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Direct Simulation Monte Carlo calculations of Gas Dynamics and Properties for Synchrotron Radiation Applications.

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Physics

A key parameter for understanding the flow behavior of gases is the Knudsen number (Kn) defined as the ratio of the mean free path to a length α characterizing the geometry of flow.

$$Kn_d = \frac{\lambda}{\alpha}$$

In gas flows with high Kn, the intermolecular collisions are reduced relative to the interaction of the gas molecules with the solid walls.

Continuum Models fail at these conditions and the flow has to be modelled on a microscopic scale with a Discrete Particle Model. These models recognize the structure of the gas as a myriad of discrete molecules and provides information on the

- Position
- Velocity
- Internal states

of every molecule at all times. The mathematical model at this level is the Boltzmann equation (**Fig 1**).

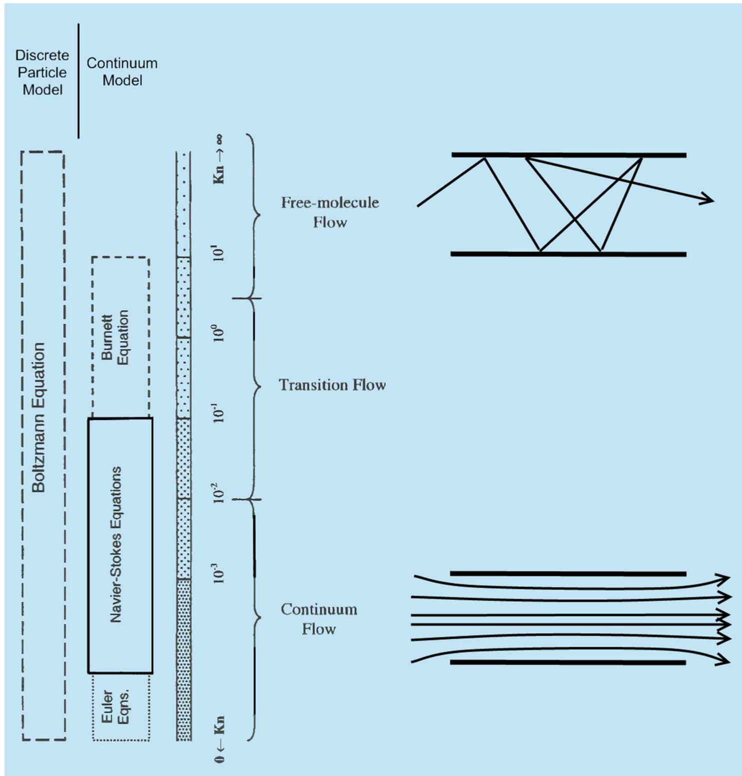

Fig 1: Kn number limits on the mathematical models [2]

Each molecule will be moving out of range of influence of other molecules for the most part. Moreover, when a collision happens, it is very likely to be a binary collision.

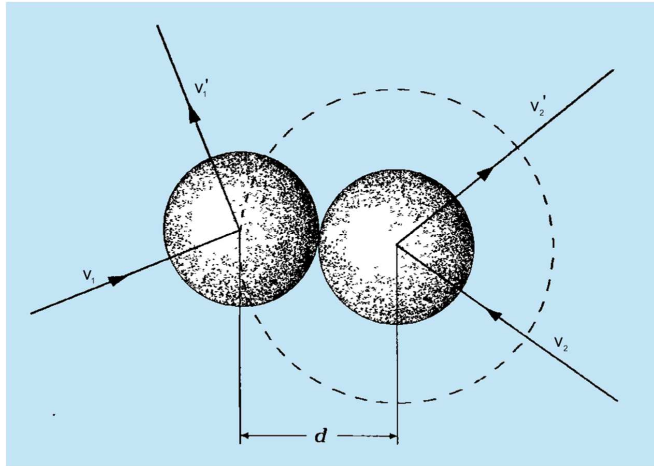

Fig 2: Collision between two hard spheres of diameter d and speeds v_1 and v_2 [2]

A hard elastic sphere of diameter d provides a simplified model of a molecule. Two of them will collide if the distance between their centers decreases to d (**Fig 2**) and can be modelled as an elastic collision.

Collisions with a wall are more complex due to engineering surfaces being microscopically mountains. The molecules suffer multiple scattering, can be momentarily trapped or become adsorbed on the surface. Most numerical studies are based on the assumption of diffuse reflection and it this appears to be adequate for the vast majority of practical gas flows. [2]

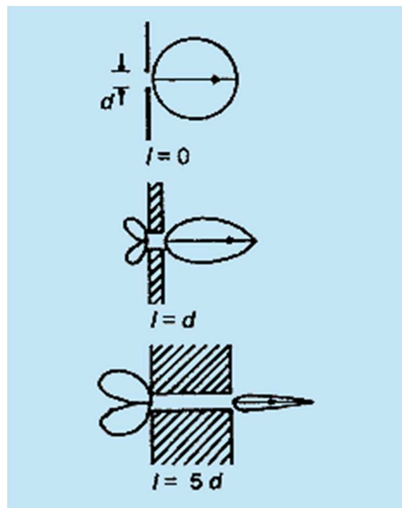

Fig 3: Angular distribution for flow through an orifice[2]

On the other hand molecular flows are very predictable in their behavior. The angular distribution of molecular gas flows into vacuum is shown in **Fig 3**.

These simple guidelines can be used to shape the flow to the desired effect, as shown below.

Gas Inlet

Gas phase photoelectron spectroscopy experiments are an example for using gas injection with molecular flow into a vacuum environment. They have special requirements to the assembly:

- Small interaction region
- High gas density
- HV environment
- Distance to metal surfaces

A conventional experiment employs a long, narrow tube that injects gas into the vacuum chamber (**Fig 4**).

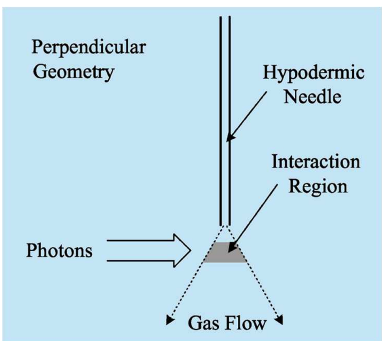

Fig 4: Conventional Geometry. [1]

The focus of this work package was to optimize the pressure in the interaction region relative to the total pressure in the vacuum chamber. Additionally, the system has to be compact in order to allow a free choice for the geometry of the spectrometer.

The optimization is done on the basis of direct Monte Carlo flow simulations (overview in [3]) and testing of prototypes in collaboration with the DynamiX group of the University of Hamburg.

For an optimization of the gas needle system these variables have most impact:

- Reservoir pressure
- Background pressure in chamber
- General geometry

The initial condition of the simulations is vacuum in the complete flow field. The reservoir pressure is 100 hPa.

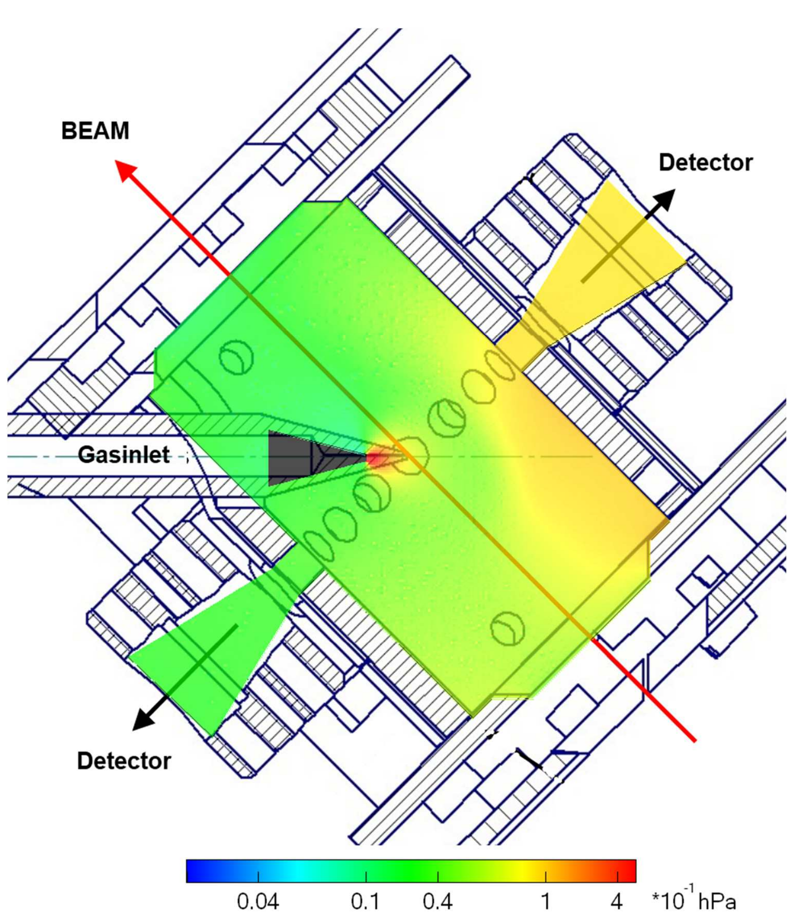

Fig 5: 2D N_2 Flow in the interaction region of a photoelectron spectroscopy experiment. [4]

The interaction region has been modeled to examine the gas flows in the existing system (**Fig. 5**). The gas needle is 3 mm away from the center. The boundaries pierced by the Beam are set to vacuum. The boundaries in the detectors are set to catch 5 % of all incoming particles, to simulate the small leaks in the closed detectors. The gas emerges directly from the tip of the needle.

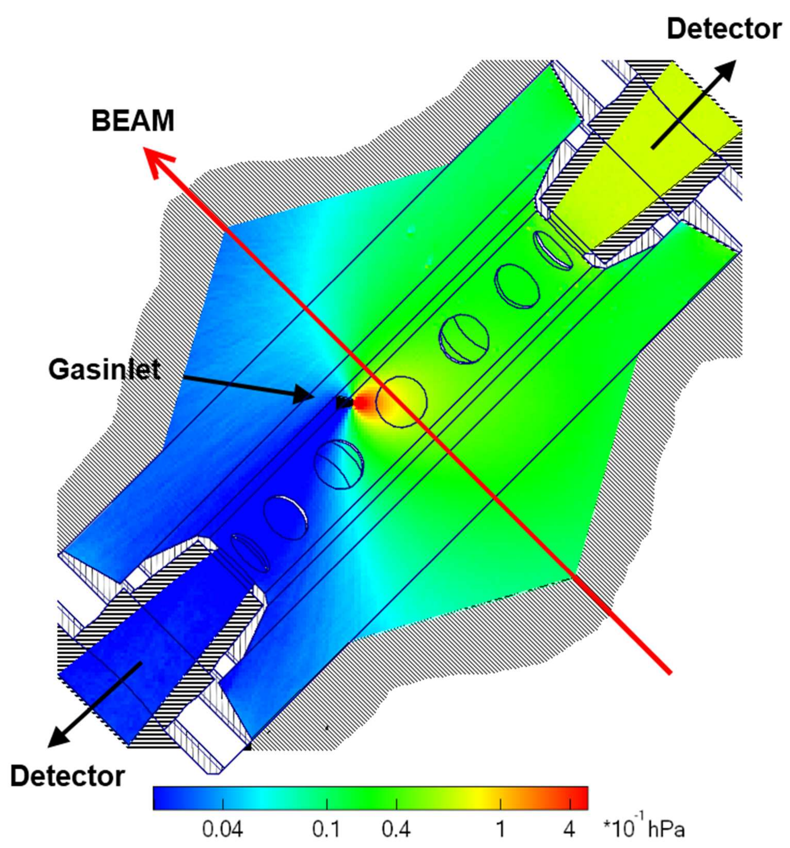

Fig 6: Optimized N_2 Flow with the same reservoir pressure. [4]

First optimizations resulted in the geometry of **Fig 6**. The pressure reduction in the whole geometry is due to the open design.

Aside from these passive optimizations of the geometry more success is gained with direct changes to the gas inlet. **Fig 7** shows 17 gas inlets focused on one point 15mm away. The point of maximum pressure moves away from the sources when molecular flow is applied (left side).

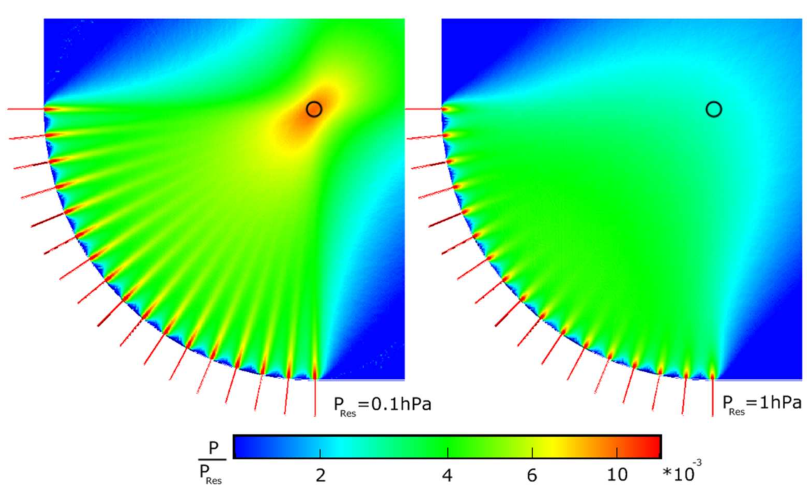

Fig 7: N_2 flow of 17 focused capillaries. Focus in 15mm distance. Circle is approx. 1mm in diameter. [4]

Given the size of a single gas inlet and the achievable distances to the focus it is possible to use several hundred inlets to maximize this effect.

These simple ideas allow modifications of the gas flow to the desired shape. Possibilities in this regard are:

- Optimized background pressure
- High pressure gradients
- Defined size of interaction region
- Lower gas flux
- Higher pressure

Differential Pumping Stage

In some applications involving synchrotron radiation beamlines it is necessary to maintain pressure differentials along the beamline. In particular, the experimental conditions may be incompatible with the usual requirements of UHV conditions at the interface with the storage ring. This can be achieved by using a high impedance connection together with additional pumping with the great advantage that the photon flux is not disturbed.

The requirements to a differential pump stage are:

- Reduction of gas flux
- Undisturbed beam passage

These contrary points need to be balanced in order to allow a good handling of the device and to minimize the needed pump stages for a given pressure difference.

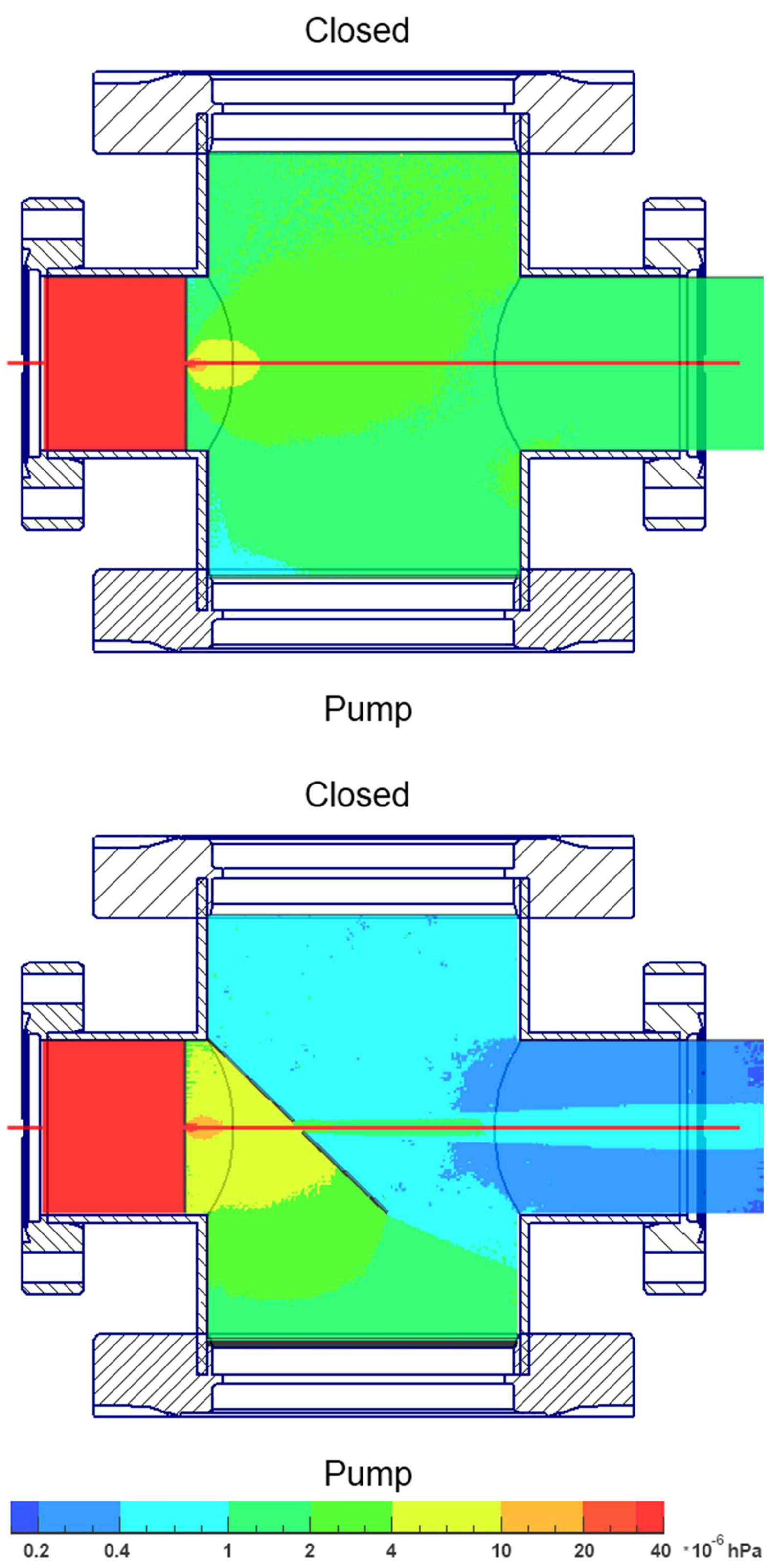

Fig 8: N_2 flow in differential pump stage with one and two apertures at 10^{-4} hPa.

Fig 8 and **Fig 9** show a differential pumping stage in a CF 63/40 cross with initial pressure of 10^{-4} hPa on the left side. The upper port is blank flanged, on the lower side is a turbomolecular pump attached. The synchrotron beam (red line) passes in horizontal direction. Mean Flux through the stage is reduced by additional factors for each aperture without further reduction of the beam opening.

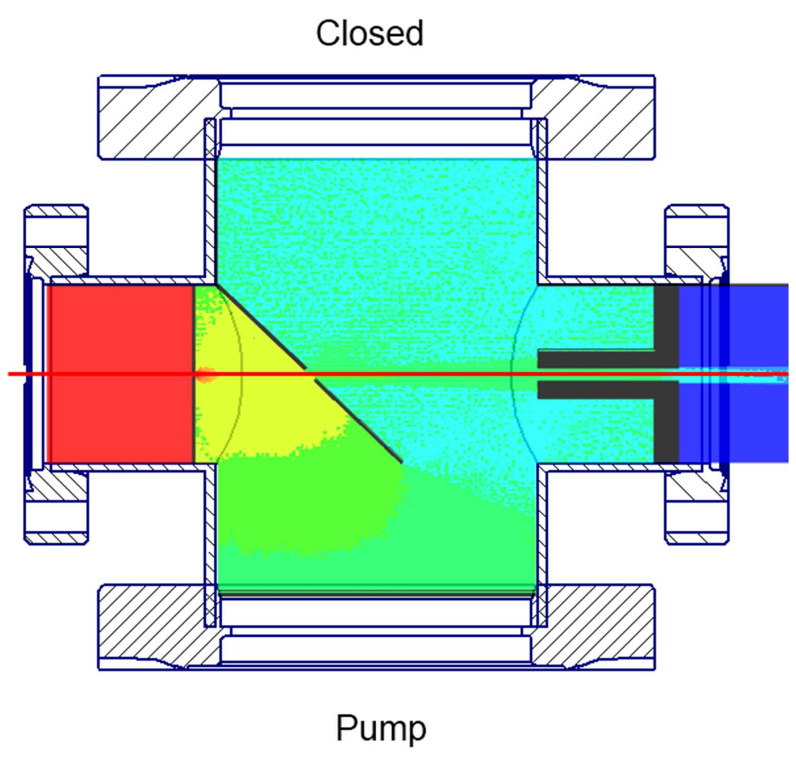

Fig 9: N_2 flow in differential pump stage with three apertures at 10^{-4} hPa.

I: Apertures	1	2	3
Opening [mm]	1mm	2mm	3mm
Length [mm]	0.5mm	0.5mm	30mm
Mean Flux [Num/m²s]	7e18	2e18	5.5e17
Flow Reduction	-	3.5	12.5
II: Apertures	**1**	**2**	**3**
Opening [mm]	1mm	2mm	3mm
Length [mm]	0.5mm	0.5mm	30mm
Mean Flux [Num/m²s]	2e23	2.5e22	1.1e21
Flow Reduction	-	8	182

Tab 1: Gas flux at 10^{-4} hPa (I) and 1 hPa (II).

With this tool it is possible to:

- Optimize design to gas flow
- Minimize required pumps
- Predict gas flux

Outlook

Gas inlet:

- Increasing number of gas inlets in Simulation
- Simulations in 3D
- Tests with a prototype
- Installing system at P04 beamline

Differential pumping stage:

- Simulation of different apertures and combinations
- Simulations in 3D
- Tests on P04 beamline

References

[1] **D.P. Seccombe, Collins, Reddish**; Rev. Sci. Instr., Vol 72, No. 6, P. 2550
[2] **G.A. Bird**; "Molecular Gas Dynamics", Oxford Science Publications
[3] **P.S. Prasanth, Kakkassery**; J.Indian Inst. Sci., Vol. 86, No. 3, P. 169
[4] **J.Seltmann**; Simulation und Test eines Gaseinlass-Systems für Synchrotronstrahlungs-Anwendungen, 2011

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More information at: http://hasylab.desy.de/facilities/petra_iii/beamlines/p04_xuv_beamline/