# Investigation of a New Monte Carlo Method for the Transitional Gas Flow

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**Abstract.** The Direct Simulation Monte Carlo method (DSMC) is well developed for rarefied gas flow in transition flow regime when 0.01<Kn<1. However, such a simulation for a complex 3D vacuum system is still a challenging task because of the huge demand on the memory and long computational time. On the other hand, if Kn>10, the gas flow is free molecular and can be simulated by the Test Particle Monte Carlo method (TPMC) without any problem even for a complex 3D vacuum system. In this paper we will investigate the approach to extend the TPMC to the transition flow regime by considering the collision between gas molecules as an interaction between a probe molecule and the gas background. Recently this collision mechanism has been implemented into ProVac3D, a new TPMC simulation program developed by Karlsruhe Institute of Technology (KIT). The preliminary simulation result shows a correct nonlinear increasing of the gas flow. However, there is still a quantitative discrepancy with the experimental data, which means further improvement is needed.

**Keywords:** Test particle Monte Carlo simulation, molecular collision, transitional gas flow
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## INTRODUCTION

The gas flow in a vacuum system is characterized by the Knudsen number Kn=λ/d, with λ being the mean free path of the molecules and d the size of the vacuum chamber. For an ultra high vacuum or a high vacuum system, the mean free path is much greater than the size of the vacuum chamber, so Kn>10. In this case, the gas molecules seldom collide with each other and the gas flow is called free molecular flow, which can be simulated by the Test Particle Monte Carlo method (TPMC). If Kn<0.01, the gas can be usually considered as a continuum fluid and the flow is called viscous flow, which can be simulated by Computational Fluid Dynamics (CFD). The gas flow regime when 0.01<Kn<1 is called transition flow regime, which can be simulated by kinetic theory or the Direct Simulation Monte Carlo method (DSMC). However, the simulation of a complex 3D vacuum system with DSMC or kinetic theory is still a challenge task because of the huge demand on the memory and long computational time. Unfortunately, the gas flows in some International Thermonuclear Experimental Reactor (ITER**)** applications, for example, the gas flow inside the neutralizer of the Neutral Beam Injection system (NBI), the gas flow before the cryogenic pump in pellet injection scenario is within the transition flow regime. So that it is reasonable to explore a new simulation Monte Carlo method for transitional gas flows.

## DEVELOPMENT OF PROVAC3D INCLUDING MOLECULAR COLLISIONS

ProVac3D, standing for "**3D** density **PRO**file in the **VAC**uum system", is a TPMC simulation program developed by the Karlsruhe Institute of Technology (KIT). In our previous works [1-3], we have well described its main ideas and successfully cross checked and used it in different applications in the free molecular flow regime.

By recording the time of flight of molecules, we can calculate the gas density distribution. The natural idea to extend ProVac3D into transition flow regime is to include the collision between gas molecules by considering appropriate interaction between the probe molecule and the gas background, which is described in Figure 1. Suppose $P(\vec{x})$ is the probability that the probe molecule meets a target molecule of the gas background before it has passed a distance $|\vec{x}|$, it reads as

$$P(\vec{x}) = 1 - \exp(-s \int n(\vec{x}) d\vec{x}), \tag{1}$$

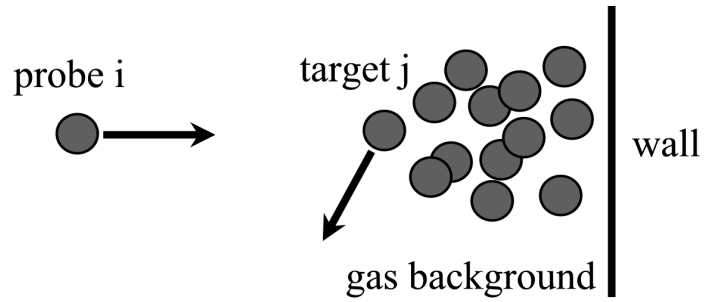


**FIGURE 1.** The collision between the probe molecule i and target molecule j.

where $n(\vec{x})$ is the density of the background gas molecules and σ the collision cross section. The integral is along the path of the probe molecule. From this relation one can derive Equation (2) to determine the collision time t of the probe molecule with one of the molecules in background.

$$\int_0^t n(x,y,z)(v_{probe} - u_{bulk})dt = -\frac{\log(rnd)}{s}, \tag{2}$$

where $v_{probe}$ is the speed of the probe molecule i, $u_{bulk}$ the bulk speed of the background gas, and rnd a random number.

Suppose τ is the possible collision time with the wall if no collision with the molecule of the background is taken into account. When $t < \tau$ the collision with the target molecule will happen at the position,

$$\vec{x} = \vec{x}_0 + \vec{v}_i t. \tag{3}$$

In such a case, the velocity $\vec{v}_i'$ of the probe molecule after the collision can be calculated, for the first attempt, by the hard sphere collision model.

$$\begin{aligned} \vec{v}_i' &= \tfrac{1}{2}\left[v_{relative}\vec{e} + (\vec{v}_i + \vec{v}_j)\right], \\ e(x) &= \sin(q_i')\cos(j_i'), \\ e(y) &= \sin(q_i')\sin(j_i'), \\ e(z) &= \cos(q_i'), \end{aligned} \tag{4}$$

with $v_{relative} = \sqrt{(\vec{v}_i - \vec{v}_j)^2}$ and $\vec{v}_j$ being the velocity of the randomly chosen target molecule j, superposed by bulk velocity $\vec{u}$,

$$\begin{aligned} v_j(x) &= \bar{v}\sin(q_j)\cos(j_j) + u_x, \\ v_j(y) &= \bar{v}\sin(q_j)\sin(j_j) + u_y, \\ v_j(z) &= \bar{v}\cos(q_j) + u_z. \end{aligned} \tag{5}$$

In Equations (4) and (5), the azimuth angles of the target molecule $(q_j, j_j)$ are randomly chosen in full space, however, the azimuth angles of the probe molecule after the collision $(q_i', j_i')$ are randomly chosen in the half-space determined by their relative velocity.

On the other hand, when $t > \tau$ the collision with the wall will happen. In such a case, Cercignani-Lampis boundary conditions have been included [4,5].

## NORMALIZATION PROCEDURE AND CONVERGENCE

The aforementioned collision mechanism has been recently implemented into ProVac3D. Naturally, it can be used to the application in which a dilute gas species is moving inside the gas background of another gas species [6]. However, the emphasis of the present work is to simulate the transition flow of single gas species through a circular tube, connecting with a dosing dome with gas density n1 and pumping dome with negligible gas density n2<<n1, as illustrated in Figure 2.

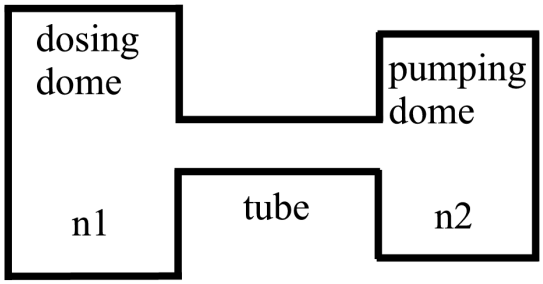


**FIGURE 2.** ProVac3D simulation model.

The gas flow is simulated as the function of the gas density n1 in the dosing dome by an iteration process

$$n1 = n_0 + k \cdot \Delta n, (k = 0,1,2,3,\cdots). \tag{6}$$

In order to start from a free molecular background, $n_0$ with k=0 must be small enough. For our simulations, Δn is chosen at least one magnitude smaller than $n_0$, so that the collisions between the probe molecules can be always negligible. For each iteration step k, a high number of probe particles representing Δn have been simulated.

As was previously mentioned, the simulation domain is divided into cells in the ProVac3D simulation [1-3]. If i is the cell index, we can calculate the average time of flight of all test particles $fts_k(i)$; here subscript k means the k'th iteration step. Even though there are collisions, the density is still proportional to $fts_k(i)$ and inversely proportional to the cell volume $V(i)$, we can normalize to obtain the density distribution until the k'th iteration step is finished,

$$n_k(i) = C \cdot (fts_0(i) \cdot n_0 + fts_1(i) \cdot \Delta n + \cdots + fts_k(i) \cdot \Delta n) / V(i), \tag{7}$$

with C being the global normalization constant.

Please note that the density distribution $n_k(i)$ is then used in Equation (2) to determine the new collision time in the next (k+1)'th iteration step. We have checked this normalization procedure with different cell shapes, cell sizes, molecular collision cross sections and increased step Δn and proven that it is convergent.

## SIMULATION RESULTS AND COMPARISON WITH EXPERIMENTAL DATA

The simulation is carried out for a circular tube of L=0.1570 m and D=0.0161 m. For this circular tube of L/D=9.75, it is not only hard to calculate with kinetic theory because the length-to-diameter ratio is too small, but also hard to calculate with DSMC because the length-to-diameter ratio is too large. The gas simulated is nitrogen at 15°C. The collision cross section is calculated from the experimental data of the viscosity [7]. The experiment was carried out in the TRANSFLOW test rig [8].

The simulation domain is only the tube itself if we neglect the collisions inside the dosing dome. In such a case, $C = \frac{1}{4} \nu A$, with ν being the thermal molecular speed and A the area of the tube cross section. Consequently, the gas flow rate Q can be determined by the transmission probabilities $w_k$ in each iteration step,

$$Q = C \cdot (w_0 \cdot n_0 + w_1 \cdot \Delta n + \cdots + w_k \cdot \Delta n). \tag{8}$$

Other macroscopic parameters, such as bulk velocity and temperature, etc., can be obtained in the similar way.

In the simulation $n_0$ is chosen as $10^{18}$, corresponding to an initial P1=$3.98\times10^{-3}$ Pa and an initial Kn=100.1. $\Delta n$ is chosen as $10^{17}$. After k=9990 iteration steps, the final n1 is $10^{21}$, which is 1000 times bigger than the initial one, corresponding to a final P1=3.98 Pa and a final Kn=0.1. So the gas flow evolves from the free molecular flow to the beginning of the transitional flow. For each iteration step, $10^5$ test particles are used, which means that one test particle represents about $2.37\times10^{10}$ nitrogen molecules. There are 5 meshes along the radial direction and 40 meshes along the axial direction of the tube. In total the simulation domain is divided into 200 cells. The simulation is finished roughly in 112 hours by a desktop PC with a CPUat 2.67 GHz.

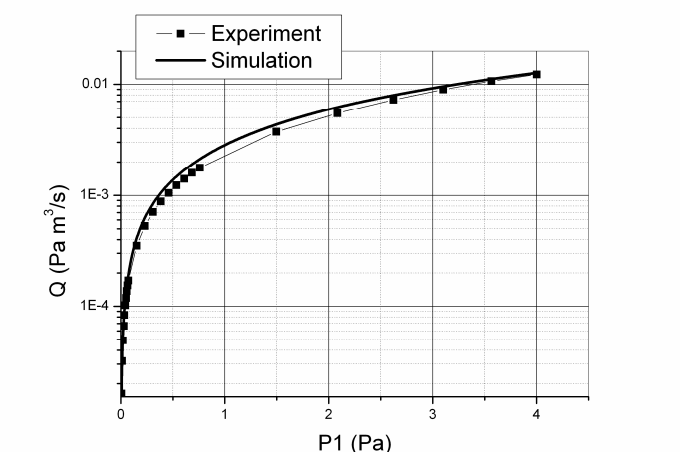


**FIGURE 3.** Comparison of experimental result and ProVac3D simulation for a circular tube of L/D=9.75.

The ProVac3D simulation result in Figure 3 shows a correct nonlinear increasing of the gas flow as P1 increases, but there is still a quantitative discrepancy with the experimental data. First of all, we have neglected the pressure in the pumping dome. From the experiment we know that the pressure in the pumping dome, though always being at least one order of magnitude lower than that in the dosing dome for this particular tube, will introduce a small back streaming. Secondly, the entrance effect or the collisions in the dosing dome may play a role. We will improve our model to include these effects.

Additionally, the simulated relative axial density and the axial bulk velocity inside the tube are shown in Figure 4 and Figure 5, respectively. We can see that the results for n1=$10^8$ and n1=$10^{21}$ are different, which is qualitatively reasonable. Unfortunately, we have neither the experimental data nor other numerical results with which to compare.

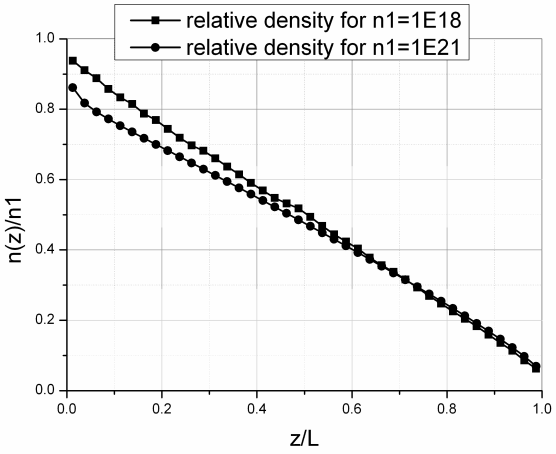


**FIGURE 4.** Relative density inside the tube for a circular tube of L/D=9.75.

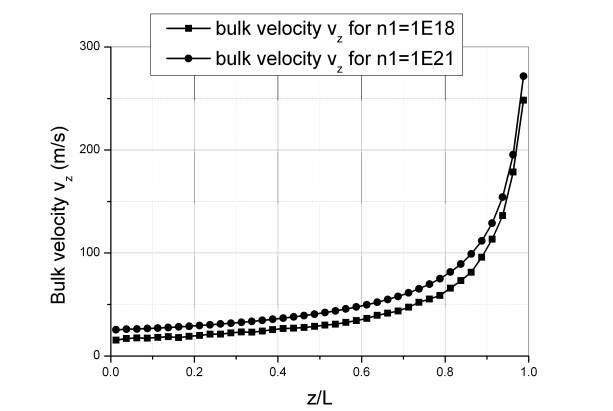


**FIGURE 5.** Bulk velocity in the axial direction for a circular tube of L/D=9.75.

## CONCLUSIONS

We have expanded our ProVac3D Monte Carlo simulation program to explore a new approach for simulating the transitional gas flow. In this new approach, the collisions between molecules are represented by the collisions of the probe particle with the target particles in the background. One convergent normalization scheme is suggested. With this procedure the gas flow through a circular tube is simulated as a function of the increasing molecular density in the dosing dome. The preliminary simulation result shows the correct nonlinear increasing of the gas flow rate. However, there is still a quantitative discrepancy with the experimental data, which means further improvement is needed.

Obviously, this new simulation approach has several advantages. First of all, like usual TPMC, the test particles are simulated one by one. So we will not need the huge memory like DSMC, which makes the simulation of a 3D problem possible. Actually, ProVac3D has implemented the entities to model a complicated 3D vacuum system. The present work shows that the computation time is much faster than DSMC. Secondly, as is well known, DSMC is very hard to parallelize. However, the parallelization of TPMC is straightforward. This work for ProVac3D is in progress. Thirdly, the gas flow is simulated by an iteration process in the suggested normalization scheme. This means that we can even interrupt the simulation process and later on continue the simulation of the further evolution of the gas flow by using the obtained result as the background. Nevertheless, the drawback of this normalization scheme is also clear since we always need to start from the free molecular flow and there are many simulation steps needed to reach the transition flow regime.

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