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Neutral-neutral interaction models in Eirene (for JET high-density regimes)

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Motivation and contents

Motivation:

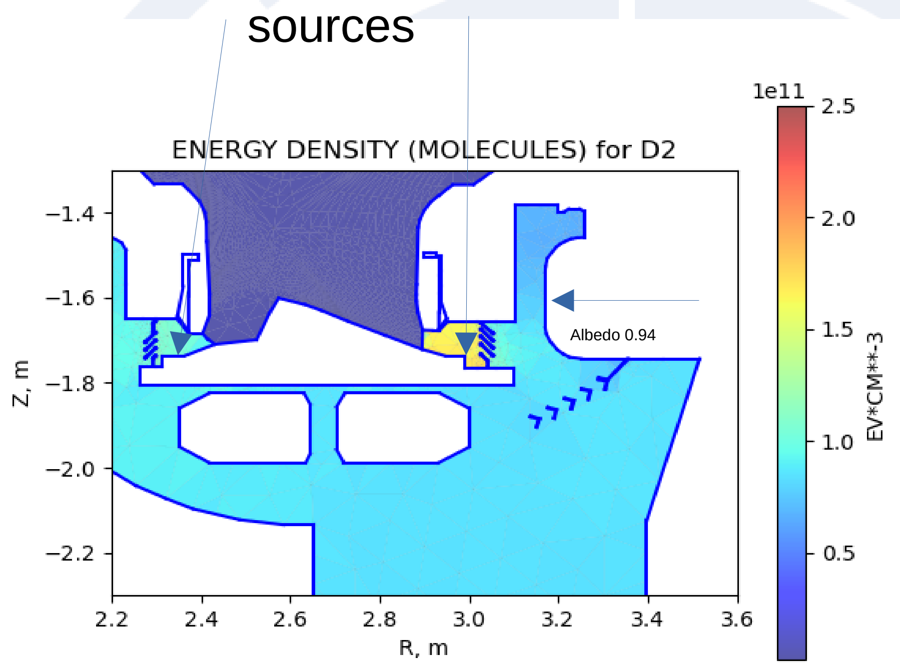
- **Validating the EIRENE simulations in high density JET cases (against experimental measurements). Characterizing the gas flow through the sub-divertor to the pump → determine the effective pumping efficiency of the JET vacuum vessel.**
- **Understanding isotope effect (H2, D2 and T2)**
- **Assessing the assumption of a pump surface at the inlet in SOLPS-ITER runs to avoid having to run with the sub-divertor included.**

Contents:

- **Simulation set up: inputs, simulation geometry etc.**
- **Testing the importance of N-N effects**
- **Testing the effects of secondary louvres**
- **(Recap of) isotope studies (just linear runs so far)**
- **Neutral-neutral collision models**

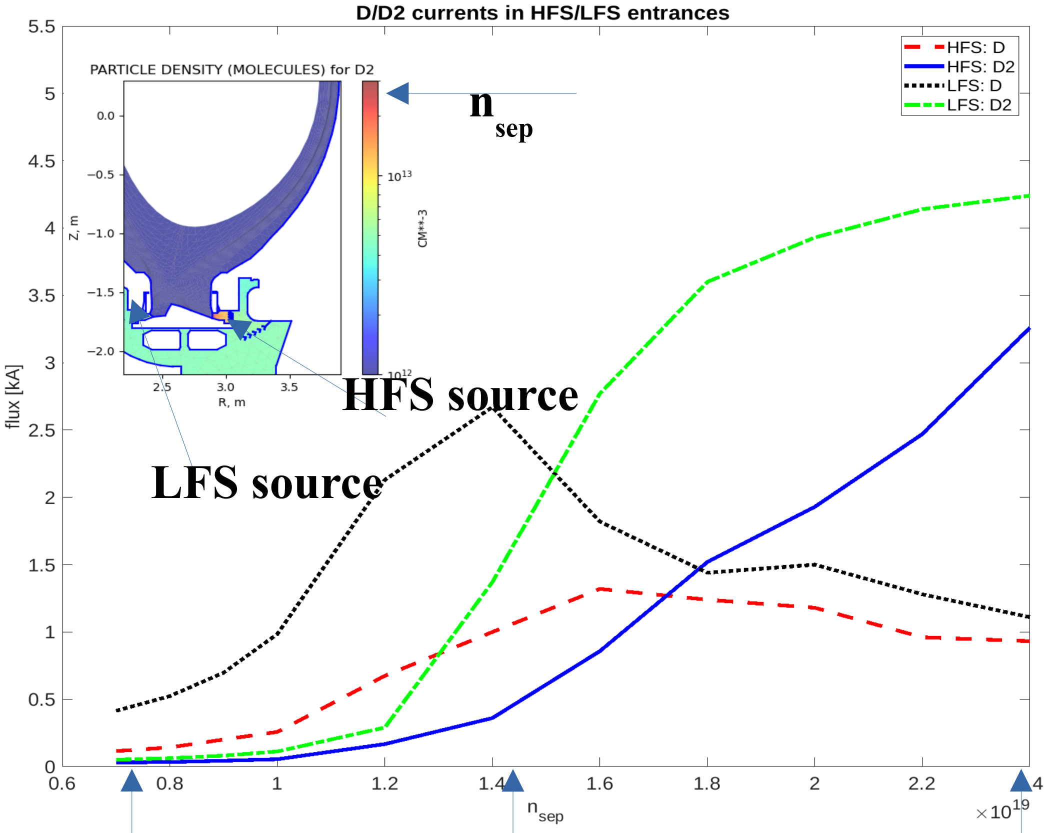
EIRENE is used to characterize the gas flow through the JET sub-divertor to the pump.

- Knudsen numbers vary between molecular flow regime transitional regime → need for N-N effects tested
- Divertor blocked (reflective surface) for simplification
- Both primary and secondary louvres are taken into acco
- Sources scanned, sinks are fixed:
  - Source: flux of molecules from divertor to sub-divert
  - Sinks: fixed sticking probabilities in pumps



T_{wall}=1160K (≈ 0.1eV, DivGeo default) in pumps, T_{wall}=300K in other components (in Varoutis 2017, surface of chevron = pumping surface at T=80K. However, impact of temperature of the pump was tested to be small)

Deuterium molecular and atomic currents from SOLPS-ITER simulations (N. Horsten et al., NME 2024) have been used as an input for sub-divertor only EIRENE simulations



n_{sep}

HFS source

LFS source

n_e at midplane of the core separatrix

Low density input fluxes taken from here

Intermediate density input fluxes taken from here

High density input fluxes taken from here

- Fluxes to the albedo pump surfaces at the subdivertor entrances evaluated with SOLPS-ITER → input to EIRENE

case	HFS current	LFS current
Low-n (free molecular flow regime)	89 A	259 A
Mid-n	861 A	2.7 kA
High-n (Kn=4 → transitional regime)	3.72 kA	4.79 kA
Ultrahigh-n	3 x high-n	3 x high-n

(Here, currents are $D2eq=0.5*D_{current} + D2_{current}$)

Knudsen below Kn<10 for highest input fluxes

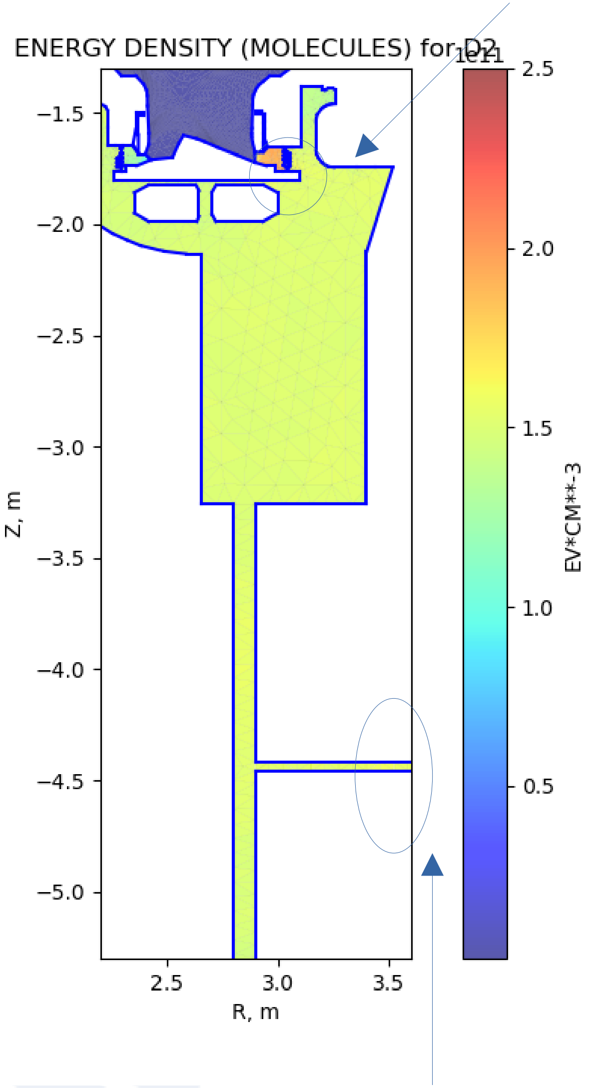
- Using estimate $Kn = 1/(\sqrt{2}\,\sigma_{el} n_N L)$ with $\sqrt{2}\,\sigma_{el} = 2\times10^{-15}\ \text{cm}^2$ Here, L=4cm for baratron and L=1cm distance between primary louvres or L=10cm distances downstream of primary louvres.

- Densities down stream from primary louvres give Knudsen numbers 1.5-83, L=10 cm:

- High density cases ($Kn \leq 4.1$) → neutral-neutral interactions required

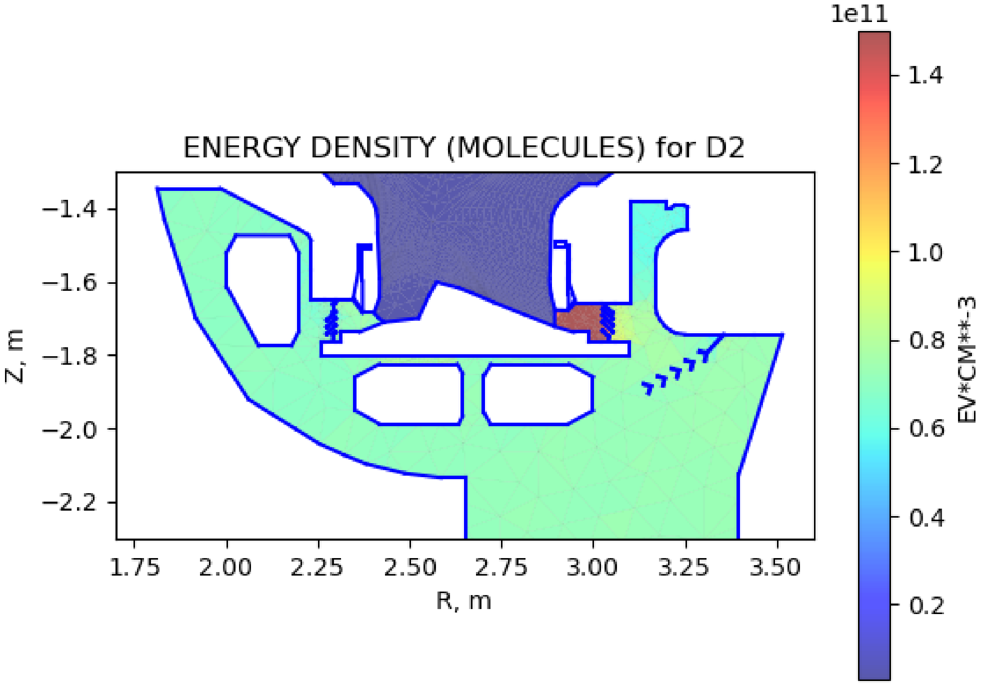
case	Neutral density	Knudsen number
Low-n	6e11 cm^{-3}	83
Mid-n	6e12 cm^{-3}	8.3
High-n	1.2e13 cm^{-3}	4.1
Ultrahigh-n	3.2e13 cm^{-3}	1.5

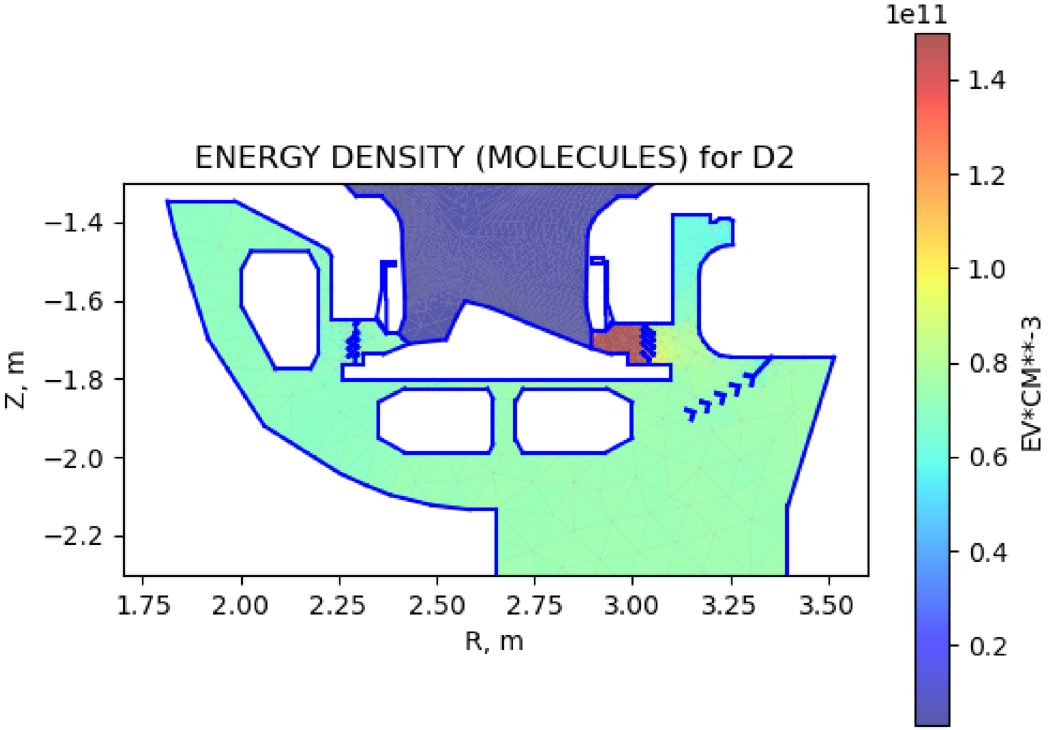
Louvres



Baratron location

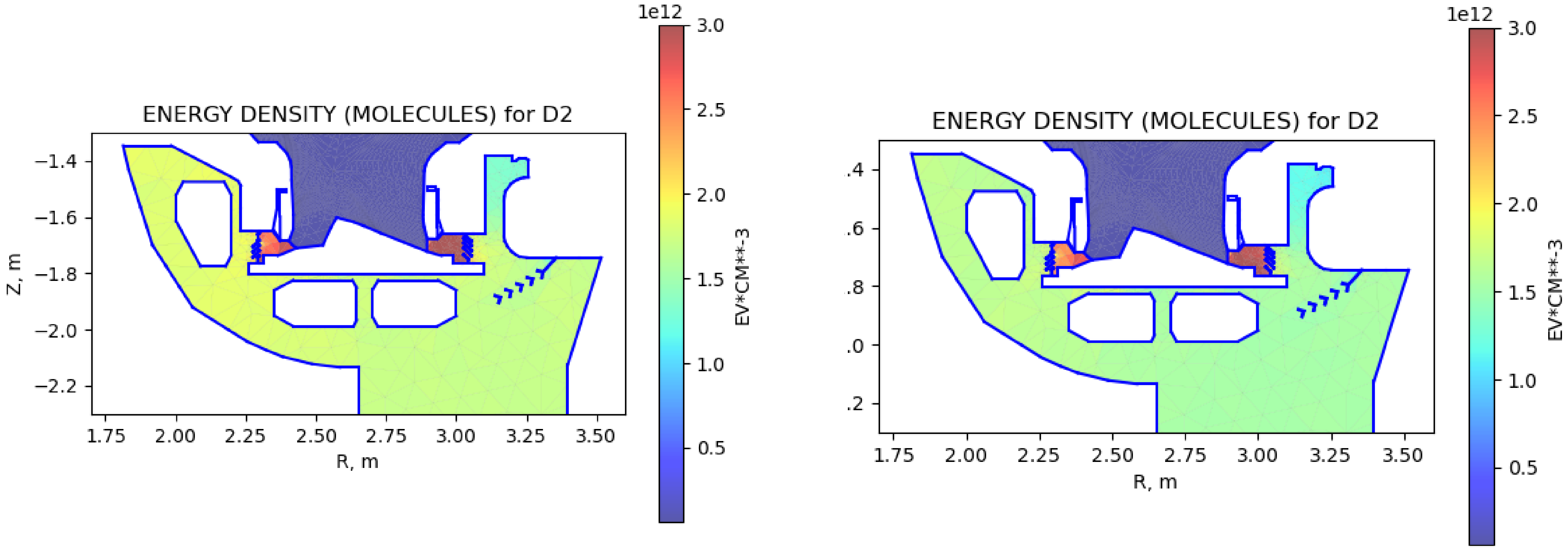
Non-linear effects (NN=1 vs NN=10 iterations) are negligible in the low density case (Kn≈80)





- Here, pumped flux in cryo pump is 21.1A (NN=1) vs. 21.7A (NN=10)
- D2 pressure downstream from primary louvre: ~12.8mPa
- The pressure at the KT5P pressure gauge however changes: 12.6 (NN=1) vs. 10.2 mPa (NN=10)

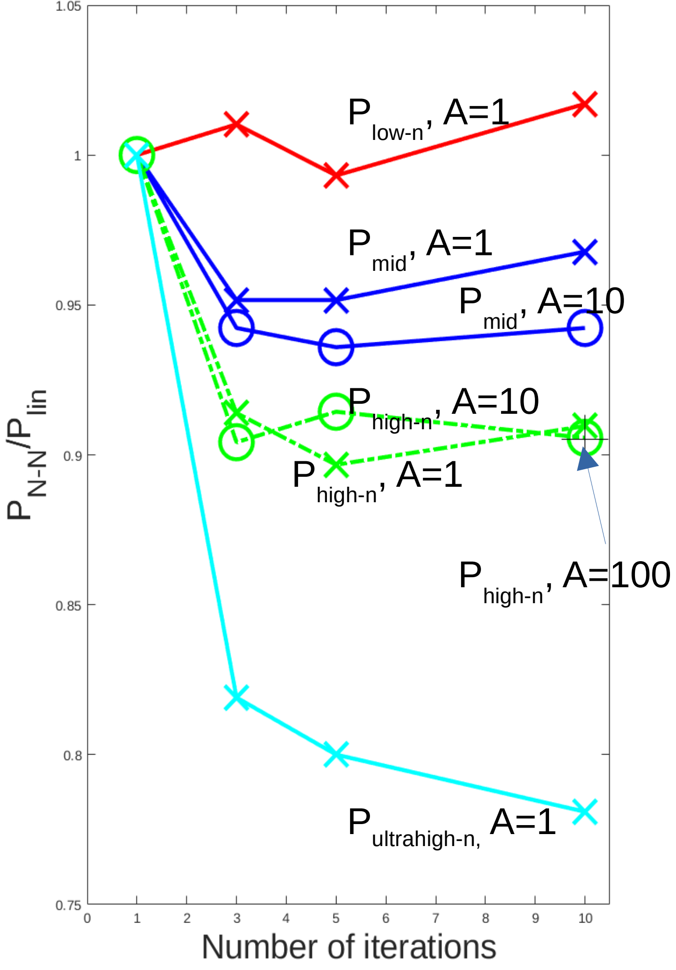
Non-linear effects (NN=1 vs NN=10 iterations) are important in the high density case (Kn≈4)



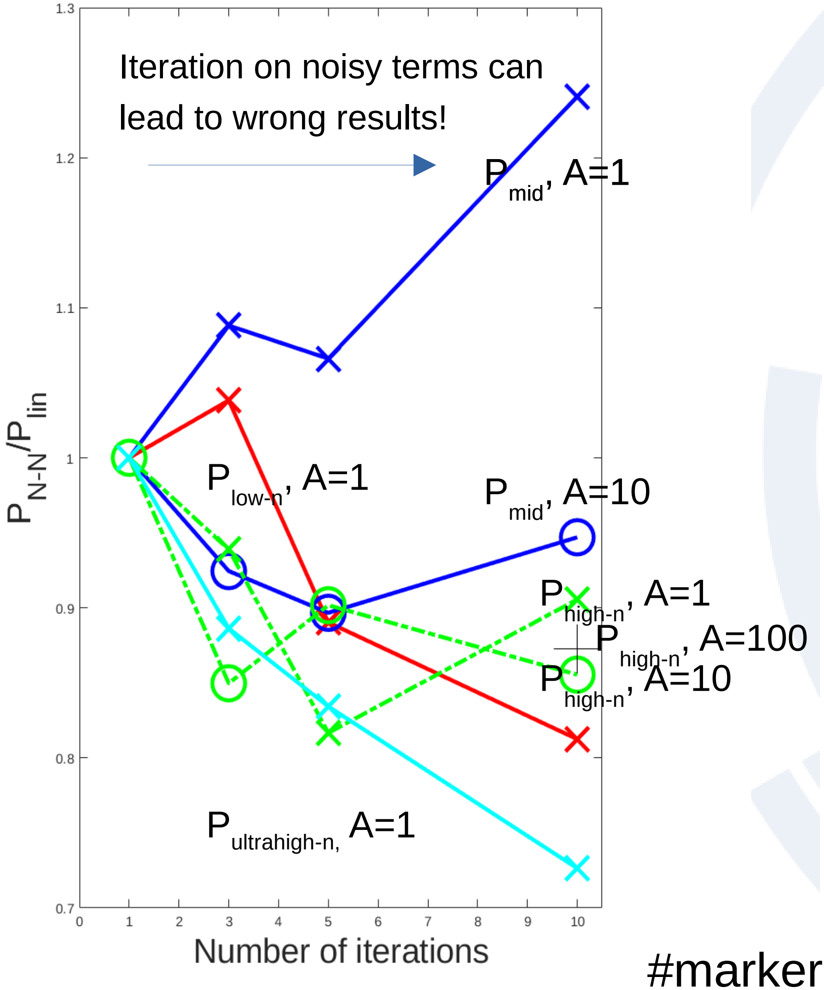
- **Here, pumped flux in cryo pump is 474A (NN=1) vs. 424A (NN=10)**
- **D2 pressure downstream from primary louvre: 272mPa vs 248mPa**
- **The pressure at the KT5P pressure gauge however changes: 288 (NN=1) vs. 261 mPa (NN=10)**

Non-linear effects are important in the high-n cases (Kn≈1-4), Results converge after NN≈5 iterations. Higher number of markers needed for local pressure values at baratron

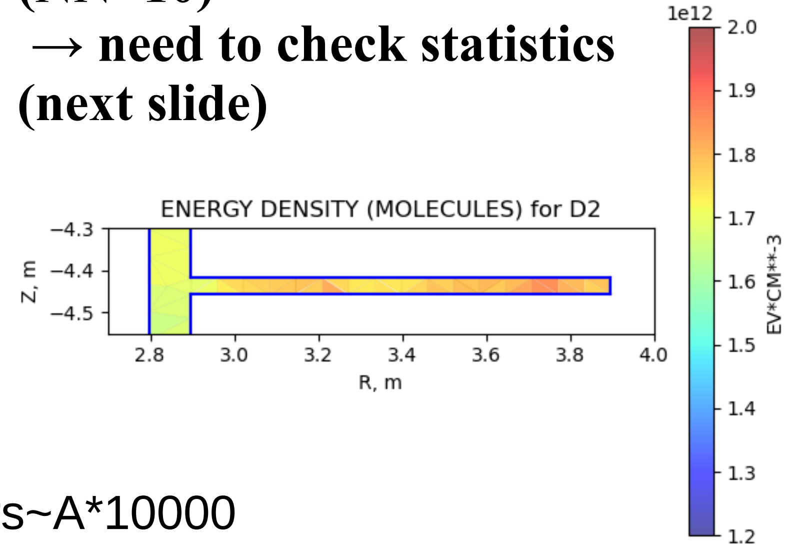
Averaged subdivertor pressure



Pressure in front of baratron


Iteration on noisy terms can lead to wrong results!

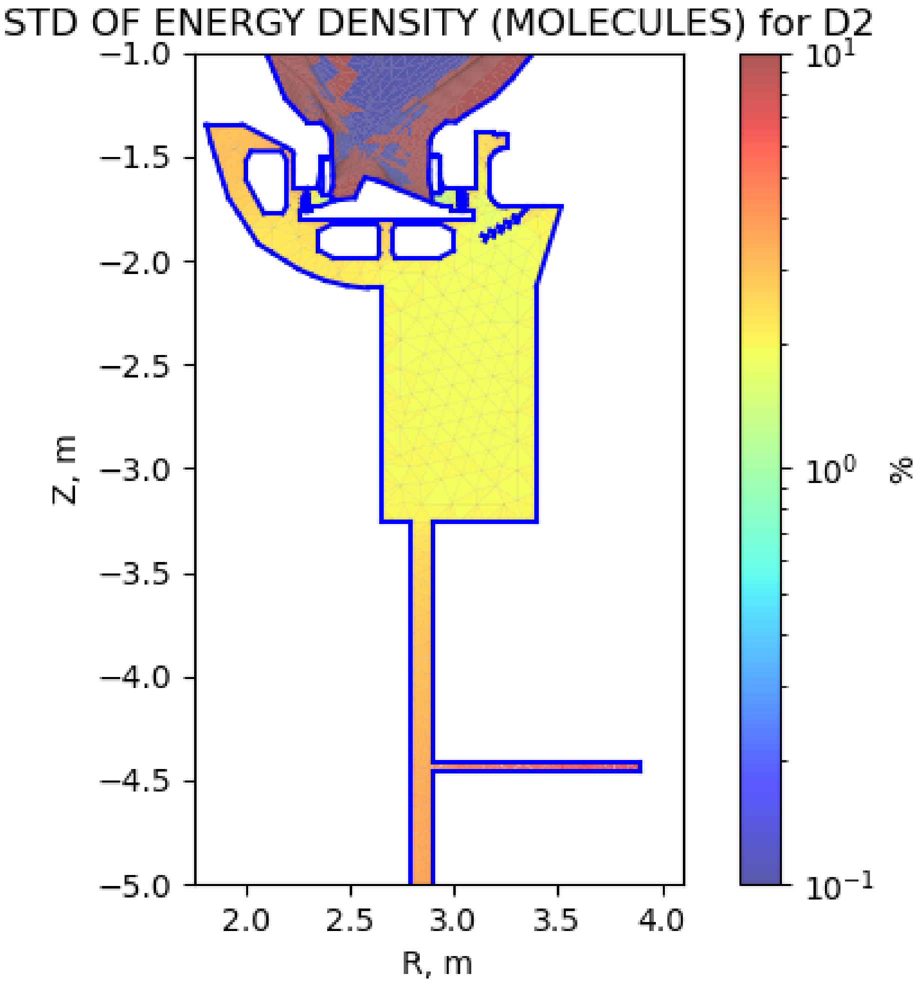
- While averaged pressures show low statistical variance, pressure in front of baratron (average over five closest points) varies more:
288 (NN=1), 271 (NN=3), 236 (NN=5) and 261 mPa (NN=10)
→ need to check statistics (next slide)



#markers~A*10000

Standard deviation shows higher noise level near baratron due to smaller grid size and lower density

AMPTS=1



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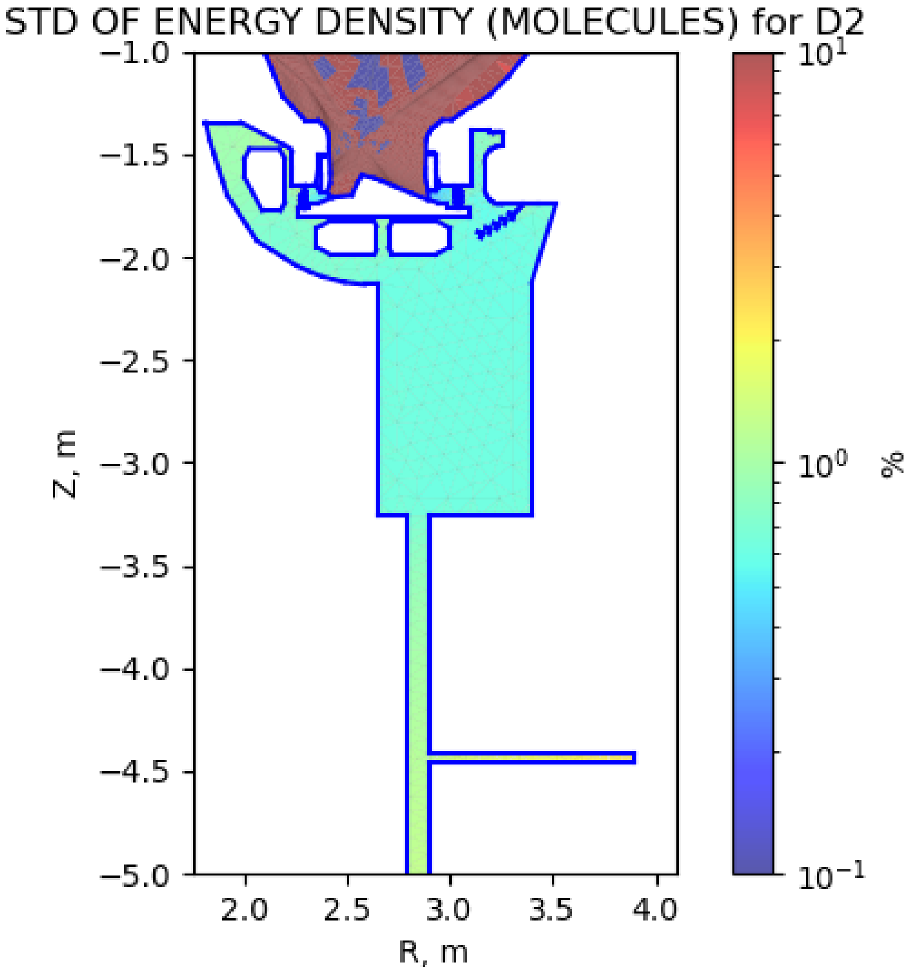
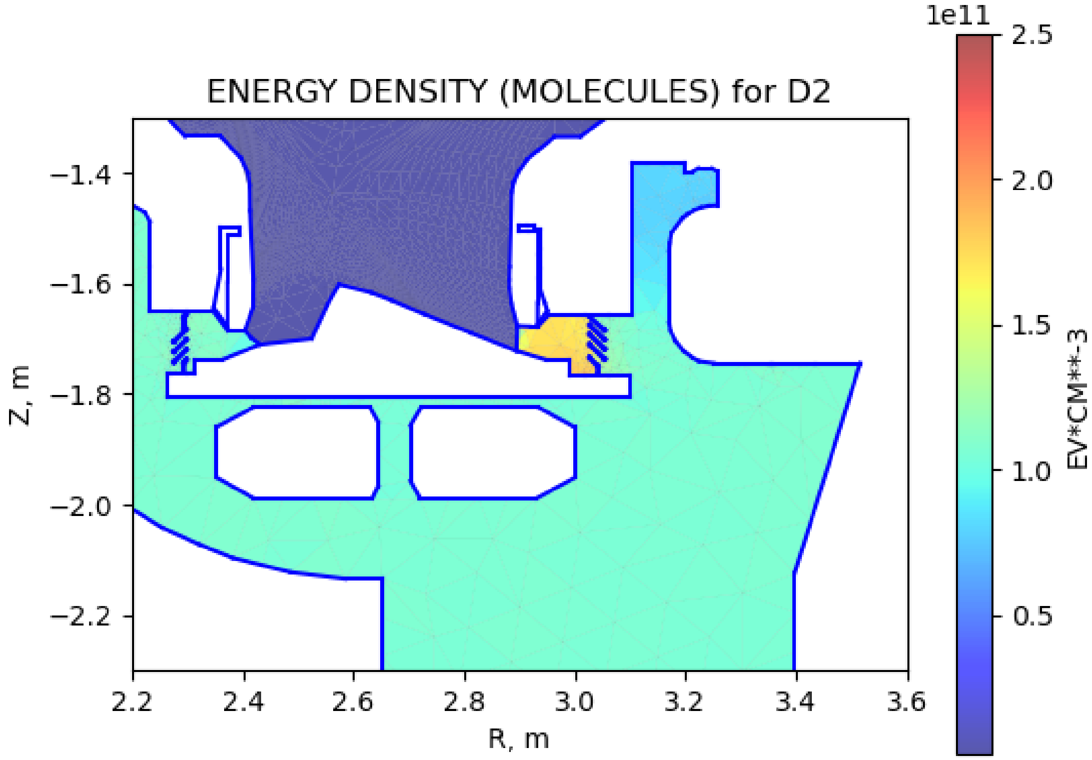
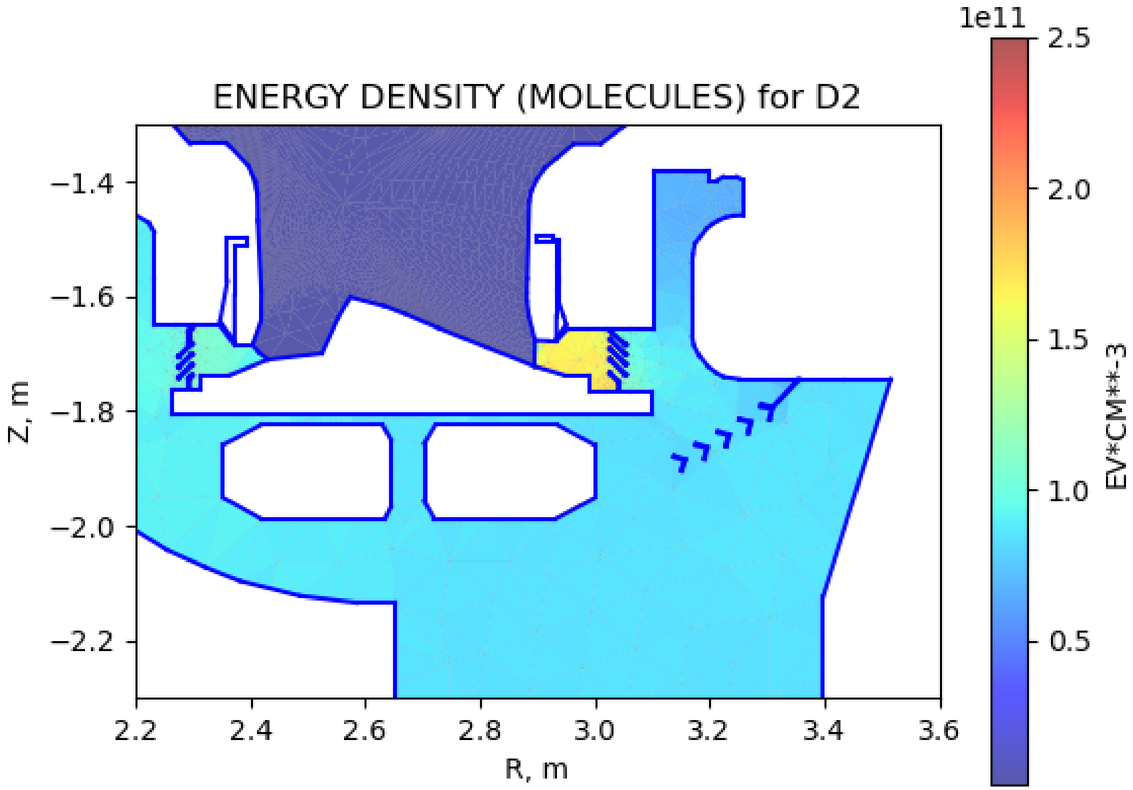


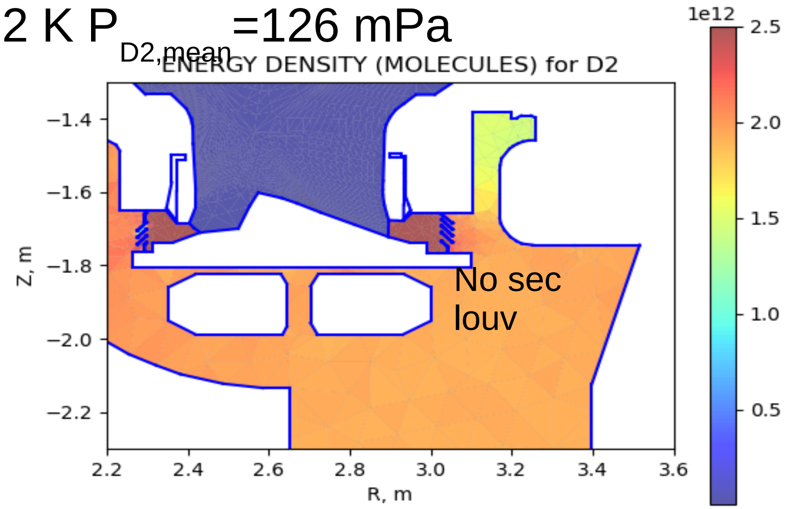
Secondary louvres reduce overall pressure level by ~15% while primary louvres causes strong local gradient in pressure (~$p_{downstream}/p_{upstream}$ ~ 0.6-0.7)



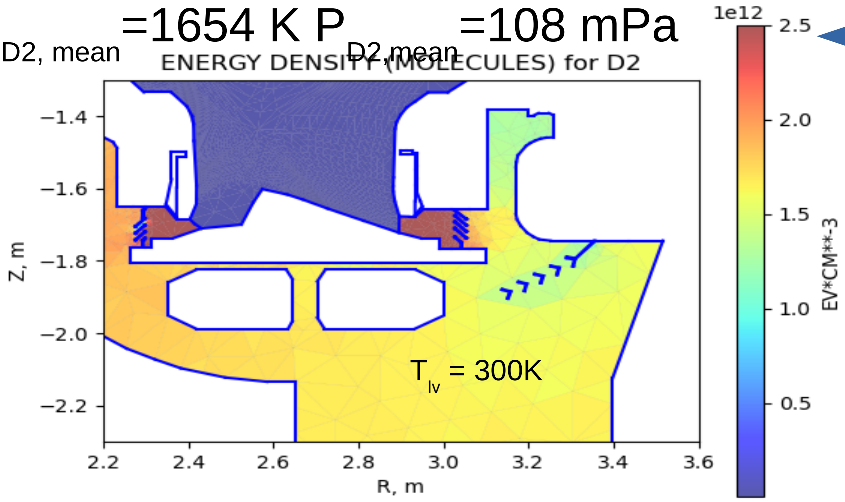


T_{louvre} scan: Effect of secondary louvres on $T_{D2, mean}$ is very small for realistic cases

$T_{D2, mean}$ = 1732 K $P_{D2,mean}$ =126 mPa

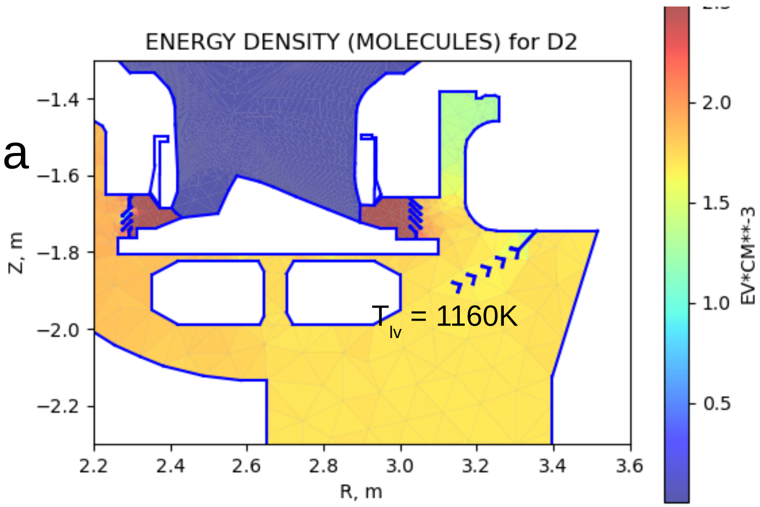


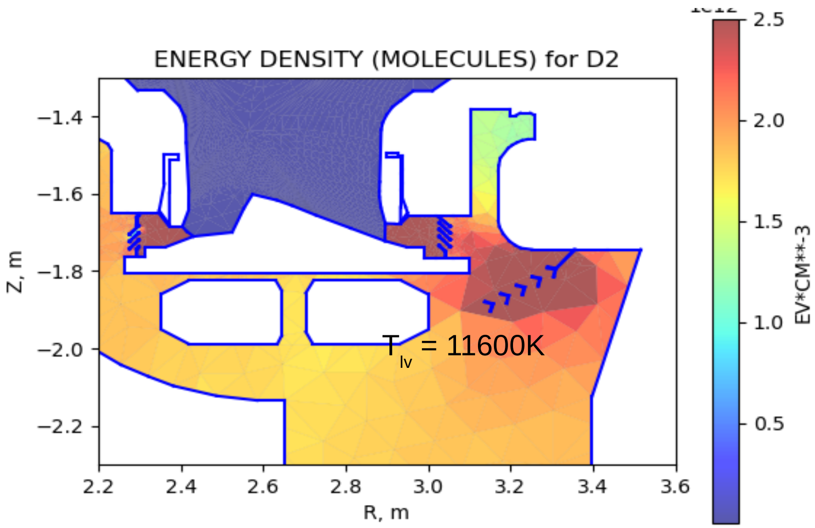
$T_{D2, mean}$ =1654 K $P_{D2,mean}$ =108 mPa



0.4Pa

$T_{D2, mean}$ =1731 K
$P_{D2,mean}$ =112 mPa

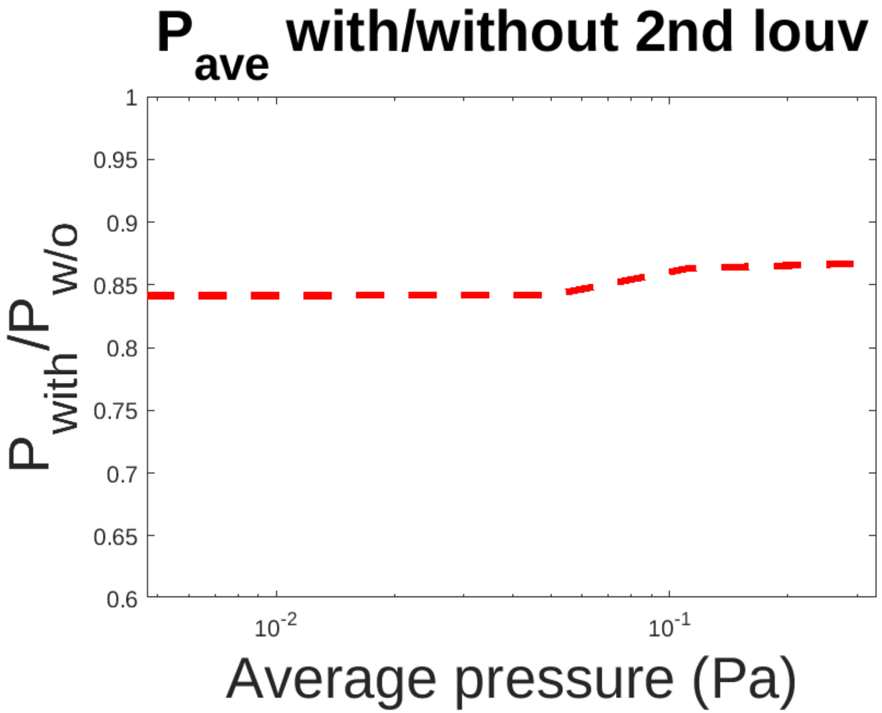


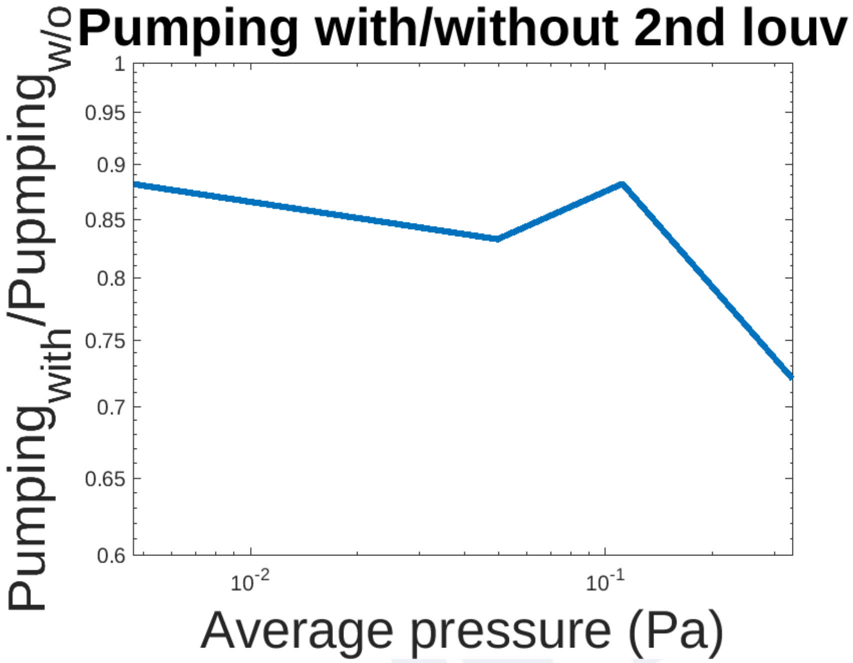


$T_{D2, mean}$ =1899 K
$P_{D2,mean}$ =119 mPa
(strong increase of temperature around louvre increases average gas temperature)

Scan is for high density case parameters

Secondary louvre drops the average pressure and pumping rate ~15% in all cases

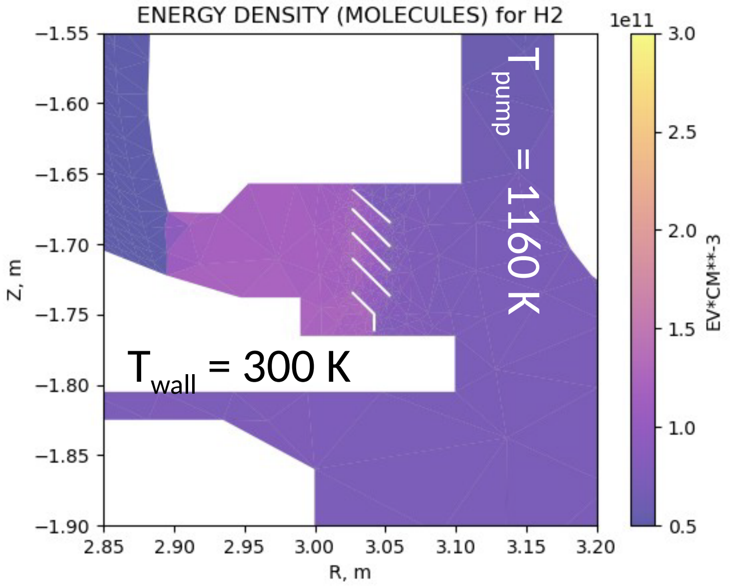

P_{ave} with/without 2nd louv

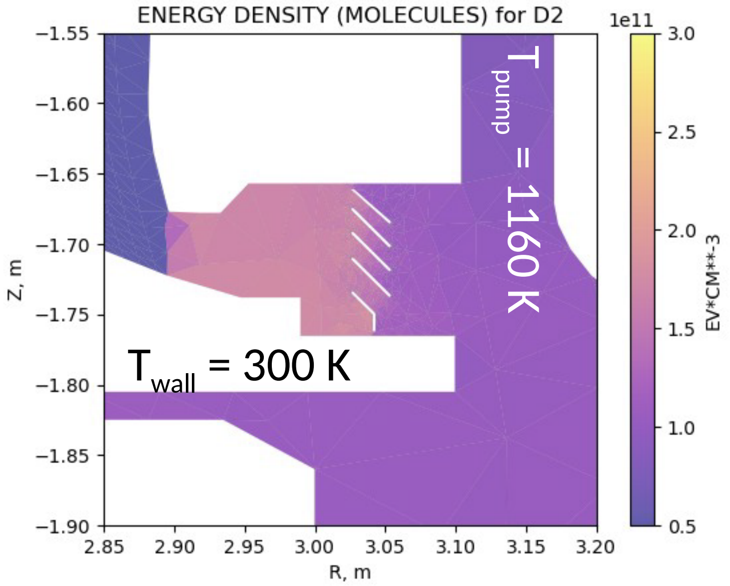

Pumping with/without 2nd louv

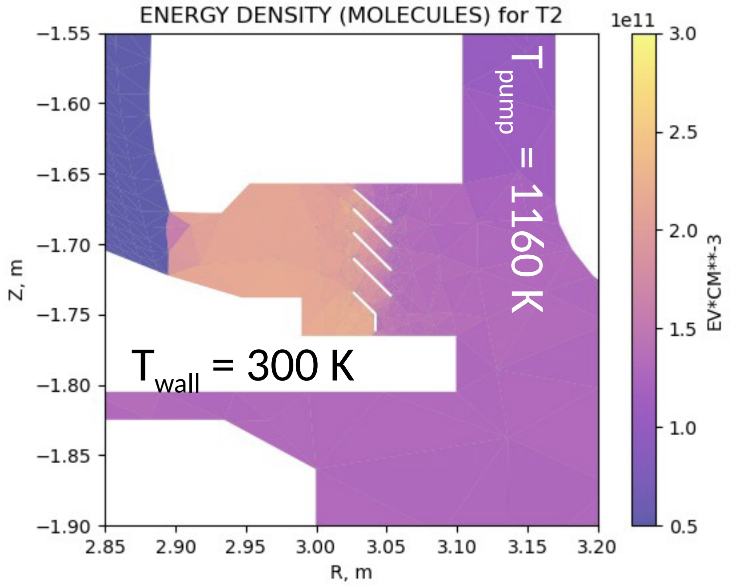
(with / w/o 2nd louvre)	low-n	mid-n	high-n	Ultra high-n
P_{ave} (mPa)	4.6/5.7	46.8/55.6	101/117	272/314
Pumped fluxes	21.6/24.5	214/257	471 /543	1160 /1610

- Note: S.Wiesen (EPS 2019 invited) showed much stronger pressures drop (~factor 3) when adding secondary louvre. There, P_{sub}=0.3 (with) and 3.8 Pa (w/o 2nd louvre, measured 0.25Pa), here 0.17 (with) and 0.2 Pa (w/o).

Raising isotope mass $H_2 \rightarrow D_2 \rightarrow T_2$ reduces thermal velocity, thus molecular pressure by factor square root of mass







- Here, same source strengths 89 A (HFS) and 259 A (LFS) are used in all cases (test is here for free-molecular flow regime)

Conductance depends inversely on the square root of isotope mass (free molecular flow regime)

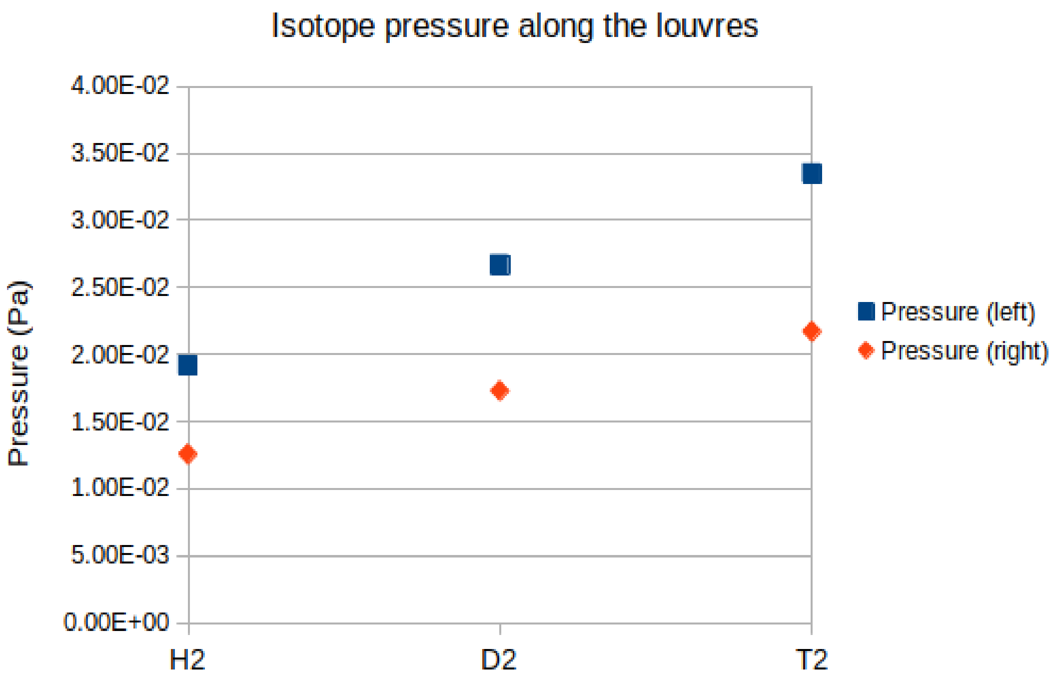
- **For fixed sources and sinks heavier isotopes just complete their trajectories factor √A slower accumulating more density → For apertures or structures like louvres this leads to lower conductance**

$$C = \alpha\sqrt{\frac{RT}{2\pi M}}A \;\sim\; \sqrt{T/M}$$

- **Lower mobility leads to higher pressures and densities**
- **Since density in linear simulation is directly proportional to source strength S it can be expressed as:**

$$n_s(x,y,z) = S*n_H(x,y,z)\sqrt{M} \quad \text{(+ effect of sink)}$$

- **Non-linear isotope effect (high-n regime) not yet tested**



Neutral-neutral models for accurate simulation of Kn<10 regime in Eirene (1/4)

- Four past/present/future options for neutral-neutral interactions in Eirene:

  a) “Bird’s DMCS" procedure which (according to Eirene manual is currently not in use)
  b) BGK approximation by using the iteration (routinely in use)
  c) BGKES (explained later)
  d) alternative(s) to BGKES

a) DSMC (Direct simulation Monte Carlo):

- Model documented in PhD thesis by T. Behringer → collision model not currently in but time-dependent option from that work is still in use in Eirene
- DSMC used e.g. in DIVGAS → simulation domain divided into network of cells → particles in each cell paired randomly → each pair of particles allowed to change momentum and energy with each other according to conservation laws and collisional cross-sections
- Model is conceptually easy to understand but requires much more CPU power and is not as straightforward to parallelize compared to iterative schemes (or linear simulations…)
- Self-consistent overall solution of combined multi species plasma and gas flows evolving together can be challenging with DSMC (compared to BGK)

Neutral-neutral models for accurate simulation of Kn<10 regime in Eirene (2/4)

b) Many variants of BGK model proposed to give correct Navier-Stokes heat conduction.
(some) basic requirements:
- **a) give non negative distributions (sanity check)**
- **b) predict Prandtl number less than one**
- **c) verify the fundamental H-theorem**

- **Here, H-theorem states that for any distribution function f(r,v,t) that evolves according to Boltzmann equation the time derivative of:**

$$\mathcal{H} = \int_D H(f(\mathbf{r},\mathbf{v},t))\mathrm{d}\mathbf{r} \quad \text{with} \quad H(f(\mathbf{r},\mathbf{v},t)) = \int_{R^3} f(\mathbf{r},\mathbf{v},t)\ln f(\mathbf{r},\mathbf{v},t)\mathrm{d}\mathbf{v}$$

is < 0 (nonporous, nonconducting wall around D).

- **In BGK model H-theorem holds, f relaxes towards Maxwellian**
- **Condition b is violated → Prandtl number corrected either with:**
  - **- relaxing to modified Maxwellian → an ellipsoidal BGK approximation (BGKES) as developed in [L.Holway, Phys. Fluids, 9, 1966.].**
  - **- with velocity dependent rate coefficients**

Neutral-neutral models for accurate simulation of Kn<10 regime in Eirene (3/4)

c) Ellipsoidal BGKES model:

- **Main advantage: includes a free parameter for adjusting a correct Prandtl number (Pr)   [Pr = momentum diffusivity / thermal diffusivity, for gases typically Pr≈1]**
- **While BGK model tries to return local drifting Maxwellian, in BGKES model additional information is of second order moments is included in this distribution**
- **BGKES model tested in EIRENE in MSc thesis (M. Simon, 2011) → The resulting conductances showed no difference to the current model, but the temperature profiles were claimed to be more realistic**
- **Code available in appendix of M.Simon’s thesis and could be adapted to present code version but alternative options to account for getting correct Prandtl number are also considered**

Neutral-neutral models for accurate simulation of Kn<10 regime in Eirene (4/4)

	Present model	Possible new model
	T_n, n_n and v_{drift} sampled in each cell	T_n, n_n sampled in each cell
Particle parameters changed based on:	Only cell background has effect on rate of parameter change: $v_{new}=v_{old}*R(T_n, n_n\ v_{drift})$.	Also, particles own velocity v_{old} has effect on rate of parameter change: $v_{new}=v_{old}*R(T_n, n_n, v_{old})$
R values	R=a*exp(bT) → 1D table for a and fixed value for b. Density n_n just scaling factor	2D polynomial fit for R on background T and particle v (as explained in Janev, Langer, Post book)
R(v,T) in section H.3	Beam-Maxwellian rates are are not used within BGK self collision terms yet	H.3 relaxation rates would be used also in BGK iteration

New model could be tested e.g. in steep temperature gradient conditions. Pure academic interest or real need?

Work plan for 2025: Improved neutral-neutral models with velocity dependent relaxation rates in Eirene

- EIRENE is used to investigate the isotope effect of JET sub-divertor in transitional area (Kn<10)

- Simulations are validated against measured pressure values at baratron

- Testing making primary and secondary louvres orifice-type for interpretative EIRENE simulations (as in work by Scarabosio and Zito for AUG) → artificial conductance adjusted to match the pressure on measurements for different isotopes

- Need for testing/developing improved BGK model(s) in JET sub-divertor is considered

Conclusions

- For fixed sources and sinks, in high Kn molecular regime isotope on densities has only √M-dependence. Possible additional effects may come in low Knudsen number regime or due to isotope effect in sources and sinks to be studied in 2025

- Primary louvre creates strong local gradients while secondary louvre drops the overall pressure level.

- N-N were shown to be off importance for high density cases (Kn<4). For pressure near baratron higher number of test particles is required due to smaller cell size.

- Different collisions models discussed, future work on testing velocity dependent relaxation rates in Eirene proposed