EUROfusion

Deterministic and stochastic modelling of particle exhaust in the sub-divertor region of W7-X

S. Varoutis, C. Tantos, Chr. Day, D. Naujoks, C. P. Dhard and W7-X Team

3rd Fusion HPC Workshop, 15-16 Dec 2022

KIT Karlsruhe Institute of Technology

Wendelstein 7-X

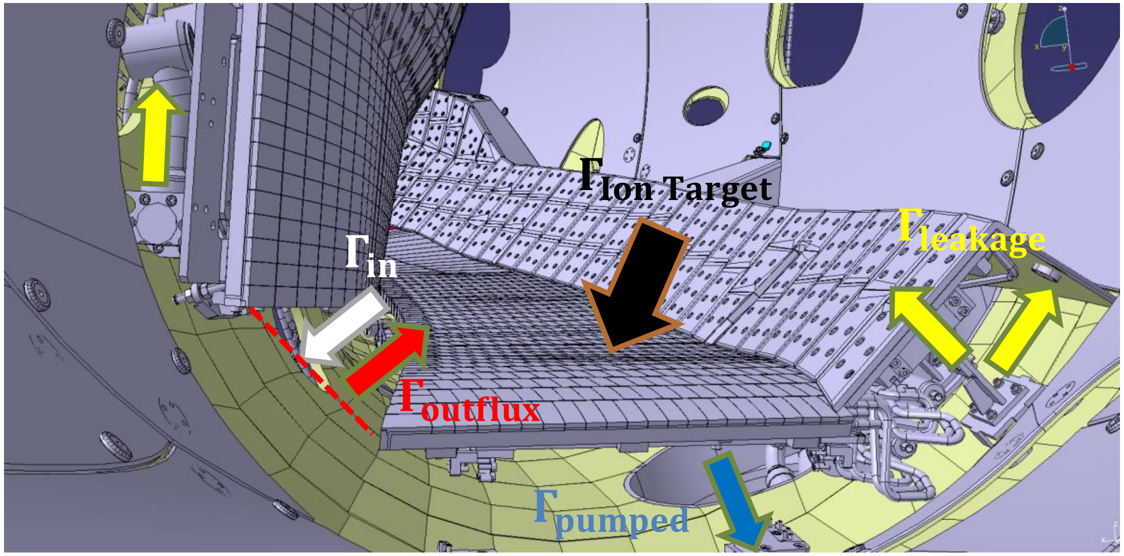
IPP Max-Planck-Institut für Plasmaphysik

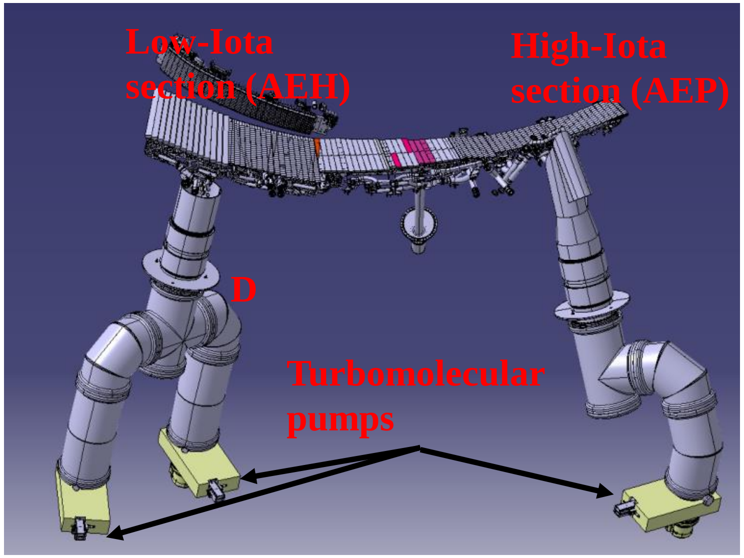
This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Outline

- Particle exhaust of W7-X – Numerical Model of Low-Iota section
- Boltzmann equation and DIVGAS code
- Deterministic (DVM) vs Stochastic (DSMC) DIVGAS solvers
- Numerical results
- Conclusions

Particle exhaust of W7-X



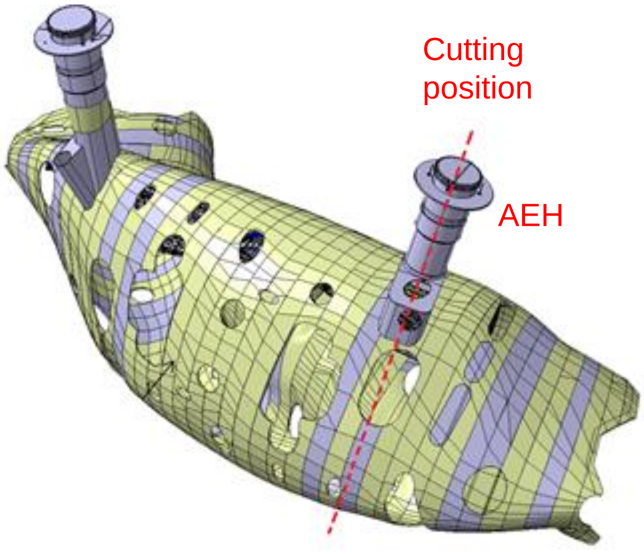


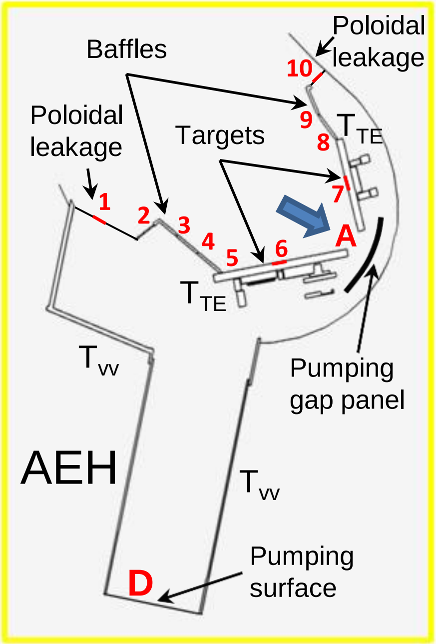
- The main objective of this work is to investigate the dynamics of neutral particles including the effects due to the geometry and the poloidal leakages, located at the divertor targets and baffles, on the achieved pumping efficiency

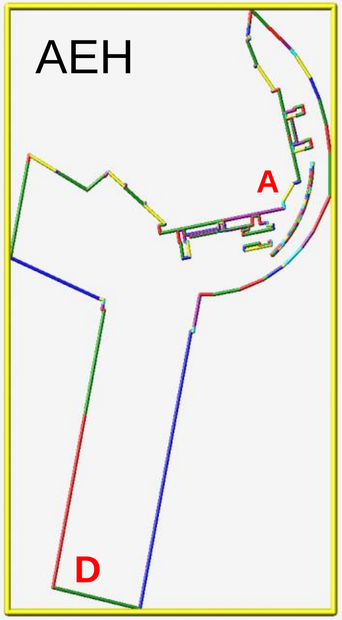
- Gas: H_2, T_{in}=600 K
- $T_{target\ elem.}$= 400 K, T_{vv}=303 K
- Γ_{in} (through pumping gap) = $10^{20} – 10^{22}$ (s^{-1})

- Low-Iota section (2 TMPs): S_{eff}=3.2 m^3/s
- High-Iota section (1 TMP): S_{eff}=1.46 m^3/s

Modelling of Low-Iota section (AEH)







- A 2D representative flow domain has been extracted from corresponding 3D CATIA files. A simplified sub-divertor geometry including internal structures has been considered.
- For the standard configuration, in total 10 poloidal leakages through the targets and baffles, have been identified. Their size ranges between 1-15 mm.
- At the pumping surface D, a capture coefficient ξ is applied. The values of ξ range between 0.1-0.5.

Boltzmann equation

- The fundamental kinetic equation, which describes the flow of a monoatomic gas, assuming **dilute gas**, **molecular chaos** and **binary collisions**, is the **Boltzmann equation**:

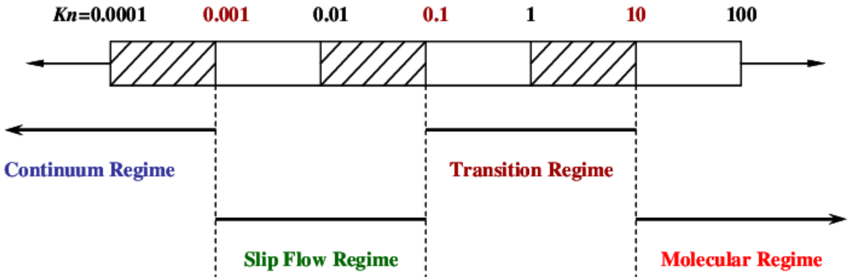
$$\left[\partial_t + \boldsymbol{\xi}\cdot\partial_{\boldsymbol{x}} + \boldsymbol{F}\cdot\partial_{\xi}\right] f\left(\boldsymbol{x},\xi,t\right) = Q\left(f\right)$$

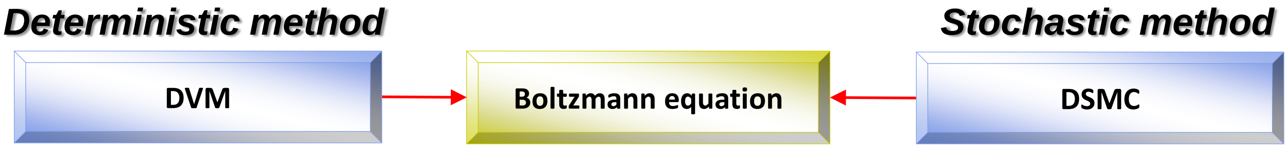
- The left hand side represents the streaming motion of the molecules along the trajectories associated with the force $\boldsymbol{F}$.
- The right hand side represents the effect of intermolecular collisions.
- The collision term $Q(f)$ could be replaced by a kinetic model: **BGK, Shakhov** etc
- **Numerical methods in the whole range of the Knudsen number**

$$Kn = \frac{\lambda}{L}$$

λ: Mean free path

L: Characteristic length (i.e diameter)





DIVertor GAs Simulator

Geometry

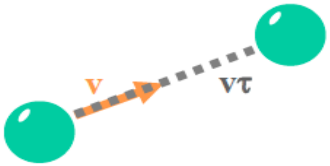
- Extraction of relevant geometry from CAD files
- Definition of interfaces between plasma and neutrals
- Plasma simulations (SOLPS, EDGE2D-EIRENE etc)
- Extraction of boundary conditions (P, T, part. fluxes)

Simulation

- Set-up of the model (2D/3D, single gas, gas mixture)
- Mesh generation
- Pump integration (i.e as a capture coefficient)
- Collisions are included
- Diffuse-specular gas-surface interaction

Post-Processing

- Evaluation of the results
- Comparison with experiments



- DIVGAS is based on the deterministic (Discrete Velocity Method) and stochastic (Direct Simulation Monte Carlo) numerical methods.
- The solution of the Boltzmann equation is reproduced.
- Conservation of momentum and energy.
- Correct estimation of transport coefficients.

DVM vs DSMC

Advantages of DVM

- Free from the statistical noise
- Good convergence rate for the slow flows
- Possibility to use the speci properties of the proble the equations (e.g. solution, lineariz n,…)
- Simple to u eady flows
- Simpl MPI/OpenMP tec l and velocity space

Details about the DVM algorithm will be presented in the following presentation by C. Tantos: *Transient deterministic modeling of neutral gas flow in DEMO particle exhaust system*

Dis s of DVM

- Di to use for the complex geometries
- More complex generalization for the polyatomic gases and gas mixtures

Advantages of DSMC

- Accurate simulation of nonequilibrium gases
- Simple to use for the complex geometries
- Simple generalization for the gas mixture and polyatomic gases
- Framework for detailed physical modelling
- Can be combined with other methods for multi-scale and multi-process systems

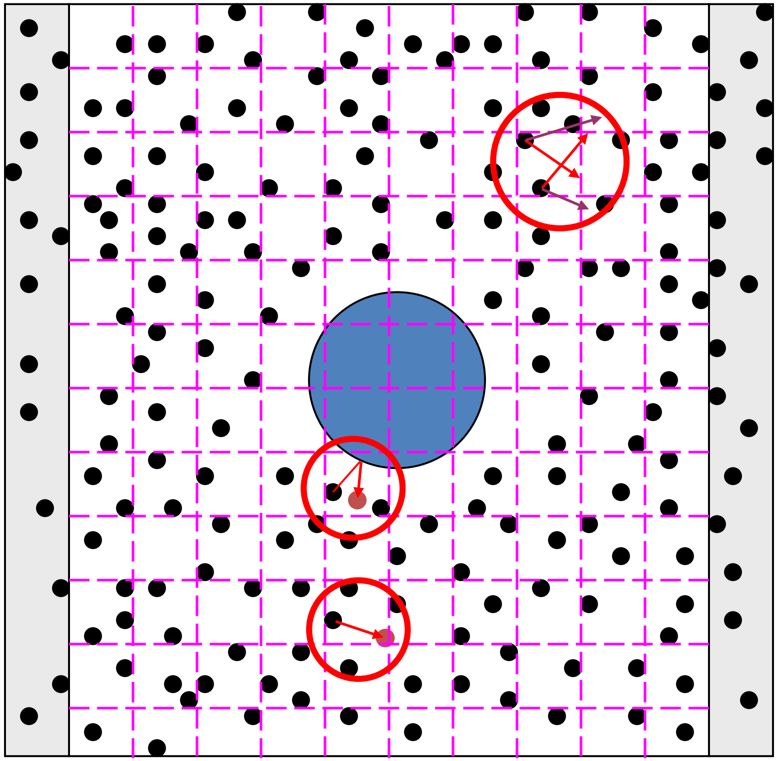
Disadvantages of DSMC

- Statistical scattering (noise)
- Slow convergence rate for the slow flows
- Expensive for the unsteady (time-dependent) flows

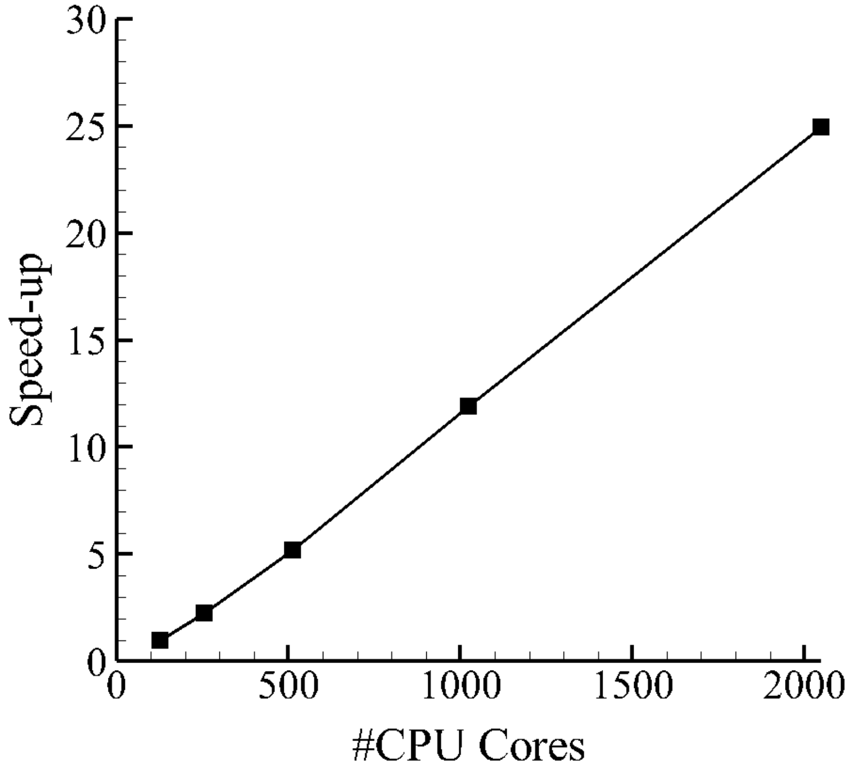
DSMC algorithm

- Initialize system with particles
- Loop over time steps
    - Create particles at open boundaries
    - Move all the particles
    - Process any interactions of particle & boundaries
    - Sort particles into cells
    - Sample statistical values
    - Select and execute random collisions

Example: Flow past a sphere



Speed-up of DIVGAS-DSMC solver



- The DIVGAS stochastic solver is based on the MPI parallelization technique
- Programming language: C++
- The code has been already tested on various HPCs i.e HELIOS, MARCONI, HoreKA, BWUniCluster
- The code performs reasonably well for both increase in load and increase in number of MPI tasks

Pumped flux (DVM vs DSMC)

Numerical Parameter	**DVM**	**DSMC**
Num. of grid cells	$2x10^4$	$2x10^4$
Num. of mol. vel.	28x28=784	-
Number of model part.	-	$8x10^7$
Time step (sec)	10^{-8}	10^{-7}

- The DVM method solves the transient **BGK** kinetic equation, ideal for non-isothermal flows.
- The DVM uses the Velocity Space Decomposition (VSD) technique.
- DVM and DSMC need $5x10^5$ and 10^7 iterations for convergence respectively.

- A very good agreement in the pumped fluxes, between DVM and DSMC is observed.
- The discrepancy between both numerical methods is less than 1% [1].

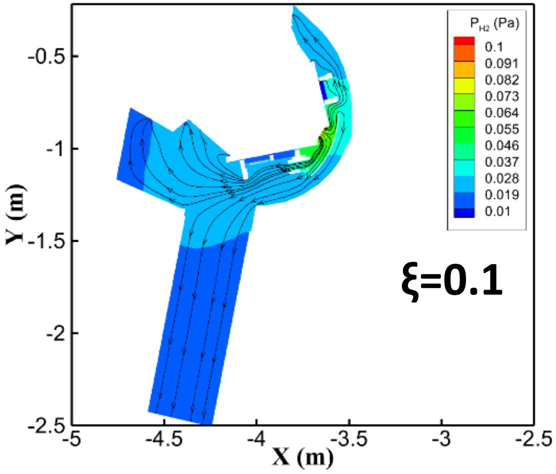
$\Gamma_{in}=10^{21}$ s^{-1}

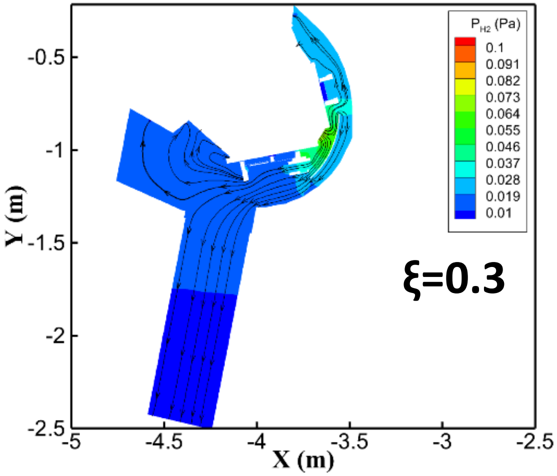
	DVM		**DSMC**	
	Open leakages	**Closed leakages**	**Open leakages**	**Closed leakages**
ξ=0.1	6.70E+19	1.04E+20	6.64E+19	1.03E+20
ξ=0.3	1.03E+20	1.39E+20	1.02E+20	1.38E+20
ξ=0.5	1.15E+20	1.49E+20	1.14E+20	1.48E+20

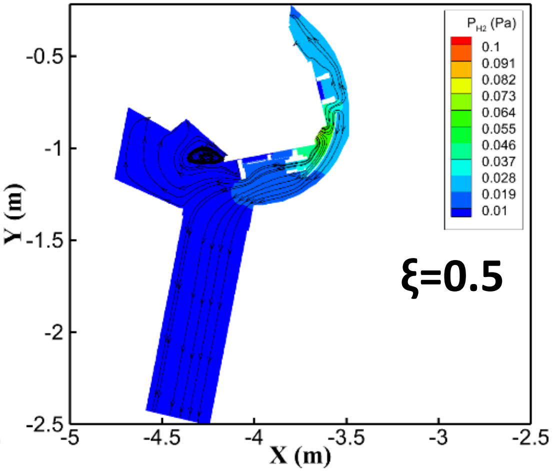
[1] C. Tantos et al., 10.1116/6.0000491.

DVM vs DSMC (pressure contours)

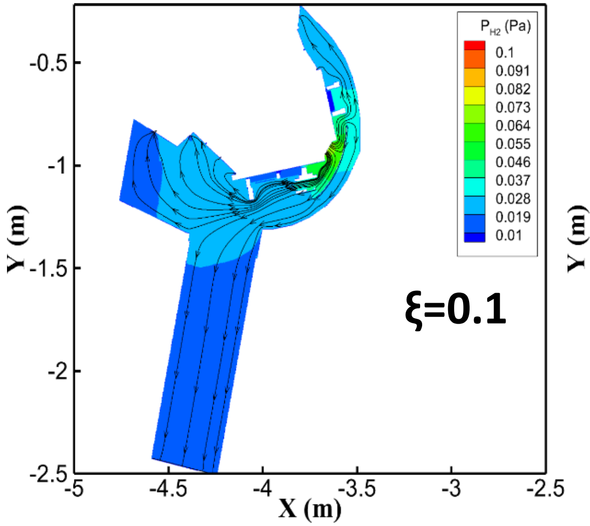
$\Gamma_{in}=10^{21}\ s^{-1}$

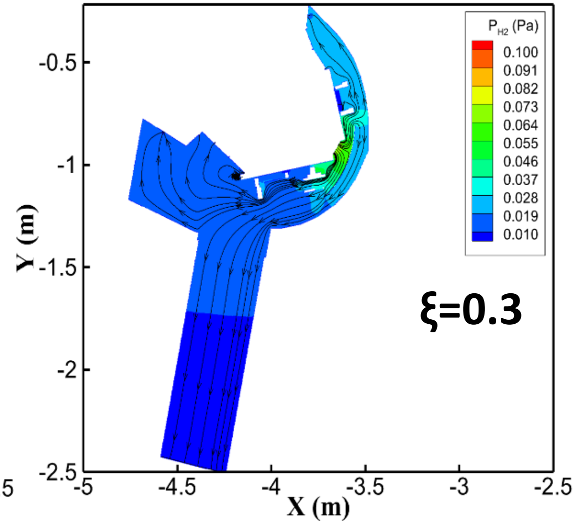


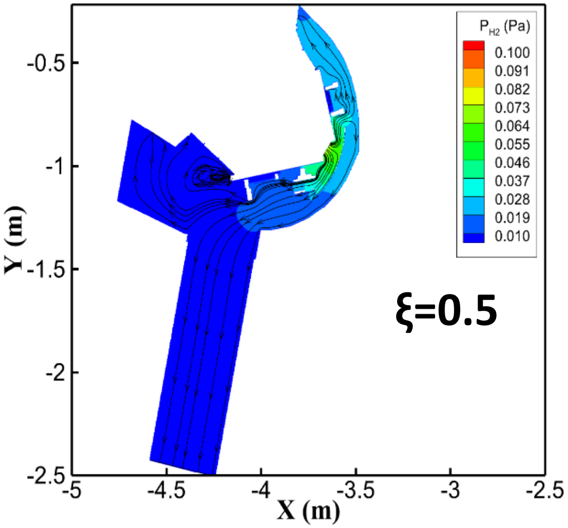




DVM

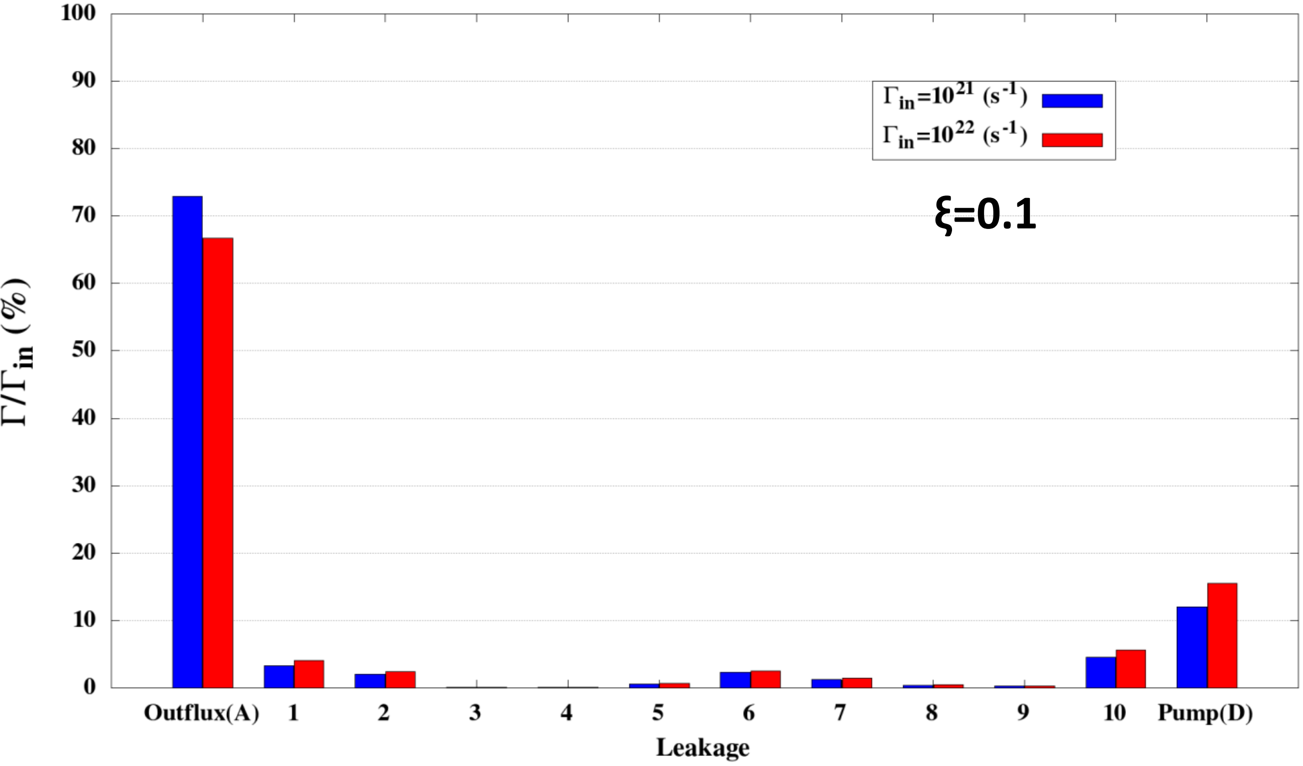


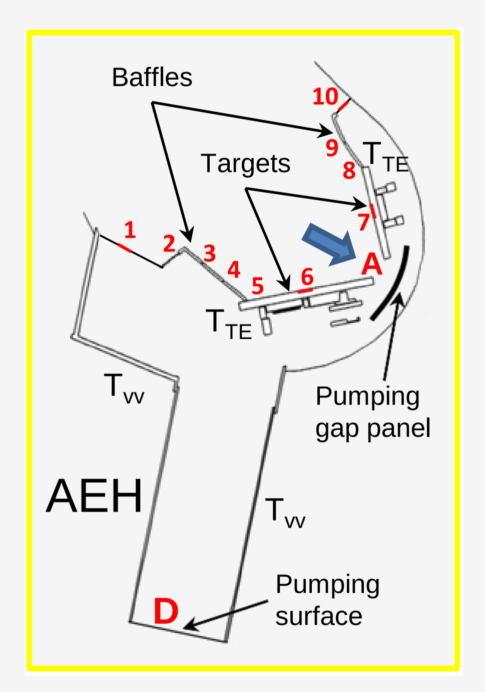




DSMC

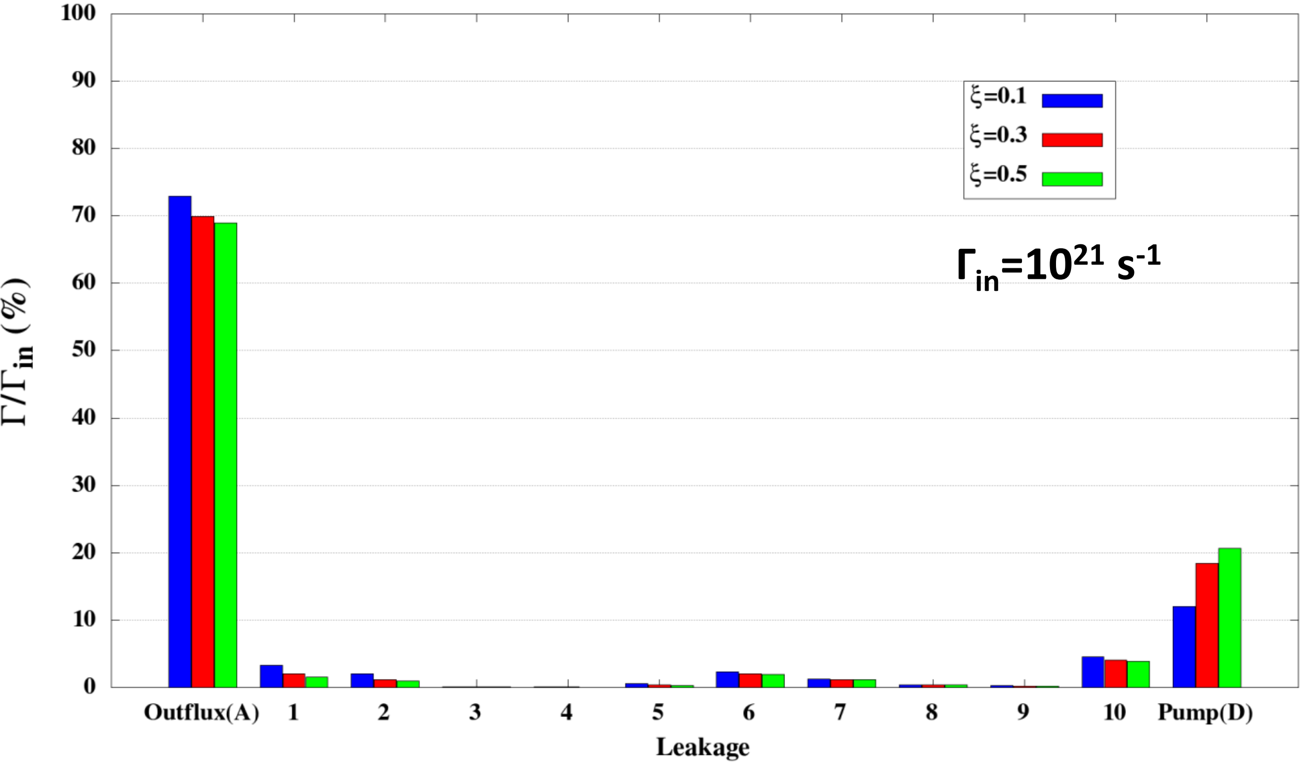
Influence of incoming neutral flux Γ_{in}

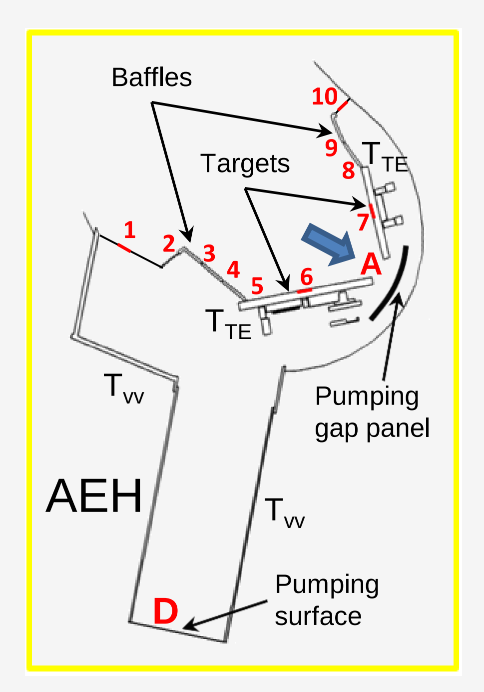




- By increasing the incoming neutral flux Γ_{in} from 10^{21} s^{-1} to 10^{22} s^{-1}, a decrease in the outflux (x1.1) and an increase (x1.3) in the pumped flux is observed.
- The flux through the poloidal leakages #1, #2 and #10 is significant, compaired to the other leakages.

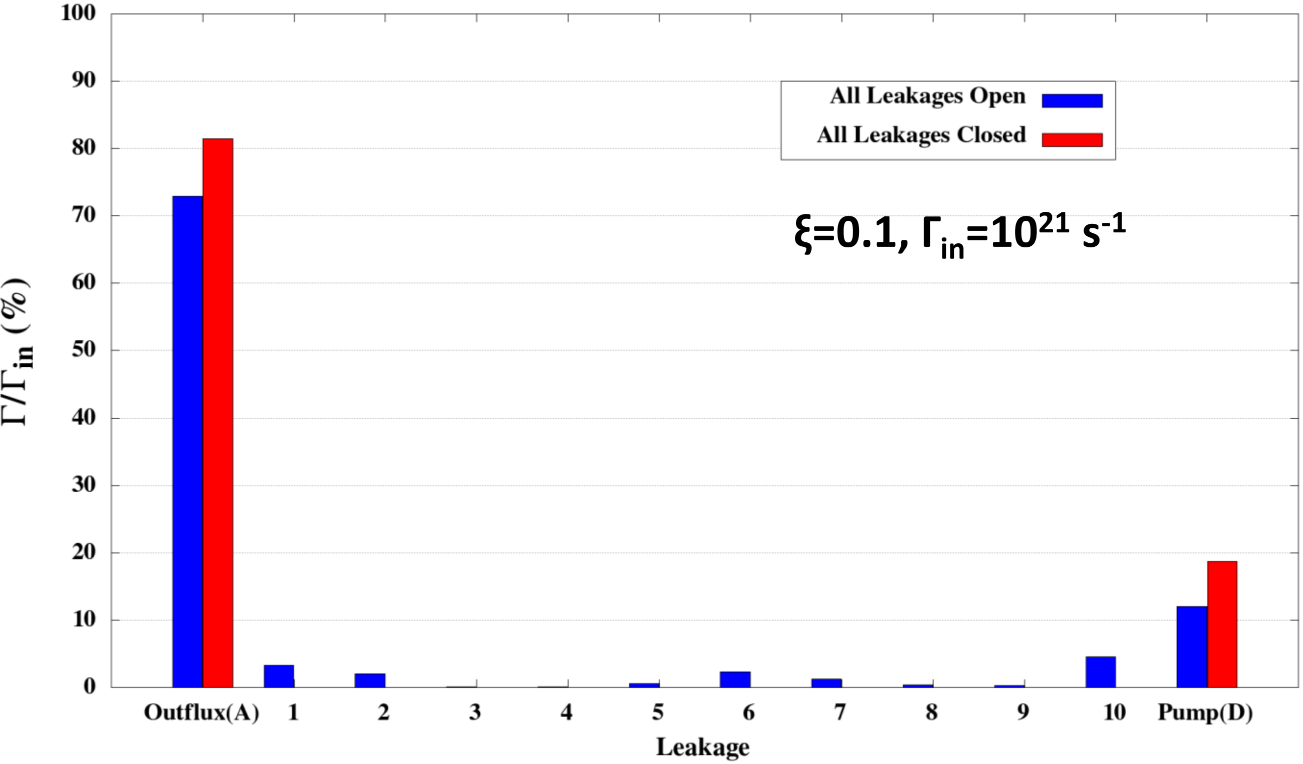
Influence of capture coefficient ξ

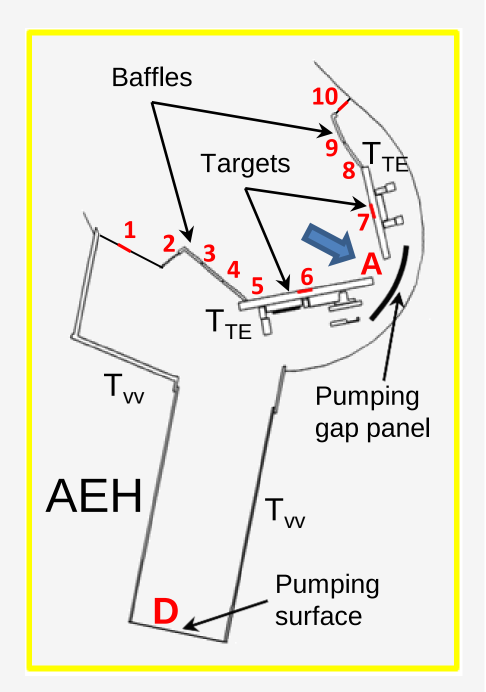




- A non-linear dependence of pumped flux as well as neutral outflux on ξ is observed.
- The pumped flux is increased by a factor of x1.7, when ξ goes from 0.1 to 0.5.
- In general, as ξ increases the pumped flux increases and the outflux decreases.

Influence of poloidal leakage closure





- The closure of poloidal leakages No. 1 - 10 facilitates the increase of the pumped flux as well as the neutral outflux towards the plasma, by a factor of x1.5 and 1.1x respectively.

Conclusions

- The DIVGAS code is a reliable tool, which can be further exploited in the design and optimisation of a stellarator particle exhaust.
- The deterministic (DVM) and stochastic (DSMC) solvers of the DIVGAS code have been applied for modelling the 2D Low-Iota configuration of W7-X.
- Both DVM and DSMC algorithms have a very good agreement and the discrepancy is less than 1%.
- Higher incoming neutral fluxes facilitate the increase of the pumped flux as well as the decrease of the outflux.
- The closure of the poloidal leakages facilitates the increase of the pumped flux as well as the neutral outflux towards the plasma.
- All the above numerical findings will enhance the optimisation of the W7-X particle exhaust.

thank you!