# TEST PARTICLE MONTE CARLO SIMULATION OF NEG COATED NARROW TUBULAR SAMPLES

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## Abstract

The pumping properties of the NEG coated vacuum chambers play an important role in the efficiency of vacuum system of accelerators. The sticking probability of the NEG films is one the most important parameters to characterise the pumping properties of the NEG coated vacuum chambers. In order to investigate the NEG film sticking probability, Test Particle Monte-Carlo (TPMC) models were used. The models were based on the design of the installed experimental setup in ASTeC Vacuum Science group laboratory at Daresbury Laboratory (DL). The results of the simulations have been used for interpreting the results of the measurements in the experimental setup.

## INTRODUCTION

Vacuum chamber coating with Non evaporable Getter (NEG) materials, developed at CERN [1], has been widely applied in vacuum systems of accelerators such as ELETTRA, ESRF, DIAMOND, Soleil, MAX IV, LHC, ILC, etc. The advantage of NEG coated vacuum chambers, such as their essentially low thermal outgassing rate, low photon and electron stimulated gas desorption and conductance-free distributed pumping ability, make it an ideal technology for conductance limited narrow-gap vacuum chambers in low emittance machines and Insertion Devices (IDs).

The properties of NEG coated vacuum chambers play an important role in the efficiency of the vacuum system of accelerators. The experimental installation for characterising the properties of the NEG coated films was designed and built in the ASTeC Vacuum Science group laboratory at Daresbury Laboratory (DL).

The sticking probability of NEG films is one the most important parameters to determine the pumping properties of the NEG coated vacuum chambers. The pumping properties of a NEG coated surface can be characterised by obtaining a sticking probability for different gases as a function of the amount of adsorbed gas per unit of its surface area $A_{NEG}$. The pumping speed S, of surface $A_{NEG}$, with sticking probability $\alpha$ can be calculated with:

$$S = \alpha A_{NEG} \frac{v}{4}$$

Where $v$ is the mean molecular velocity of the gas. To apply this equation a uniform molecular velocity distribution is required [1-3]. When desorption and pumping surfaces are located in different parts of the vacuum system, especially when $\alpha \approx 1$, this condition fails. This condition with the contribution of the strong beaming effect in narrow tubes may lead to a significant error in the sticking probability.

The previous study showed that the data obtained with TPMC modelling can be used to accurately determine the sticking probability of the NEG coating for various gases [4].

In order to investigate the relationship between measured pressures and the NEG film sticking probability, Test Particle Monte-Carlo (TPMC) models were built for each configuration with the use of the MOLFLOW program written by R. Kersevan [4, 5].

## TEST PARTICLE MONTE-CARLO (TPMC) MODEL

The models were designed based on the installed experimental setup in ASTeC Vacuum Science group laboratory at Daresbury Laboratory (DL) which is described in [4, 6].

The NEG coated samples are tubes with a large L/d ratio where L and d are the length and diameter of the tube, respectively. The bottom end of the tube is connected to a vacuum chamber equipped with a pumping system, gas injection, an extractor gauge and an RGA. Another RGA is installed on the top of the NEG coated tube.

For narrow tube measurement, a bypass system was added to the system to allow faster pre-evacuate. The 3D model of one configuration is shown in Fig.1.



Figure 1: 3D model used for TMPC simulations.

The TPMC model consists of a number of vertexes (points) in 3D space which create the facets (flat surfaces). The facets must create a closed volume. The parameters of each facet including sticking probability, desorption law, reflectivity law, temperature, and opacity determine the case of use of the facet.

In this model, one of the ports in the big chamber (at the bottom of Fig.1) was assigned as an inlet. The internal NEG sample surfaces were adsorbing surfaces. The second port and the upper chamber were used as gauges which are RGAs in the installed experimental chamber.

The discrete numbers of sticking probability in the range $10^{-4} < \alpha < 1$ for the facets representing the NEG coated sample was applied to the models. The average pressure P at each facet can be calculated from the impingement rate [5].

A number of TPMC models were built and run for different tubular samples. In this study, we will focus on narrow tubes with 0.5 m length and 5 mm, 7 mm and 9 mm diameter. The model assumes that that the sticking probability is uniform along the entire surface of the sample tube.

## RESULTS

There are different methods to calculate the sticking probability from the experimental and simulation results. According to previous studies [5], the most accurate result can be obtained by taking the ratio between two pressure readings (P1/P2) where P1 and P2 are the pressures on the bottom chamber and top of the NEG coated tube respectively. This method is independent of the injected gas flow in the molecular flow regime leading to an accuracy of 10%.

However, this method is time consuming. Computing each point related to the various sticking probability for different configurations takes significant time.

For $10^{-4} < \alpha < 10^{-3}$ the number of test particles (around few $10^5$) is enough to have 10% error that takes one or two days per CPU core. For $\alpha \approx 1$ it needs at least few $10^7$ test particle to have a similar error. It takes few weeks per CPU core.

In addition, by decreasing the diameter of the NEG coated tube, the time required to compute increases.

The results for the 0.5m NEG coated tube with 5 mm, 7 mm and 9 mm diameter are shown in Fig 2.

The fitting formula for the results obtained with the TPMC simulations can be used for practical calculations of the sticking probability of systems with similar length and configuration:

$$Log\left(\frac{P1}{P2}\right) = \frac{0.6(Log\alpha)^3 + 6.2(log\alpha)^2 + 23.4Log\alpha - 0.5d + 37}{(Log\alpha)^2 + 5Log\alpha + 8}$$

Where $\alpha$ is the sticking probability and $d$ is the tube diameter.

The normalised pressure profile in the NEG coated tube with a diameter of 9 mm for various sticking probability is shown in Fig 3. The fluctuation in $\alpha=0.7$ indicates that the error in the pressure profile in the sample NEG coated tube is more than P1/P2. In this case, the $1.2\times10^7$ test particles that are produced required 3 weeks per CPU core.
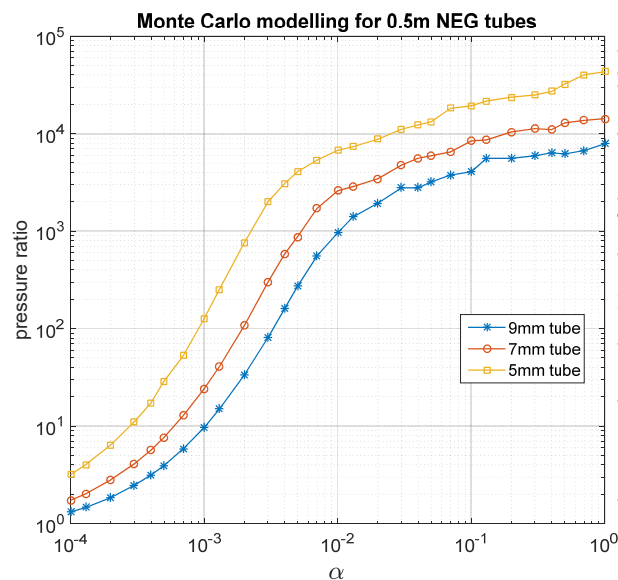
Figure 2: Pressure ratio P1/P2 as a function of sticking probability of the NEG coating for the 0.5m long tubular samples with 5mm, 7mm and 9mm diameter.

At the end of the sample NEG coated tube the pressure slightly increases. This increase is higher for the larger sticking probability. This is due to the beaming effect in the system. Some of the gas molecules arriving at the RGA inlet return to the sample tube and cause a rise in pressure at the end of the tube. By decreasing the tube diameter this effect is stronger.
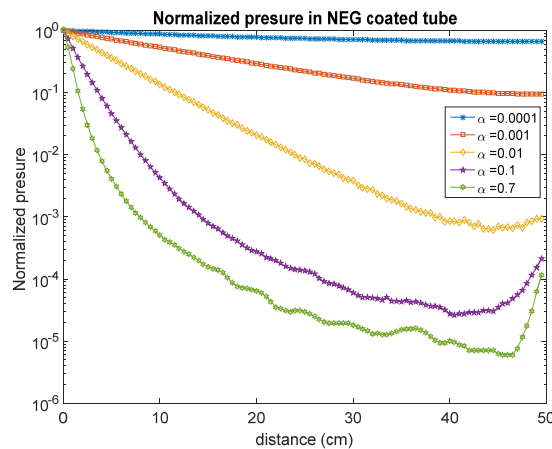
Figure 3: Normalised pressure profile for the 0.5 m long NEG coated tube with the diameter of 9 mm

A further set of simulations were done to investigate the effect of the RGA location on the pressure ratio. Results show that by increasing the distance between the RGA installed on the top of the sample tube and the end of the tube under test, the pressure ratio P1/P2 decreased.

This decrease in pressure ratio increases with increasing sticking probability. For example, if the distance between the RGA and the tube is increased by 135 mm, for a 0.5 m long sample tube with a diameter of 9 mm, the pressure ratio is decreased by 0.70 when $\alpha=1$. While for $\alpha=0.001$, this reduction is 0.8. This means that the sensitivity of the

experiment is decreased by increasing the distance of RGA from the tube.

## CONCLUSION

TPMC modelling was used for accurate calculating of sticking probability of NEG coated narrow tubes. Results of the TPMC modelling and fitting formula will be used for experimental evaluation of the sticking probabilities for NEG coated narrow tubes. The results show the strong beaming effect in the NEG coated narrow tubes with large sticking probability. This effect increases with decreasing tube diameter and increasing the sticking probability.

The effect of the RGA location on pressure ratio was investigated. Results show that the sensitivity of the experiment is decreased by increasing the distance of RGA from the tube.

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