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Simulations of Effusion from ISOL Target/Ion Source Systems *

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Abstract

Monte-Carlo simulations of the low- and high-conductivity Target/Ion Source systems used at Oak Ridge National Laboratory for effusion measurements are performed. Comparisons with the corresponding experimental data for the different geometries are presented and discussed. Independent checks of the simulation using data for simple geometries and using the conductance approach well known in vacuum technology are performed. A simulation based comparison between the low- and high-conductivity systems is also presented.

Key words : ISOL targets; Release curve; Effusion; Monte-Carlo simulation.

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1 Introduction

In a previous work [1], we reported on the implementation of a Monte-Carlo calculation to simulate the release process of radioactive isotopes from ISOL-Targets. In this calculation, the effusion process is simulated using the tool-kit Geant-4 [2] by tracking the particles through the target until released from the ion source. The diffusion is treated analytically using the solution of Fick's diffusion equation [3] for the considered form of the target material: foils, fibers or grains. We have also shown that it is possible to characterize the release process and extract its important parameters, the diffusion coefficient (D) and the sticking time per collision (τ_s), by fitting the simulated release curve to the experimental one measured with a given target geometry for a given isotope. The extracted information can then be used to improve the efficiency of existing targets and design new geometries more suitable to produce beams of rare isotopes.

In the same study, the simulation of the whole release process (diffusion, effusion and decay) of ^{8}Li from the RIST target [4] tested online at ISOLDE-CERN has revealed that the diffusion coefficient D can be determined only if the diffusion process is faster than the decay of the considered isotope. To determin D when the decay is faster than the diffusion (case of ^{8}Li), we could use the value measured for the closest stable isotope (^{7}Li).

To better characterize the diffusion and effusion processes and avoid the uncertainty coming from the undertermination of D, we propose here to deconvolute the two processes and study them separately. This will allow the unambiguous extraction of the release parameters from the appropriate measurements: τ_s from effusion measurements and D from diffusion measurements. It will also provide an independent benchmark of the effusion and diffusion parts of the calculation.

In this paper, we focus on the study of the effusion part of the release process. The only parameter in this case is the sticking time τ_s. Furthermore, if we consider non-sticky particles (τ_s=0), noble gases for example, there will be no parameters at all and the problem is fully determined for a given geometry. Using effusion measurements for non-sticky particles, we can perform a direct and independent benchmarck of the effusion part of the calculation. The calculation will provide us with information like the total path length and number of collsions for a given geometry which could later be used to measure the sticking time of other particles.

We report here on the simulation of three Target/Ion Source systems used at Oak Ridge National Laboratory [5, 6] to measure effusion times of different rare gases. Both low- and high-conductivity systems were used in these measurements. In the next section, the principle and the conditions of these measurements will be presented. In section 3, the results of the simulation of the low-conductivity systems will be presented and compared with the corresponding data. Some checks of the simulation using data for simple geometry components and using the conductance approach will be presented and discussed in section 4. Section 5 is a comparison between the low- and high-conductivity systems based on the simulation. Our concluding remarks will be given in the last section.

2 Effusion Measurements at ORNL

In these measurements, the considered gas is admitted to the system at a controlled rate through a needle-valve (see figure 1.a) until a steady flow is reached. Then, a fast valve system closes the inlet in about 0.1 ms and the decay rate of the ion source current is measured, see figure 1.b. The characteristic effusion time, τ_e, is determined by fitting the decay curve using an exponential form: $\alpha\ e^{-t/\tau_e}$.

The measurements were performed for different noble gases: He, Ne, Ar, Kr and Xe at different temperatures: 1073-1473 K. Two kinds of geometries were used: low- and high-conductivity systems. The low-conductivity geometry is characterised by small section tubes connecting the target chamber to the ion source, see figure 2.a. In the high-conductivity geometry, a more open connection is used, see figure 2.b.

For each geometry, the data were taken for both an empty target chamber and one filled with a Reticulated Vitreous Carbon Foam (RVCF) matrix. The simulation is performed only for the case of empty target chambers.

3 Simulation of the Low-Conductivity Systems

There are two low-conductivity systems for which effusion times were measured. They differ by the size of the target chamber. In the first (figure 1.a), the target chamber was a 1.5 cm diameter and 19.3 cm long tube. In the second (figure 2.a), a larger tube was used: 2.4 cm diameter with the same length. In both cases the target was connected to the ion source using an elbow (0.87 cm diamter, 3.5 cm total axis length) and a tube (0.87 cm diameter and 10 cm long).

The simulation of the first system (figure 1.a) showed that particles travel on average 125 m before leaving through the ion source and collide about 11000 times with the internal surfaces of the system. The effusion time calculated for ^4He at 1473 K is 44.9 ms which is about twice the measured value ($\sim$ 23 ms). Trying to understand the extra delay in the simulation, we simulated the case without the ion source in order to estimate its contribution to the delay, the results are summarised in table 1.

We notice that by removing the ion source, the simulation is faster than the data which seems to be consistent with the data because the ion source will introduce an additional delay anyway. The question now is: what is the real delay introduced by the ion source? Since we don't simulate the ionisation process in the calculation, it is possible that we predict more delay than the experiment where particles could be extracted faster once ionised in the ion source. A possible precise measurement of the delay introduced by the ion source could be carried out by using a simple tube connected to the ion source instead of the whole system.

The simulation of the second low-conductivity system (figure 2.a) showed that on average particles travel about 300 m and collide about 15000 times before leaving the system. For ^4He at 1473 K, the calculated effusion time is 105.6 ms which is about 3 times the experimental value ($\sim$ 38 ms). And more surprisingly, even after removing the ion source the simulation predict more delay than the experiment, see table 2. This is of course inconsistent with the data and with the first geometry, because the argument of the accelerating effect of the ion source can't explain this discrepancy.

The present conclusion is that the quantitative increase in the delay time calculated for the larger tube is in the right direction, but it is larger than seen experimentally. In order to find the source of this discrepancy, we have performed some independent checks of the simulation. Tests using basic geometry components were carried out and confronted to experimental data. They are discussed in more details in the next section.

4 Test of the Simulation

4.1 Using Data for Simple Shapes

In 1960, Levenson et al. [7] reported on measurements of transmission probability of particles through simple shapes: tubes, elbows, etc. The measurements were performed by admitting a gas into one end of the considered shape and measuring the pressure at entrances and exits. The transmission probabilities from one end to another were then determined using the pressure difference.

After adapting the calculation to give the transmission probability, the simulation was performed for the tube and elbow shapes, the basic components of ORNL's systems. Tubes and Elbows with different length-to-radius ratios (L/R) were considered. In the case of elbows, L is the total axis length.

Comparisons to the data are shown in figure 3.a for tubes and figure 3.b for elbows.

We notice that the simulation agrees very well with the data within error bars. This test provides an important validation of the Monte Carlo simulations.

This first test dealt only with transmission probabilities of particles through basic shapes and did not test the delay time predicted by the simulation. In order to check the timing from the calculation, we have used the conductance approach well known in vacuum technology.

4.2 Using the Conductance Approach

The problem of unsteady molecular flow through a long tube could be resolved by analogy to the one-dimension heat-conduction problem, see ref. [8]. Consider the case of N_0 particles trapped between the two ends of a long tube (L >> R). At t = 0, one end of the tube is opened and particles start leaving the tube. This is of course a non steady flow of particles because the number of particles leaving the tube is varying in time until no particle is left inside the tube.

Based on the above analogy, the number of particles leaving the tube at a time t is given by :

$$N(t) = N_0 \times \frac{8}{\pi^2 \tau_0} \sum_{n=0}^{\infty} e^{-(2n+1)^2 \frac{t}{\tau_0}},$$

τ_0 is the characteristic delay time (effusion time) given by the following expression :

$$\tau_0 = \frac{4}{\pi^2} \frac{V}{C}$$

where $V = \pi R^2 L$ is the volume of the tube, $C = \frac{2}{3}\pi \frac{R^3}{L} v$ is the conductance of the tube assuming L >> R. $v = \sqrt{\frac{8kT}{\pi M}}$ is the average Maxwell velocity for a particle of mass M at a temperature T.

The simulation was run for $N_0 = 10^5$ particles using a 1 cm diameter and 100 cm long tube ($V = 78.5\ cm^3$). The conductance calculated for ^{4}He at 1473 K is $C = 730.8\ cm^3/s$ resulting in a delay time $\tau_0 = 43.5\ ms$. The value determined from the simulation is 42.8 ms, in a good agreement with the conductance approach.

The comparison of the simulated N(t) with the conductance formula is shown in figure 4. A very good agreement is seen except at longer times where the end effect of the tube manifest itself by liberating all particles at a finite time.

The simulation gives a delay time in good agreement with the conductance approach for a simple tube. In the next section we consider more complicated systems composed of connected simple components

4.3 Conductance of the Low-Conductivity Systems

Because the geometry of the low-conductivity systems is essentially simple tubes with different lengths and sections connected to each other, it is possible to treat it like the serial coupling of these same tubes. In this case, the conductance C of the whole system could be obtained by :

$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2} + \frac{1}{C_3} + ...$$

where 1,2,3,... denote the tubes. The total volume of the system is simply the sum of volumes $V = V_1 + V_2 + V_3 + ...$ The characteristic delay time in the system could be determined using the same expression for τ_0.

Applied to the two low-conductivity systems, this approach gave the results shown in table 3.

We notice a good agreement between the simulation and the conductance approach for both geometries. Note that in table 3 neither the Monte Carlo simulation nor the conductance calculation include any delay from the ion source.

5 Comparison of the Low- and High- Conductivity Systems

The simulation of the high-conductivity system (figure 2.b) showed that on average, particles travel about 355 m and collide about 22000 times inside the system including the ion source. The delay time calculated for ^{4}He at 1473 K is 127.3 ms which is more than 3 times the experimental value: 34.8 ms, see table 4. Simulating the case without the ion source gives a delay time of 33.5 ms which is smaller than the measured value. This result is consistent with the first low-conductivity geometry because the difference with the data could be explained by an eventual effect of the ion source.

The high-conductivity system was designed with more open geometry in the purpose of a faster release, but the experiment showed that the first low-conductivity system is faster. In order to understand the reason for that, we will use the conductance approach which gives almost the same results as the simulation.

In the conductance approach, the delay time τ_0 is proportional to the ratio volume-to-conductance (V/C) of the system. So, in order to compare the conductance of two systems, we should consider the same volume V. In this case, the faster system is the one with the higher conductance C. Comparing the high-conductivity system with a low-conductivity system having the same volume showed that the high-conductivity system is about 2 times faster than the low-conductivity one (71.1 ms for the low-conductivity case vs. 33.5 ms for the high-conductivity case). This confirms that using a more open geometry helps make the release faster. (Again the delay times are calculated without including the ion source.) However, the geometry of figure 1.a is faster than that of the more open geometry of figure 2.b, because it is dominated by the smaller overall geometry.

6 Concluding Remarks

Monte-Carlo simulations of the low- and high-conductivity Target/Ion Source systems, recently tested at Oak Ridge National Laboratory, were performed. Compared to the experimental data, the simulation predicts more delay for all the systems. The simulation of the first low-conductivity and the high-conductivity systems without the ion source seems to give closer results to the data. However, the discrepancy seen for the second low-conductivity geometry can not be explained by an eventual effect of the ion source. On the other hand, the simulation seems to agree well with data measured for simple geometries and with the results obtained using the conductance approach well known in vacuum technology. The same conductance approach showed that the comparison of the low- and high-conductivity systems should be done for systems with the same total volume. In this case, the high-conductivity system is faster confirming the advantage of using more open geometries if the total volume is not increased.

At this stage, we consider that the simulation is partially validated. However, other verfications are needed. In collaboration with the ORNL's group, we propose special measurements to study the effect of the ion source. This could be done by replacing the target by a simple tube directly connected to the ion source. It will also be important to perform other measurements to confirm the data obtained for the second low-conductivity system.

Once the simulation is validated using the experimental data from noble gases, the calculated total path length and number of collisions will be fully determined for a given geometry. This information could then be used to extract the sticking time of more reactive species in future measurements. Combined with the future diffusion measurements at the UNISOR facility at Oak Ridge, a complete release study of an important range of rare isotopes will be possible.

References

[1] B. Mustapha and J.A. Nolen, Proceedings of the 14th International Conference On Electromagnetic Isotope Separators And Techniques Related To Their Applications, May 6-10, 2002, Vectoria, Canada, to be published in Nucl. Instr. and Meth. B.

[2] Geant4 home page : http://geant4.web.cern.ch/geant4/.

[3] "The mathematics of diffusion" by John Crank, Clarendon Press, Oxford, 1975.

[4] C. J. Densham et al, Nucl. Instr. and Meth. B 126 (1997) 154.

[5] J.C. Bilheux, G.D. Alton et al, Proceedings of the Particle Accelerator Conference, June 18-22, 2001, Chicago, Illinois.

[6] J.C. Bilheux, G.D. Alton et al, Proceedings of the International Conference on the Application of Accelerators in Research and Industry, Nov. 12-17, 2002, Denton, Texas, to be published by AIP.

[7] L.L. Levenson et al, Proceedings of the 7th National Symposium on Vacuum Technology Transactions, American Vacuum Society, Oct. 12-14, 1960, Cleveland, Ohio.

[8] "Foundations of Vacuum Science and Technology", edited by J. M. Lafferty, John Wiley & Sons, 1998.

Table 1 : Results of the simulation as the average number of surface collisions and total path length of particles for the first low-conductivity system (figure 1.a) with and without the ion source. The calculated delay times for ^{4}He at 1473 K are compared to the measured value in the bottom line.

	W/ Ion Source	*No Ion Source*	*Experiment*
$< N_{collisions} >$	10987	4466	–
$< Path\, length > (m)$	125.3	90.3	-
$\tau(ms)$	44.9	19.1	23.0

Table 2 : Results of the simulation as the average number of surface collisions and total path length of particles for the second low-conductivity system (figure 2.a) with and without the ion source. The calculated delay times for ^{4}He at 1473 K are compared to the measured value in the bottom line.

	W/ Ion Source	*No Ion Source*	*Experiment*
$< N_{collisions} >$	15550	6540	–
$< Path\, length > (m)$	294.7	130.6	-
$\tau(ms)$	105.6	46.8	38.1

Table 3 : Comparison of the simulation with the conductance approach for the two low-conductivity systems.

	V (cm^3)	C (cm^3/s)	Conductance τ_0 (ms)	Simulation τ_0 (ms)	Experiment τ_0 (ms)
1^{st} *system*	40.3	803.4	20.3	19.1	23.0
2^{nd} *system*	97.0	856.9	45.9	46.8	38.1

Table 4 : Results of the simulation as the average number of surface collisions and total path length of particles for the high-conductivity system (figure 2.b) with and without the ion source. The calculated delay times for ^{4}He at 1473 K are compared to the measured value in the bottom line.

	W/ Ion Source	*No Ion Source*	*Experiment*
$< N_{collisions} >$	22155	5784	–
$< Path\,length >$ (m)	355.5	93.5	-
τ(ms)	127.3	33.5	34.8

Figure captions :

Figure 1 : Principle of ORNL measurements : a) A typical geometry used to measure effusion times (1st low-conductance system) showing all geometry components including the Gas Inlet/Valve system. b) A typical measured release curve showing the steady flow while the valve is open (the plateau) and the exponential decrease after the valve is closed.

Figure 2 : Low- and high-conductivity systems : a) Geometry of a low-conductivity system (2nd low-conductivity system). b) Geometry of the high-conductivity system.

Figure 3 : Test of simulation using experimental data : a) case of a tube and b) case of an elbow. Open circles with error bars are data from [7] and dashed line is the result of the simulation.

Figure 4 : Comparison of the simulation with the conductance approach for a long tube

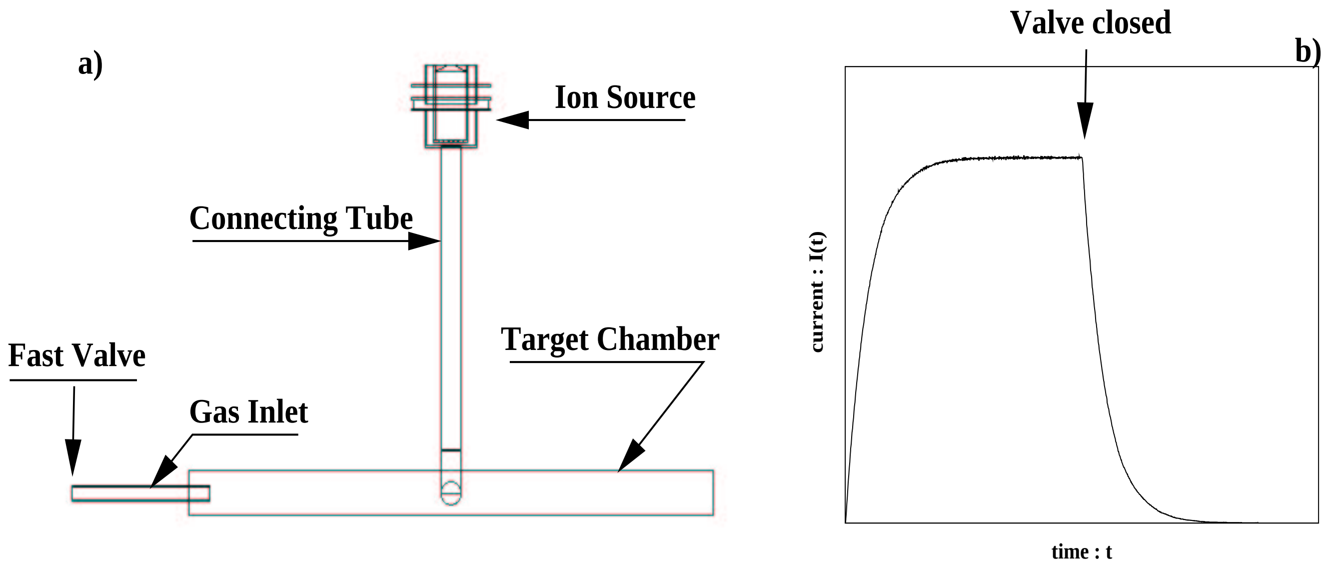

Figure 1.

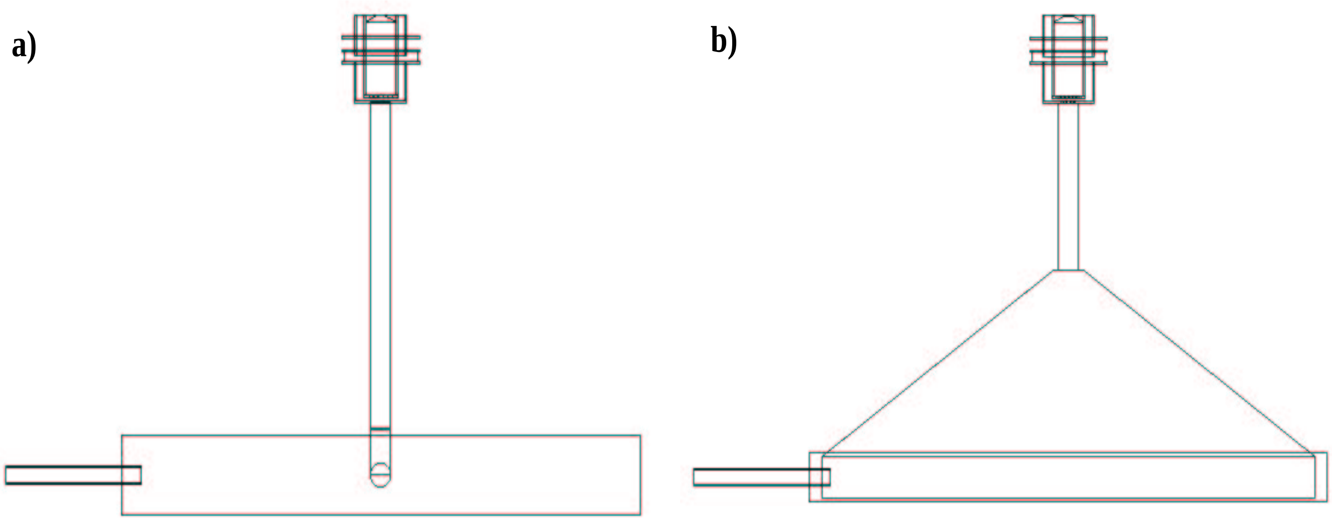

Figure 2.

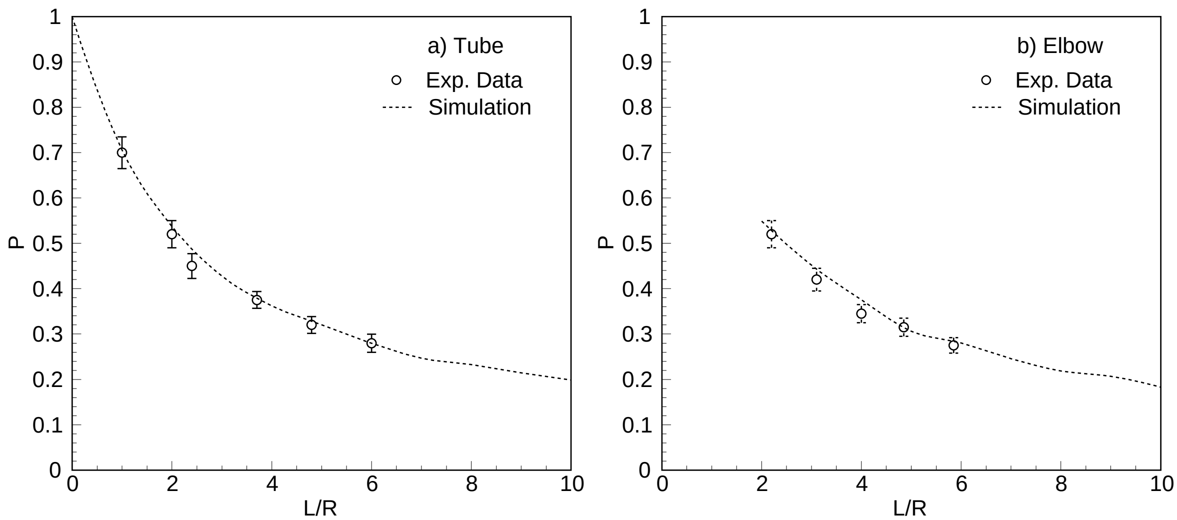

Figure 3.

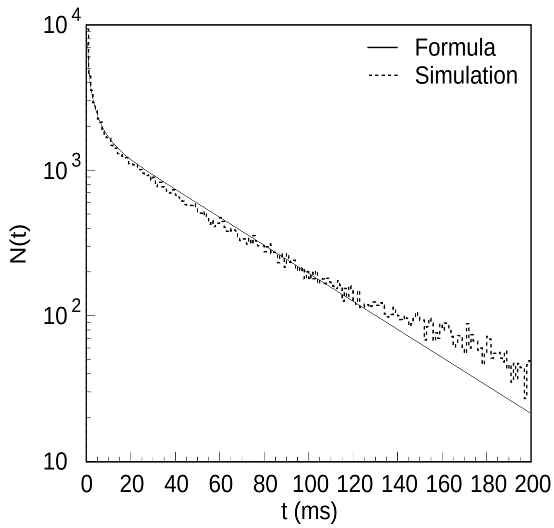

Figure 4.