

KINETIC SIMULATION OF MOLECULAR DRAG PUMPS



Direct Simulation Monte Carlo

The Direct Simulation Monte Carlo method in PICLas is suitable for rarefied gas flows and has a multitude of features:

- 1D, 2D, axisymmetric (including a radial weighting) and 3D simulations
- Mesh independence with on-the-fly octree-based mesh refinement and a nearest neighbour algorithm
- Broad range of available species from electrons to polyatomic molecules such as CO₂ and CH₄

Application areas of DSMC range from atmospheric entry and in-space propulsion to terrestrial applications such as micro-channel flows and vacuum pumps.

Other methods, which can be coupled with DSMC, are implemented within PICLas:

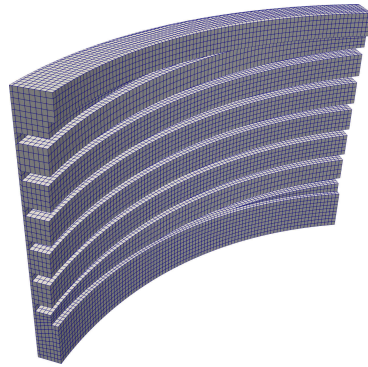
- **Particle in Cell** for the electromagnetic interaction of charged particles
- **Bhatnagar-Gross-Krook** for the efficient simulation of denser gas flows

Available on GitHub:

[/piclas-framework/piclas](https://github.com/piclas-framework/piclas)

Holweck / Helical-type vacuum pump

Numerical setup

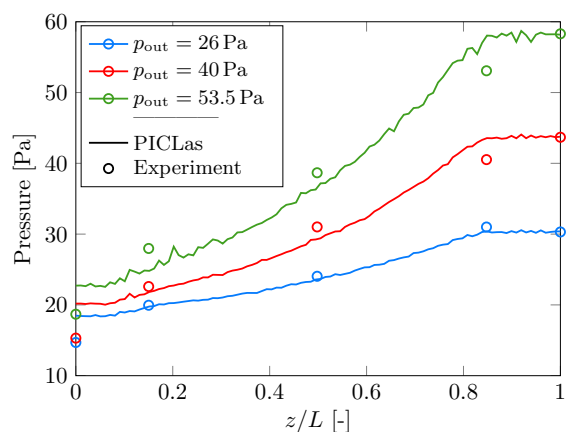


The setup is a single stage helical-type (Holweck) molecular drag pump in the transitional flow regime. The rotor has a diameter of 169 mm and a height of 41 mm. The simulation domain extends 11 mm below (outlet) and 5 mm above (inlet) the rotor. The clearance to the outer stator cylinder is 0.5 mm. The number of grooves is six, allowing to exploit rotational symmetry with a 60° slice. The simulation is performed in the rotational frame of reference. The

test gas is diatomic nitrogen (N₂). The discretized geometry is shown on the left and further details on the experiment are provided by Kim et al. (2008). The boundary conditions are summarized below, where a fixed outlet pressure and a constant mass flow at the inlet are defined. Complete diffuse reflection and full thermal accommodation is assumed as the gas-surface interaction. The simulation is performed at three different outlet pressures, in particular 26 Pa, 40 Pa and 53.5 Pa.

\dot{m}_{in} [sccm]	T_{in} [K]	ω_{rot} [rpm]	T_{wall} [K]
66	297	24 000	293.15

Experimental measurements



The experimental measurements from the literature have been performed by Kim et al. (2008) at five different points along the outer cylinder height, where p_{out} corresponds to P_5 in the publication. The pressure measurements are compared to the simulation results, where good agreement can be observed. The increased deviation at the inlet for all three cases might be attributed to the influence of the boundary condition and/or inaccuracies of the pressure measurement at low pressure conditions.

Reference:

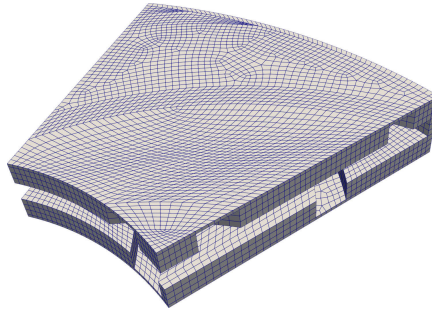
- Kim, D.-H., Kwon, M.-K., Hwang, Y.-K., & Abe, T. (2009). A Study on the Pumping Performance of a Helical-type Molecular Drag Pump. AIP Conference Proceedings 1141–1146. <https://doi.org/10.1063/1.3076453>

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Siegbahn / Disk-type vacuum pump

Numerical setup

The experimental configuration involves a single-stage disk-type (Siegbahn) molecular drag pump operating within the transitional flow regime. The system comprises a grooved rotor (Type-II) and plane stators positioned both above and below the rotor. Featuring ten grooves, the rotor allows the utilization of rotational symmetry within a 36° slice. The simulation is conducted in the rotational frame of reference, with diatomic nitrogen (N_2) as the test gas. The discretized geometry is presented on the right, and additional experimental and geometric details can be found in the work by Kwon et al. (2004). Boundary conditions include a fixed outlet pressure and a constant mass flow at the inlet. Complete diffuse reflection and full thermal accommodation is assumed as the gas-surface interaction. The simulation is carried out at various outlet pressures with different mass fluxes, specifically at 13.35 Pa, 26.65 Pa, and 40 Pa, combined with a mass flux of 0 sccm, 10 sccm, 30 sccm, and 60 sccm per pressure level.

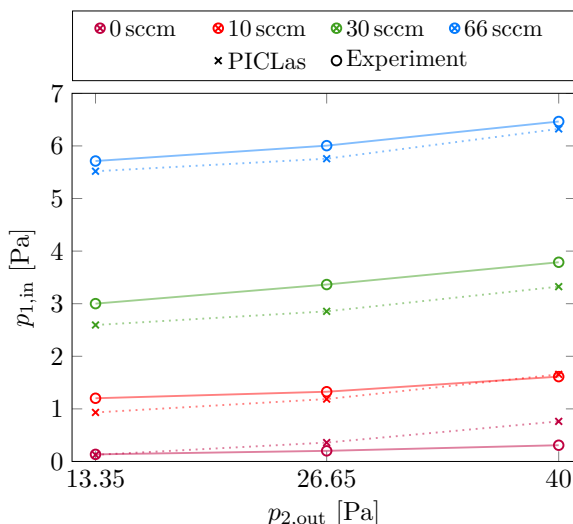


boltzplatz - numerical plasma dynamics GmbH offers engineering services such as simulation projects, technical support and workshops & training around the open-source software PICLas.

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T_{out} [K]	ω_{rot} [rpm]	T_{wall} [K]
295.15	24 000	295.15



Experimental measurements

Experimental measurements were conducted by Kwon et al. (2004) at two distinct locations: the inlet $p_{1,in}$ and the outlet $p_{2,out}$. The pressure readings obtained from the inlet are compared to the simulation results on the left-hand side and show good agreement. It should be noted that the accuracy of the simulation results strongly depends on the accommodation coefficient of the surface boundary, which is a function of the surface material, its finish temperature, and the gas species.

Finally, predictive simulations can be performed to investigate new concepts and gain detailed insights into the pumping mechanisms in the transitional flow regime. In addition to simulating individual helical-type (Holweck) and disk-type (Siegbahn) molecular drag pumps, it is possible to simulate multiple stages within a turbomolecular pump.

Reference:

- Kwon, M. K., & Hwang, Y. K. (2004). A study on the pumping performance of the disk-type drag pumps for spiral channel in rarefied gas flow. *Vacuum*, 76(1), 63–71. <https://doi.org/10.1016/j.vacuum.2004.05.011>