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Molecular Gas Flow in a Fish Trap Nozzle – Challenge to the Second Law of Thermodynamics

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Introduction: During examination of molecular gas flow in freeze dryers in near-vacuum properties, an idea came up to model a molecular fish trap nozzle (Figure 1). An appropriate shape of this fish trap nozzle allows to separate free flowing molecules into 2 chambers, and obtain a pressure gain in a isothermal environment (molecular flow "diode"). While particles don't change their magnitude of momentum after reflection at the walls, observed separation can be considered as isothermal compression. On first impression this behavior conflicts with the Second Law of Thermodynamics. But this is not the case. By focusing this problem on stochastic (molecular flow) scale, and not on continuum gas mechanics, there is no problem with any physics laws. For example, probability of separating N molecules to exactly one half of a room by random movement is [1 : 2^N]. Therefore it is not impossible, but very unlikely, to separate 1 mol of gas without a rectifier. The only constraint is to ensure a big Knudsen Number (say: Kn > 2 or more). This work shows an approach for a suitable rectifier.

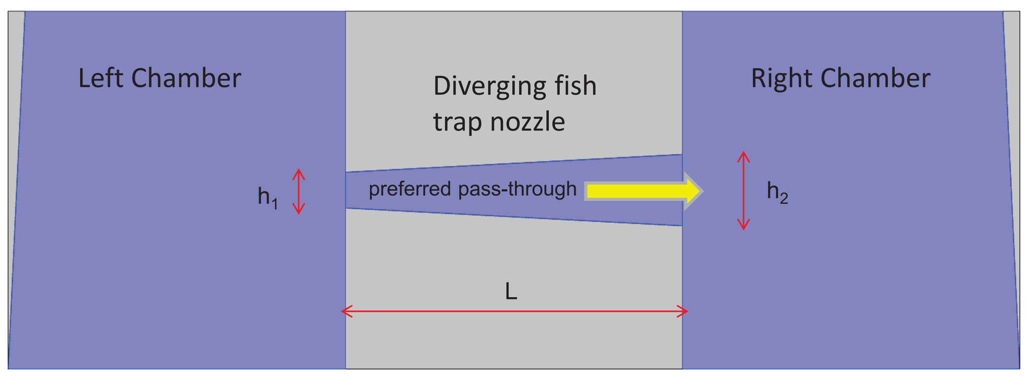


Figure 1. Geometry of Fish Trap Nozzle and Chambers

Computational Methods: Mathematical Particle Tracing module with simple Newtonian particles was used to model this case. Particle-particle collisions and molecular surface adsorption were not considered in reference to the Knudsen Number and simplicity of this model. Modeled particles are fully elastic with "bounce" condition on wall contact. Equal numbers of particles were released in 2 chambers with mirrored velocity vectors and random start positions.

$$\frac{d(m\,v)}{dt} = F_t$$

where
m : mass of particle
v : velocity
F_t : force on particle

Results: Simulation results show a significant separation and accumulation into the chamber on the diverging part of the fish trap nozzle (Figure 2), (Figure 3). Real fishes would take the other way around. In contrast to "Maxwell's Demon" this fish trap nozzle is a fully passive device and needs no kind of valves or moving parts. It is a kind of "thermodynamic diode". Best results on separation seem to appear on L>>$h_{1,2}$, where L is length and h gap size of the fish trap nozzle. Understanding the mechanism of separation is very simple. A converging nozzle will behave like a prism mirror by adding reflection angles after several reflections in the nozzle, a diverging nozzle lets particles pass through (Figures 4,5,6,7). Distribution ratio r_{dist} will fit to the ratio of pass-through probabilities P_{div} and P_{conv} , where "div" is pass in divergent direction (left -> right), and "conv" is pass in opposite direction. Probabilities P are described by geometrical properties in both chambers, where Ω is the sector "valid inlet area" shown by the red arc, and orientation angle α is the yellow zone of "valid inlet vectors" (Figures 6,7). Therefore $P_{div,conv}$ are dimensionless integrals over area Ω and zone α by the fraction of valid incoming particle directions and full circle (2π) in 2D case. Positions of PONR (Figure 7) can be determined by Rendering equations.

$$r_{dist} = \frac{P_{div}}{P_{conv}} \qquad P = \iint_{\Omega,\alpha} \frac{1}{2\pi}\, d\varphi$$

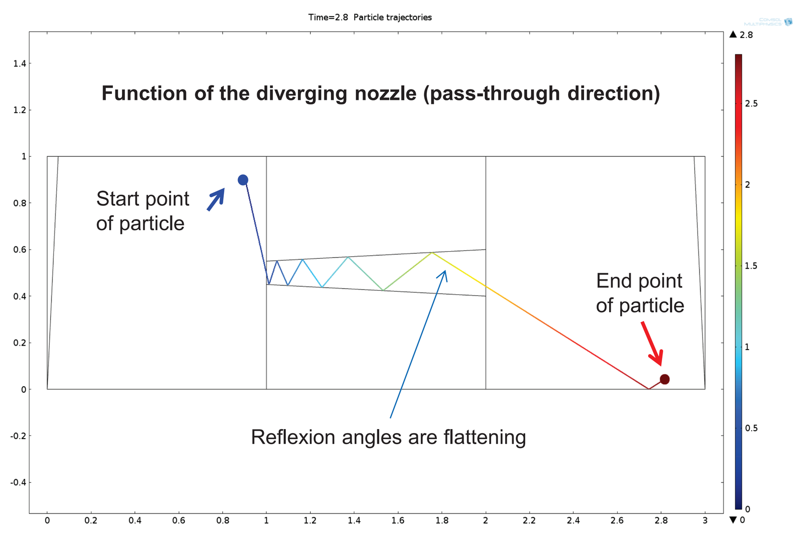


Figure 4. pass-through direction of nozzle

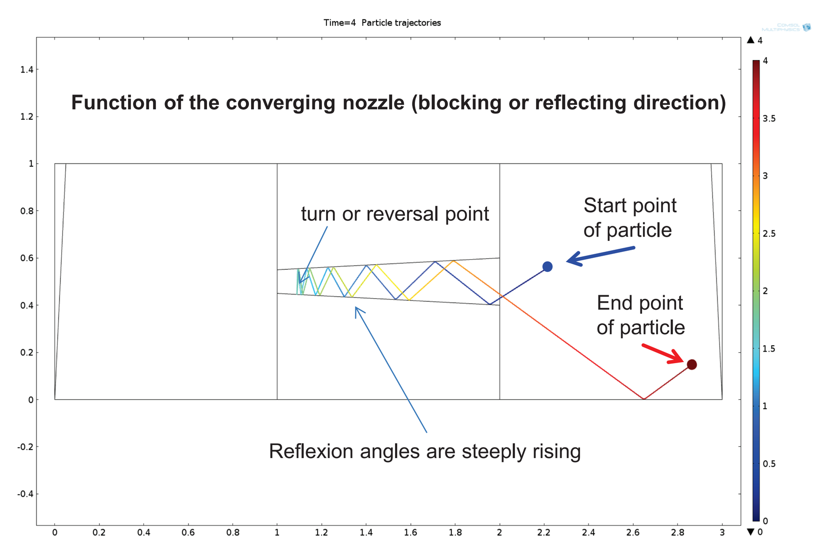


Figure 5. blocking direction of nozzle

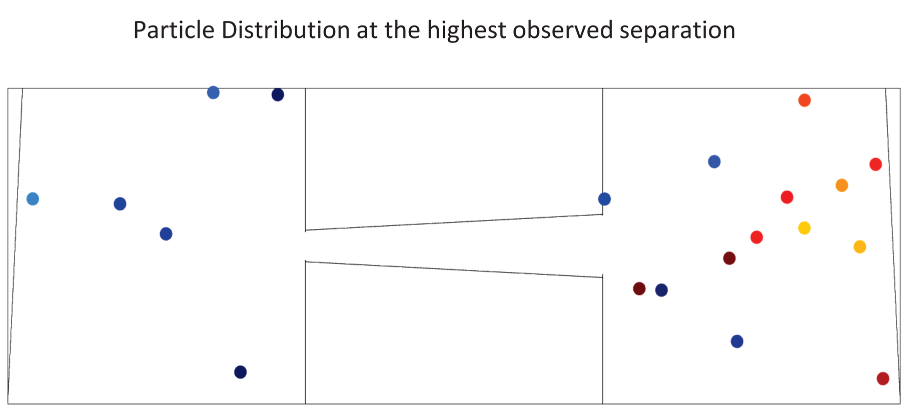


Figure 2. Distribution of Particles after specific time

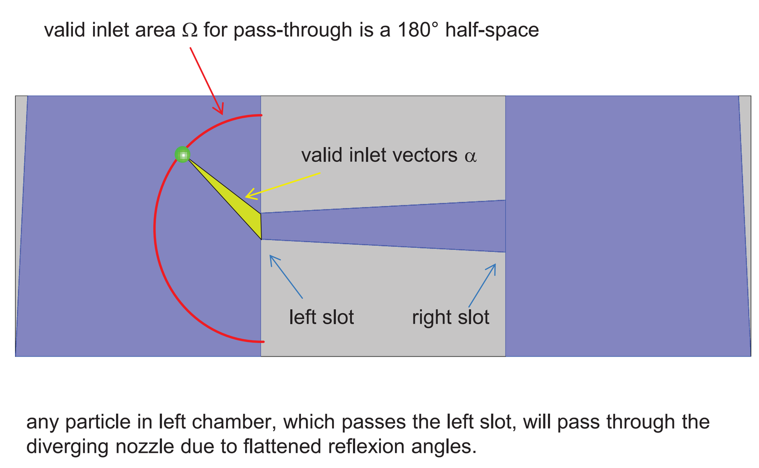


Figure 6. pass-through conditions of diverging nozzle

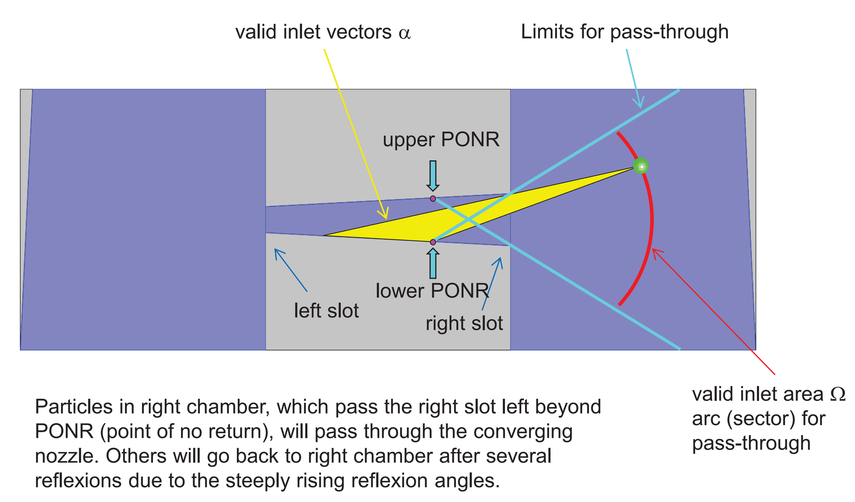
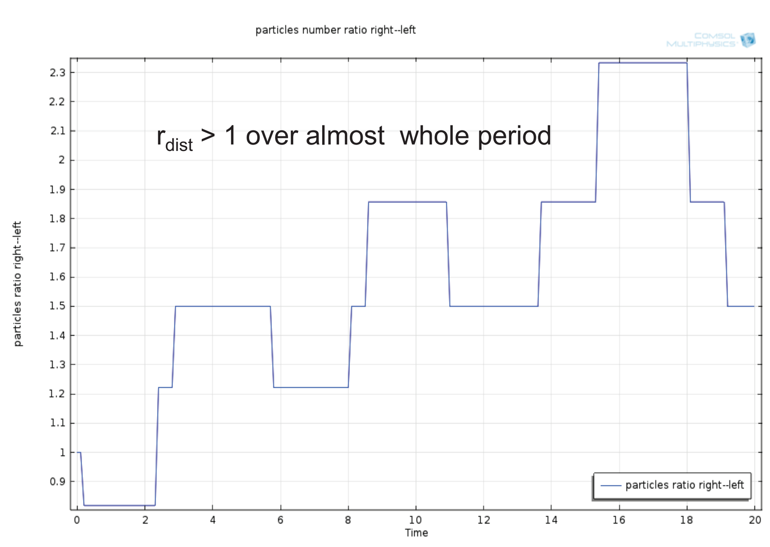


Figure 7. pass-through conditions of converging nozzle



highest separation rate is [2.3 : 1] in this small study

Figure 3. Distribution Ratio r_{dist} of Particles over time

Conclusions: Further scientific work can help optimize the fish trap geometry, i.e. L/h and different shapes like sawtooth or curved slots. Maybe this approach will lead to new technologies like passive vacuum pumps or energy harvesting with nano-scale sieves at atmospheric pressure (if surface absorption and particle-particle collisions really can be neglected)

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References:

1. Vladislav Cápek et al., Challenges to the Second Law of Thermodynamics, Springer, 2005.