertor entrance







Trying to understand the differences…



- radiation increases & power to target decreases
- Power to north wall and PFR roughly constant

However, the κ-model shows

- Slightly smaller power to targets
- Slightly larger radiation
- Near zero power to PFR due to zero-gradient BC there, this power difference seems to be directed to north wall

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Conclusions and next steps

First application of model calibration framework in SOLPS-ITER on TCV-X21

1. How does κ-model compare to standard models? → Very similar results
2. Is the κ-model better at *predictions*? → Not better, not worse (so far)

Planned next steps:

- Finish up last optimizations with radial profiles of diffusion coefficients
- Predictions: use higher density TCV-X21 data (waiting for Diego's paper…) to validate and better understand density scan results
- Kinetic cases with Carbon sputtering included

Future steps (not planned by Stefano)

- Bayesian estimation: can **tell if model 1 is actually better than 2** and get **uncertainty estimates on the calibrated parameters**