Development of vacuum flow modeling tools

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- Why vacuum flow modeling?
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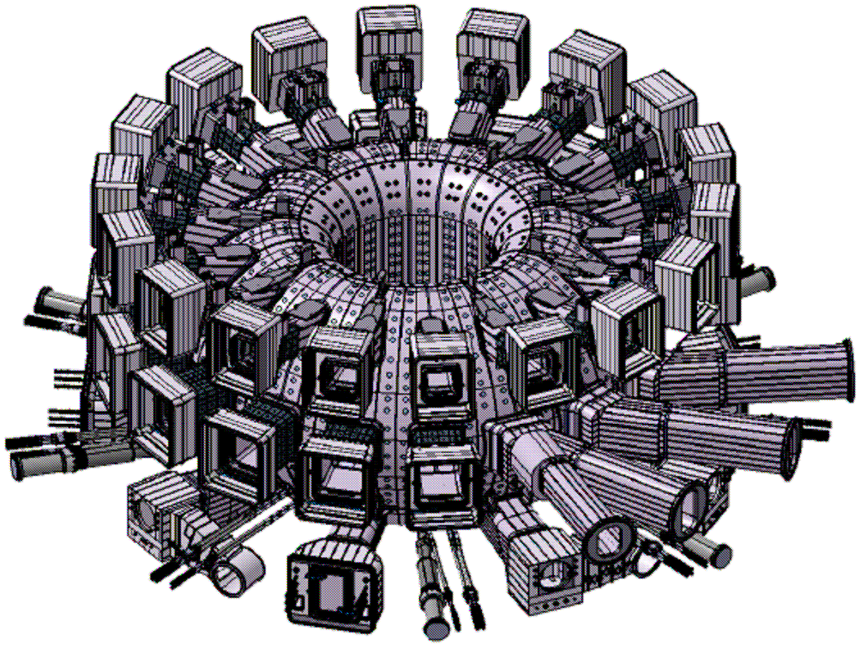
Why vacuum flow modeling?



- For a proper design, all conductance values of the system have to be known
- Important for the function of the whole system ("black hole pumping speed" can not be exceeded; conductance loss due to ducts has to be taken into account)
- Important for a economic design (oversized pumps are expensive)

Introduction to vacuum flow modeling

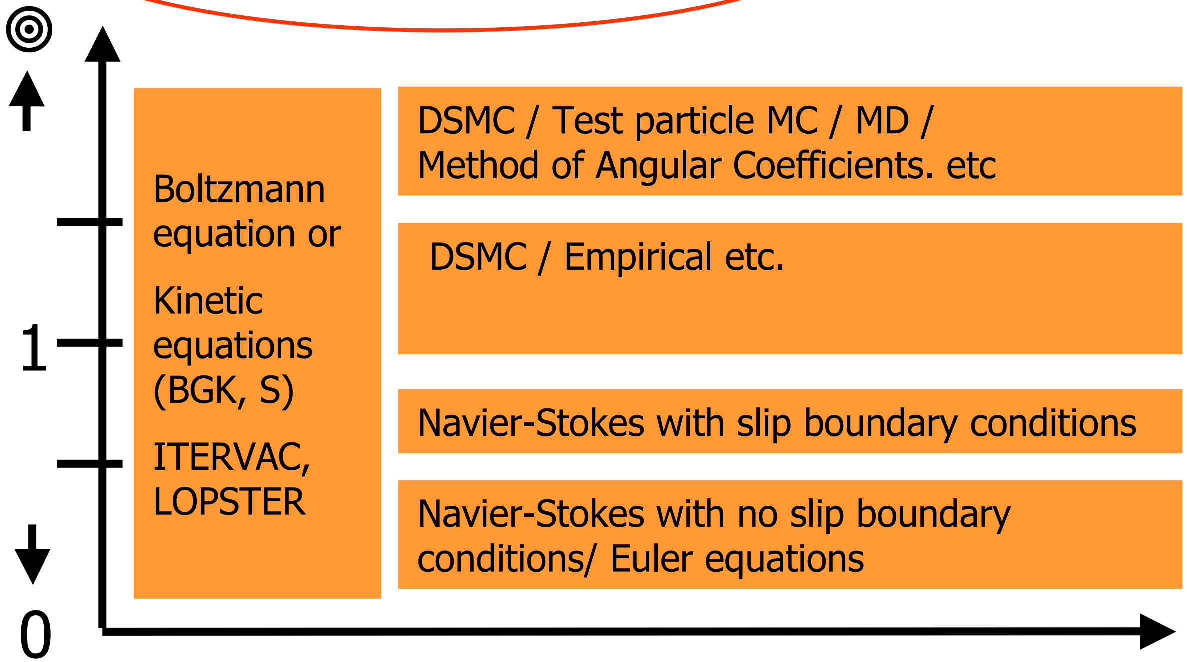
- Most important number for the design of vacuum systems is the Knudsen (Kn) number
- Kn gives the flow regime:

viscous: Kn << 1

transient Kn ≈ 1

free molecular Kn >> 1

$$Kn = \frac{\text{mean free path}}{\text{characteristic dimension}}$$



Boltzmann equation

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$f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}$ number of molecules in $\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}$

velocity distribution function

$n(t, \boldsymbol{r}) = \int f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - number density

$\boldsymbol{u}(t, \boldsymbol{r}) = \frac{1}{n} \int \boldsymbol{v} f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - bulk velocity

$P(t, \boldsymbol{r}) = \frac{m}{3} \int V^2 f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - pressure

$T(t, \boldsymbol{r}) = \frac{m}{3nk} \int V^2 f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - temperature

$\boldsymbol{q}(t, \boldsymbol{r}) = \frac{m}{2} \int V^2 \boldsymbol{V} f(t, \boldsymbol{r}, \boldsymbol{v})\mathrm{d}\boldsymbol{v}$ - heat flux vector

Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} = Q(f f_*)$$

$$Q(f f_*) = \int (f' f'_* - f f_*) \, |\boldsymbol{v} - \boldsymbol{v}_*| b \mathrm{d}b \, \mathrm{d}\varepsilon \, \mathrm{d}\boldsymbol{v}_*$$

$\boldsymbol{v}'$ and $\boldsymbol{v}_*'$ - pre-collision molecular velocities

$\boldsymbol{v}$ and $\boldsymbol{v}_*$ - post-collision molecular velocities

simplifying of the collision integral:

BGK model

$$Q(f f_*) = \nu \left(f^M - f\right)$$

S model

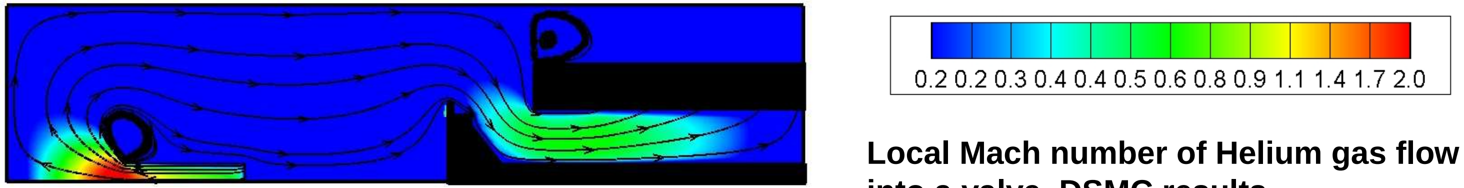
$$Q(f f_*) = \nu \left\{ f^M \left[1 + \frac{2m(\boldsymbol{q} \cdot \boldsymbol{V})}{15n(kT)^2} \left(\frac{mV^2}{2kT} - \frac{5}{2}\right)\right] - f \right\}$$

TPMC / DSMC

Test Particle Monte Carlo

Direct Simulation Monte Carlo

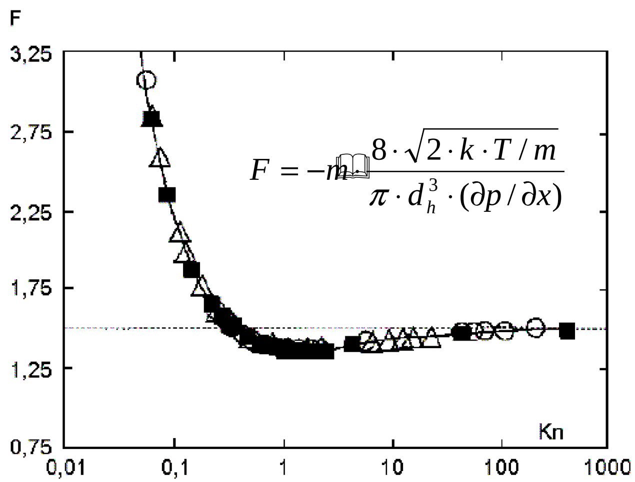
- Methods are based on particle tracking
- Transmission probability is calculated for the geometry
- Millions of particles have to be simulated, leads to a very high computational effort
- TPMC: Interaction of particles with walls is regarded, i.e. method can only be used at high Kn
- DSMC: Interaction of particles with walls and other particles is regarded, i.e. method can be used in high vacuum up to viscous



Local Mach number of Helium gas flow through a pipe into a valve, DSMC results

Empirical methods

- When the conductance as the function of Kn is known for every geometry, the conductance can be calculated easily by using a fit function
- Problem: Conductance function must be available for a lot of different geometries
- These results can be obtained by TSMC / DSMC / Boltzmann or experiments



4 parameter fit →

$$F = \frac{c_1}{Kn} + c_2 + \frac{c_3 \cdot Kn}{c_4 + Kn}$$

Programs available on the market

For vacuum flow modeling, only few programs are available.

For **TPMC**:

- ProVac3D (suitable for transient problems)
- MOVAK3D
- Molflow
- … (many in-house codes)

For **DSMC**:

- Open Foam
- SMILE
- … (many in-house codes)

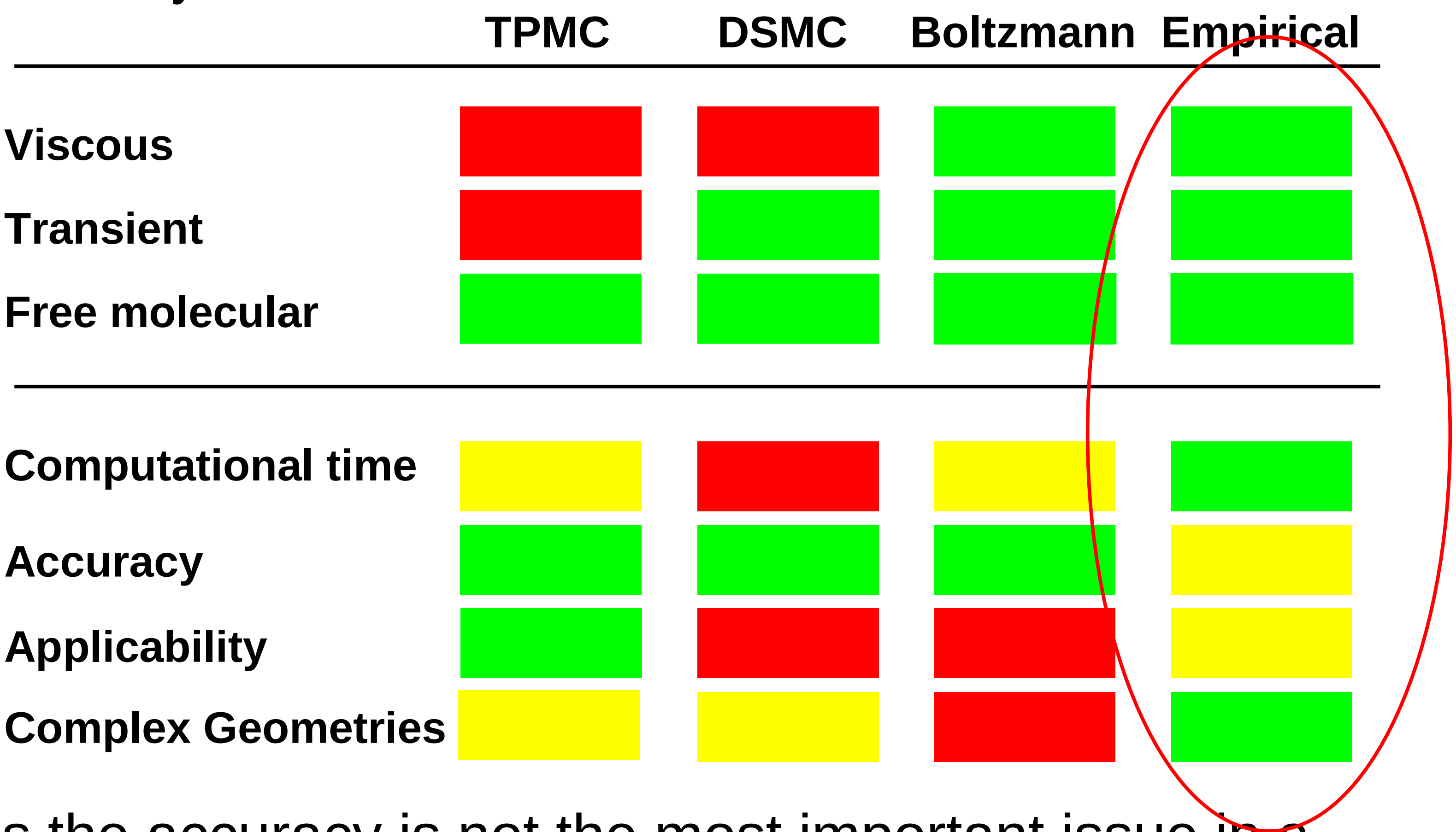
For **Boltzmann**:

- Unified Flow Solver, UFS
- … (many in-house codes)

Empirical methods: (allow network modeling)

- ITERVAC
- In Future: LOPSTER

Which one should be used for modeling of complex vacuum systems?



As the accuracy is not the most important issue in a complex, technical vacuum system, the <u>empirical method</u> would be favorable!

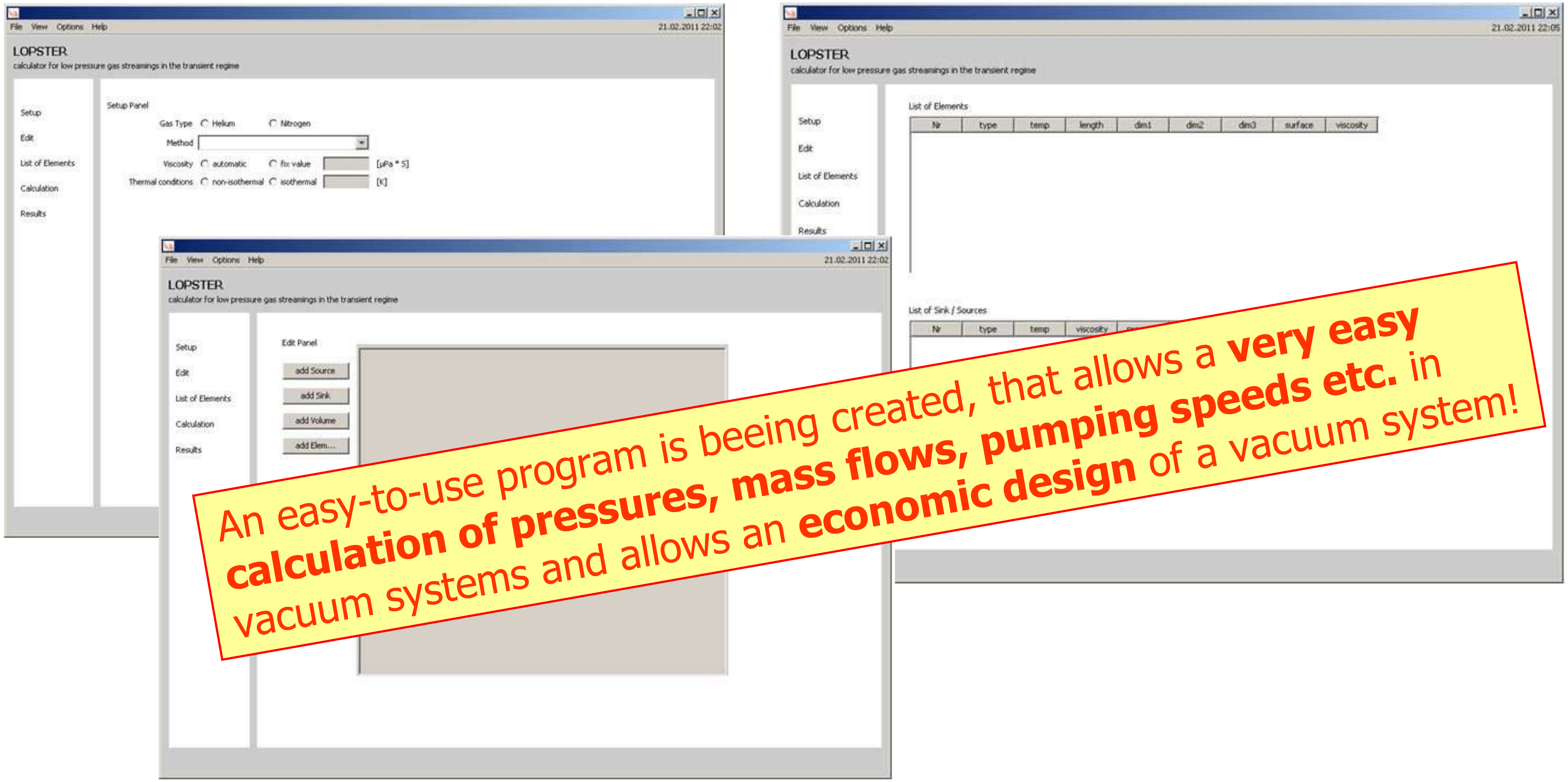
ITERVAC

- ITERVAC was developed at the former FZK (today: KIT) in 2002
- Based on few experimental data
- Low accuracy, especially for very short geometries (error of some 10 percent)
- Difficult to use
- Some important functions not available (calculation of pump size etc.)

Development of LOPSTER

Calculator for low pressure gas streaming in the transient regime

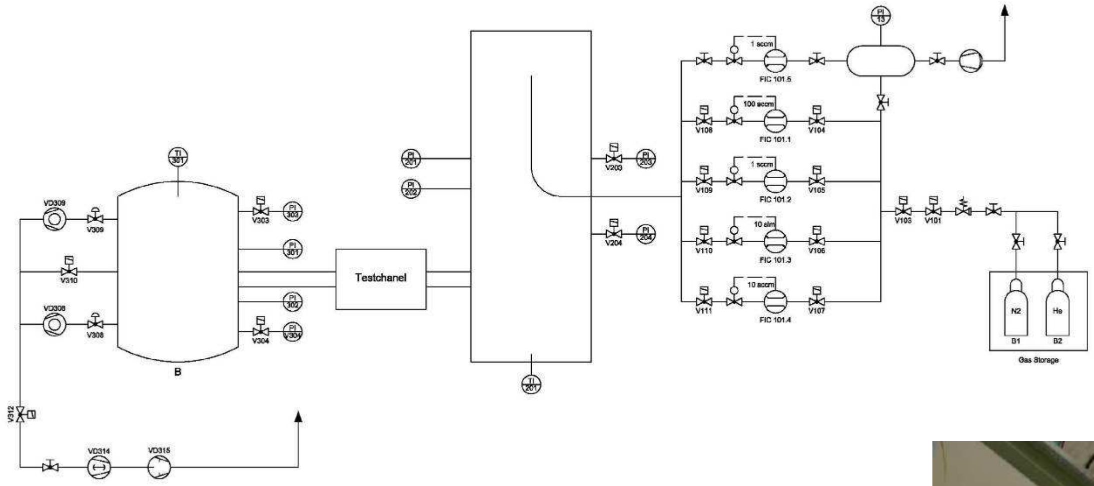
Due to the mentioned problems with ITERVAC and a grown experimental and theoretical database, the decision was made to develop a new program.

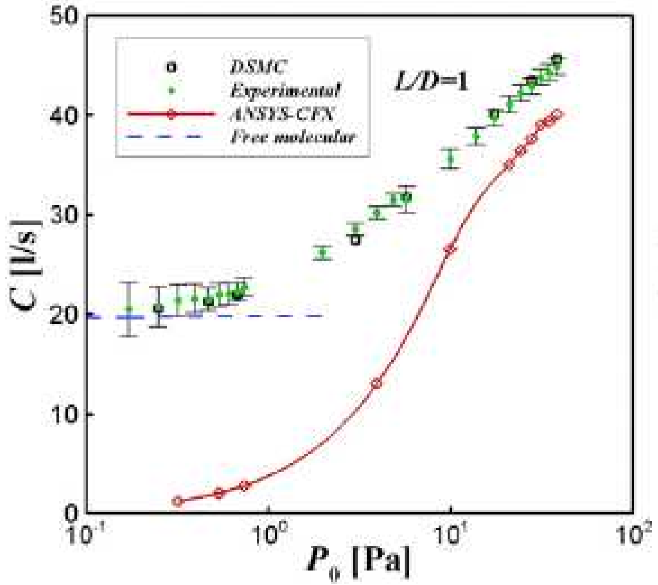


An easy-to-use program is beeing created, that allows a **very easy calculation of pressures, mass flows, pumping speeds etc.** in vacuum systems and allows an **economic design** of a vacuum system!

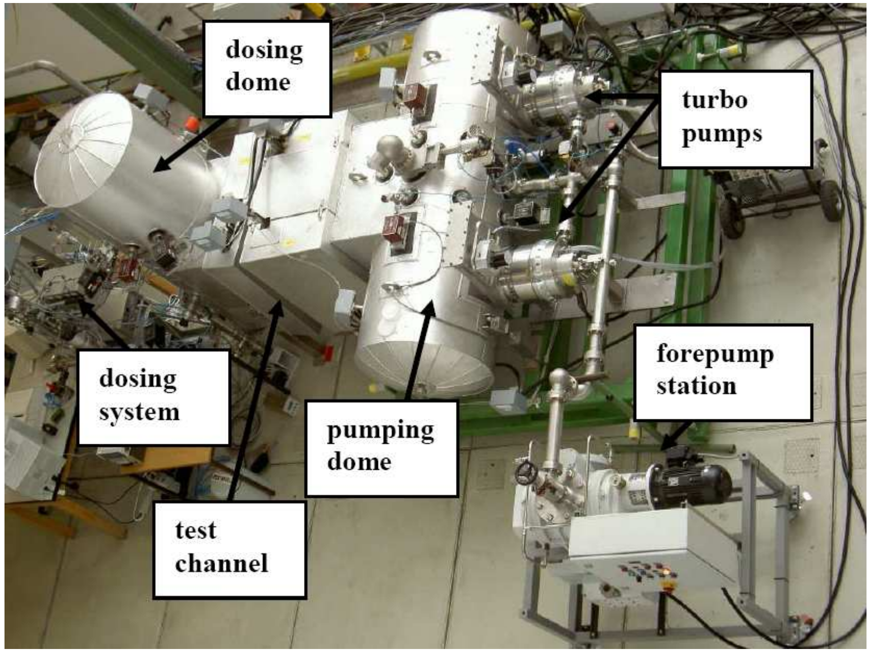
Benchmark tests in TRANSFLOW

Test facility for transitional flow range experiments





- Measurements are based on the 'direct approach' (pressure drop is measured over the geometry at a known gas flow rate)
- Test geometries up to 600 mm in diameter and 1200 mm in length can be measured in TRANSFLOW
- The results can be used to benchmark the results obtained by new codes or calculators



Conclusion and Outlook

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- Development of LOPSTER is ongoing at KIT
- First results will be available in the next months
- For complex geometries, ProVac3D and DSMC codes are available
- Benchmark tests can be done in TRANSFLOW

Thank you!

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LOPSTER filed for patent