

Direct Monte-Carlo Simulations In a Gas Centrifuge

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Abstract. The study is related to the centrifugation process for isotope separation. In a gas centrifuge, the major part of the rotating gas is modeled by fluid equations with this gas flow described by suitable Navier-Stokes. Nevertheless, a kinetic description of the gas is necessary for the feed gas expansion from the central pipe, and for the residual gas contained in the casing in which the cylinder rotates. For these rarefied regimes, we use Direct Monte-Carlo Simulations. In the first case, the simulations provide more realistic boundary conditions for fluid flow calculations. In the second case, we use DSMC to determine the mechanical power of the rotating cylinder and the heat flux dissipated on this cylinder and the fixed cylinder of the casing.

INTRODUCTION

Our work is carried out as part of modeling isotopic separation by centrifugation using the principle of a cylinder rotating at high speed in a vacuum casing. As in the most widely used configuration (1), the gas containing the isotope mixture is introduced by a fixed axial feed pipe and expands in the cylinder. It is subjected to high centrifugal acceleration, it undergoes rigid body rotation and stratifies radially according to a barometric-type pressure law. By pressure diffusion, the heavier isotopes migrate to the cylinder wall and the lighter ones to the center. A temperature gradient on the wall, and the presence of a scoop in the fluid enabling recuperation of the gas depleted in light isotopes, produce a vertical countercurrent which transforms the radial separation effect into an axial effect. The enriched and depleted fractions can then be extracted through scoops. Practically all the gas is governed by the Navier-Stokes equations in 2D axial symmetry. The linearization of these equations leads to a differential equation called Onsager's equation (2). The fluid equations are then coupled to the solution of the isotope diffusion equation (3). Due to the high pressure stratification, the continuous fluids equations are not valid throughout all the cylinder. Schematically, we can distinguish two zones (Fig.2). The first one, dense and close to the rotational wall, is described by the Navier-Stokes equations. In the second one, rarefied and close to the center, these equations are not valid. In the fluid calculations, an internal boundary separates the continuum domain from the rarefied domain in which the feed gas expands. The radial position of this cut-off becomes closer to the wall with increasing gas density and rotation speed. In the rarefied domain, the Boltzmann equation is solved by the DSMC method (4). The complete simulation of the feed gas expansion interacting with the rotating gas makes it possible to give more realistic boundary conditions to codes which treat the fluid domain. This is the first study. The cylinder spins in a vacuum casing, limited by an external cylinder. From a technological viewpoint, it is essential to determine the mechanical power of the rotating cylinder and the heat flux dissipated on the two cylinders, as a function of the residual pressure in the casing. In this second study, we also use the DSMC code.

MONTE-CARLO SIMULATIONS OF THE FEED GAS

The reference centrifuge is a hypothetical and non-classified machine enabling the scientific community to compare results obtained for the optimization of separation performances (3). Its radius a is 6 cm, its peripheral speed Ωa is 600 m/s. The selected gas is UF_6 . We set the UF_6 pressure at the cylinder wall at 100 Torr and the gas temperature at 310 K at the feed pipe outlet. The domain studied with DSMC has a cylindrical symmetry around the feed pipe axis

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and extends radially up to $r_{\max} = 5$ cm, i.e., outside the estimated fluid limit r_f of around $r_f = 4.5$ cm where the local Knudsen number is around one. As the Monte-Carlo code is valid in the fluid region, it is better that the computed domain overlaps this dense region. The domain is axially limited to $z_{\max} = 5$ cm. At the center, the radius of the feed pipe is taken at $r^\circ = 0.5$ cm. The axial extension h of the outlet orifice is 1 cm and there is a symmetry plane at $z = 0$ (Fig. 1). The feed rate through the half-hole is 10 mg/s and the outlet condition is assumed to be sonic. The rotating gas is simulated by an emission from the internal boundary, at $r = r_{\max}$. Because of the rigid-body rotation in the fluid region, the gas is emitted over a half-maxwellian shifted by $v_\theta = \Omega r_{\max}$. The domain, which is initially empty, is divided into uniform, 100×100 cells. The time step is $5 \cdot 10^{-7}$ s. In the fluid region, the density profile $n(r)$ for a gas of mass M is given by the barometric-type density law :

$$n(r) = n(a) \exp\left(-\frac{1}{2} \alpha [1 - (r/a)^2]\right) \text{ with } \alpha = (\Omega a)^2 / (RT_0 / M) \quad (1)$$

In reality, UF_6 gas can contain traces of HF. Contrary to UF_6 , this lighter gas has a low stratification in the fluid region (see eq. 1). Moreover, considering the collisionless expansion of a gas from the fluid boundary it is easy to show that the maxwellian distribution function, shifted by Ωr in the angular direction, with an equilibrium molecular density profile (eq. 1), is a solution of the collisionless stationary cylindrical Boltzmann equation with the equilibrium boundary condition in r_f . Consequently, the two gases have an equilibrium density profile even up to the axis, and the central region contains essentially HF molecules. We have confirmed this result with DSMC, considering the collisional mixture expansion from the internal rotating boundary, at zero feed. Thus, we simulate UF_6 expansion in a UF_6 -HF mixture. We fix the HF pressure at $2 \cdot 10^{-5}$ Torr at the outer wall, and we consider the density of the gases, at $r = r_{\max}$, according to the equilibrium law. We consider the molecules as hard elastic spheres with diameters of $4 \cdot 10^{-10}$ m and $6 \cdot 10^{-10}$ m for HF and UF_6 , respectively. During the expansion, the rotation of the feed is induced by collisions with the rotating gas, and reaches a velocity close to those of the local velocity of the latter, i.e., $v_\theta = 500$ m/s at 5 cm from the axis (Fig. 2). The expansion leads first to an increase in the radial speed v_r . Then, the radial speed drops drastically due to the collisions with the background gas (Fig. 3).

At the limit of the fluid domain, DSMC calculations give information on the feed mass profile, the feed momentum profile and the feed energy profile. These sources are then used as boundary conditions for the Navier-Stokes calculations in order to estimate the separation performance of the centrifuge, which is dependant in some degree of the feed model (5).

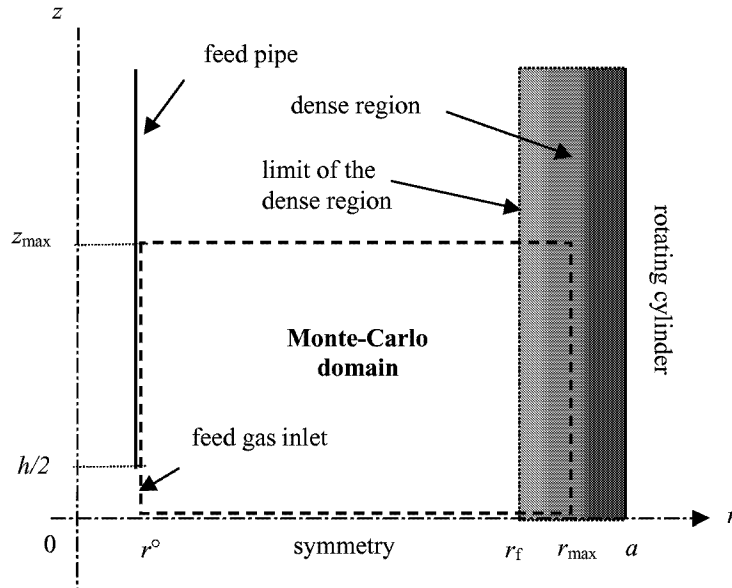


FIGURE 1. Schematic of the Monte-Carlo domain (dotted line). The centrifuge radius is a . The emission of molecules from the rotating boundary at $r = r_{\max}$ enables simulating the rotation of the gas in the dense region.

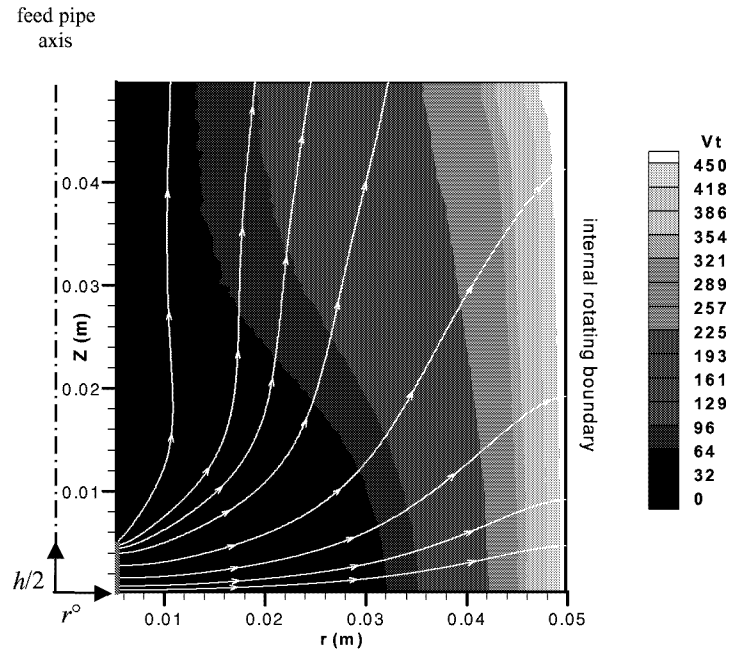


FIGURE 2. Rotational speed v_θ (m/s) and stream function of the feed gas, emitted from $r = r^\circ$ on a ring of height $h/2$. The internal rotating boundary is at $r_{\max} = 5$ cm.

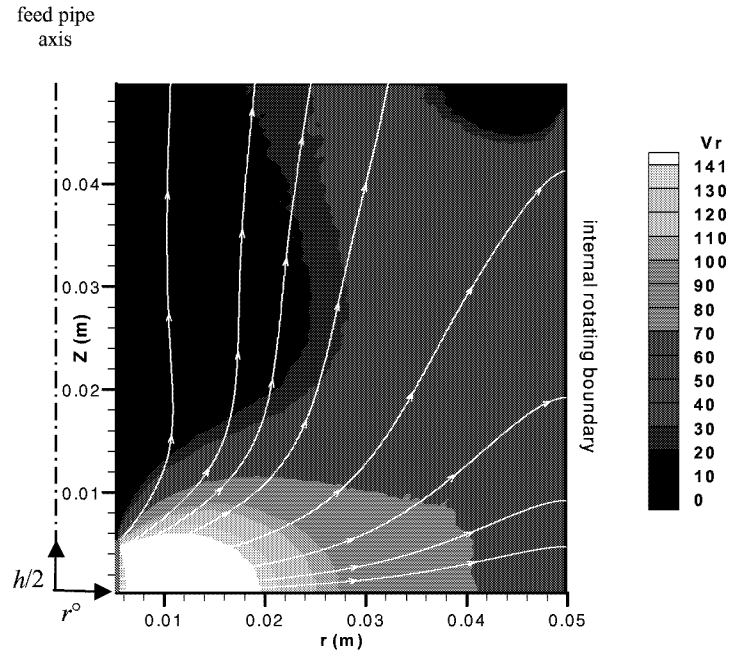


FIGURE 3. Radial speed v_r (m/s) and stream function of the feed gas, emitted from $r = r^\circ$ on a ring of height $h/2$. The internal rotating boundary is at $r_{\max} = 5$ cm.

MONTE-CARLO SIMULATIONS IN THE CASING

In a gas centrifuge, the internal cylinder is spinning and the external cylinder is fixed. The region between these two cylinders communicates with the center of the machine and so contains essentially HF gas. The overheating produced by the rotation can degrade materials and also the temperature profile on the rotating wall, source of the axial countercurrent. Thus, it is useful to determine this overheating in terms of residual pressure in the casing. This vacuum is enabled by the rotation itself, by use of a molecular pump. We study here the Couette flow in the casing between the rotating cylinder and the fixed outside cylinder and we use for this, like other authors (6), the DSMC code. In the limit of the low residual pressure, we have a collisionless regime and analytical solutions can be given. The conservation equations, in a 1D cylindrical geometry (r, θ, z) , with $v_r = v_z = 0$, for any surface $S(r)$, lead to :

$$(q_r - \tau_{r\theta} v_\theta) S(r) = \text{constant} \quad (2)$$

According to the kinetic theory (4), the shear stress $\tau_{r\theta}$ and the radial heat flux q_r in the gas for molecules with mass m , velocities $\vec{w}$ and density n are the average quantities :

$$\tau_{r\theta} = -nm \overline{(w_r w_\theta)} \quad (3-1)$$

$$q_r = \frac{1}{2} nm \overline{w_r w^2} + v_\theta \tau_{r\theta} \quad (3-2)$$

We can also define these quantities as surface properties (4), considering the incident (i) and reflected (r) contributions, with diffusion reflection on each cylinder, internal (int) with rotating speed v_p and external (ext), where x and y are the opposite direction to the normal and the tangential direction respectively. In particular :

$$\tau^{int} = \tau^{i,int} = nm \overline{(w_x (w_y - v_p))}^i = nm \overline{w_x w_y} \quad (4-1)$$

$$q^{int} = q^{i,int} + q^{r,int} = \frac{1}{2} nm \overline{w_x (\vec{w} - \vec{v}_p)^2} = (\frac{1}{2} nm \overline{w_x w^2})_{int} - \tau^{int} v_p \quad (4-2)$$

And similarly for τ^{ext} and q^{ext} . Using the fluid relations (eqs. 3) at the internal radius r_i , we obtain from eqs. 4 :

$$q^{int} = -q(r_i) - \tau_{r\theta}(r_i) (v_p - v_\theta(r_i)) \quad (5)$$

$$P_c = -\tau^{int} v_p S^{int} = -\tau_{r\theta}(r_i) v_p S^{int} = q^{int} S^{int} + q^{ext} S^{ext} \quad (6)$$

In eq. 6, P_c is the mechanical power of the cylinder, entirely dissipated in heat on both the cylinders.

In the molecular regime, the analysis of the velocity distribution function, as sum of the internal and external contributions, leads to a semi-analytical complete solution for the macroscopic quantities in the whole domain, that we successfully compared to collisionless DSMC calculations. In particular, at $r = r_i$, and for the same temperature T_s at cylinder surfaces, the heat flux is zero and the gas velocity is half the wall velocity. Thus it is easy to show (eq. 6) that the heat flows on internal and external cylinders ($W s^{-1}$) are identical and half of P_c . Moreover, the shear stress at the internal radius can be written :

$$\tau_{r\theta}(r_i) = -\phi^{int} m v_p \quad (7)$$

For an analytical solution of the mechanical power in the molecular regime, the internal flux ϕ^{int} can be assumed to be those of an equilibrium gas where the pressure p is the homogeneous pressure before rotation. Indeed, the pressure profile is relatively flat for HF whose mean velocity is close to the rotation speed. Thus to a first approximation, the mechanical power for the molecular regime can be written :

$$P_c^{mol} = \left(\frac{m}{2\pi k T_s} \right) p v_p^2 S^{int} \quad (8)$$

The DSMC calculations (Fig. 4) are done with HF gas, an internal and external radii of 0.06 m and 0.085 m respectively, with $T_s = 310$ K. For high pressure, the regime becomes fluid and the power consumption has an analytical expression, a function of gas viscosity in the 1D Navier-Stokes problem (7). For this, the viscosity is estimated by kinetic theory for the hard sphere model (4). DSMC results are in good agreement with the analytical model for the lower pressures, and tend to the viscous limit when the pressure increases. (Fig. 4).

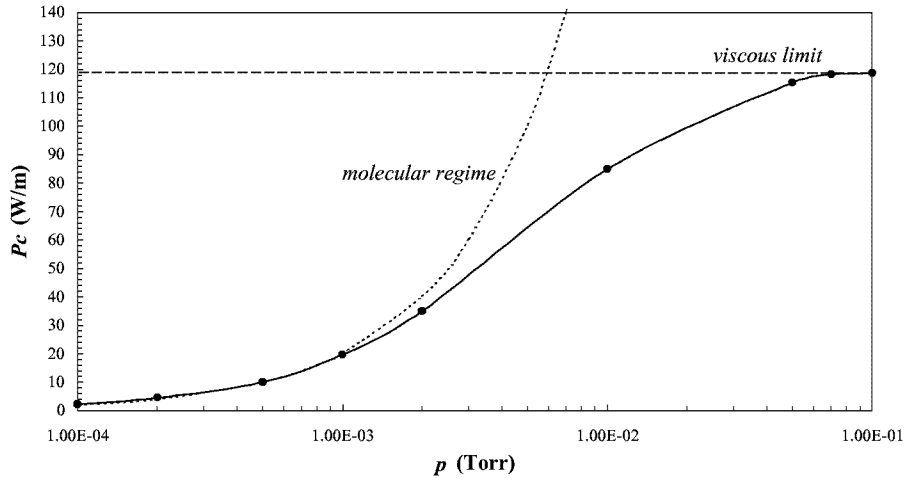


FIGURE 4. Mechanical power P_c (W/m) of the rotating cylinder versus the residual pressure p (Torr) in the casing (DSMC results). Analytical model for molecular regime (dotted line) and viscous limit.

CONCLUSION

The internal flow in a centrifuge is described by codes solving Navier-Stokes equations but some rarefied regions in the centrifuge require a kinetic description. This is true for the feed gas expansion interacting with the rotating gas. The Monte-Carlo simulations enable this description and can give realistic boundary conditions for the fluid mechanics codes that we developed. We have also used Monte-Carlo calculations to determine the friction of the rotating cylinder in the casing. We determined the mechanical power of the rotating cylinder and the heat flux dissipated on the two cylinders as a function of the residual pressure in the casing, which gives information on the tolerable pressure, taking into account a number of mechanical and thermal constraints. We developed analytical solutions in the rarefied domain and show that they provide a good approximation of the DSMC results in the pressure range used in practice.

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