

# ISOL TARGET–VAPOR TRANSPORT SYSTEM SIMULATIONS \*

Y. Zhang, I. Remec, Z. Liu,  
Oak Ridge National Laboratory, Oak Ridge, TN 37831, U.S.A.

## Abstract

Computational simulation studies offer cost effective techniques for ISOL target designs with optimized diffusion release properties and vapor transport systems with shorter effusive-flow distances. In this paper, analytic solutions to the diffusion equation involving radioactive decay are compared with those obtained from a finite-difference code for rare isotopes diffusion release from simple geometry targets. The viability of the Monte Carlo technique as a practical means for optimally designing vapor transport systems is demonstrated by simulations of neutral particle effusive-flow through several complex target-vapor transport systems. Important issues which affect the yield rates of short-lived species generated in high power ISOL targets are also discussed.

## INTRODUCTION

Intensities of beams of short-lived species, generated with the Isotope Separator On-line (ISOL) techniques, are limited by decay losses associated with times required for diffusion from target materials and effusive-flow from the target to the ion source. For example, times needed for diffusion of particles from solid targets may range from a few seconds to hundreds of hours, while the effusive-flow times for particle transport to the ion source - depend on the mass of the species, the porosity of the target material, the temperature, the geometry and size of the target-vapor transport system and the chemistry between the particle and materials from which the system is built. Therefore, to provide useful beam intensities of short-lived isotopes, it is imperative to minimize delay times for these limiting processes by optimally designing both production targets and vapor transport systems [1].

Following diffusion–release from a production target, particles must be transported through a highly permeable target matrix and a transient vapor transport system to an ion source, where a fraction of the particles are ionized, extracted from the source and accelerated. Time delays for diffusion are usually longer than those for effusive-flow for elements with low enthalpies of adsorption. However, for electronegative elements with appreciable enthalpies of adsorption, the delay times may be reversed. Target-vapor transport systems can be optimized in terms of geometry and size to minimize particle travel distances and numbers of surface collisions during the transport [1]. In this paper, analytic solutions to the diffusion equation involving radioactive decay are compared with those from a finite-difference code; simulation with a Monte Carlo effusion code is applied to optimize target-vapor transport

systems for faster particle effusive-flow, and combined decay losses in the two processes are calculated.

## DIFFUSION AND RADIOACTIVE DECAY

The diffusion process for a short-lived isotope of concentration  $C$  and decay constant  $\lambda$  can be described by Fick's second equation [2]:

$$\frac{\partial C}{\partial t} = D \cdot \nabla^2 C + S - \lambda \cdot C \quad (1)$$

where,  $D$  is the diffusion coefficient and,  $S$  is the production rate of the species. The diffusion coefficient  $D$  depends on the physical and chemical properties of the binary diffusion couple – target material and diffusing particle, as well as target temperature.

For a simple geometry, homogenous target materials operated at uniform temperatures, constant production rates and initial conditions, the above partial differential equation (PDE) has analytic solutions for one dimensional diffusion in planar geometry targets fabricated with thin films and thin slabs. Analytic solutions to Eq.1 can be derived out by separation of variables and the Fourier transform techniques:

$$\text{Thin film: } J(t) = \frac{2SD}{d^2} \cdot \sum_{k=0}^{\infty} \left\{ \frac{1 - e^{-\left[ \frac{D \cdot (k+0.5)^2 \cdot \pi^2}{d^2} + \lambda \right] t}}}{\frac{D \cdot (k+0.5)^2 \cdot \pi^2}{d^2} + \lambda} \right\} \quad (2)$$

$$\text{Thin slab: } J(t) = \frac{8SD}{d^2} \cdot \sum_{k=0}^{\infty} \left\{ \frac{1 - e^{-\left[ \frac{D \cdot (2k+1)^2 \cdot \pi^2}{d^2} + \lambda \right] t}}}{\frac{D \cdot (2k+1)^2 \cdot \pi^2}{d^2} + \lambda} \right\} \quad (3)$$

where,  $J$  is the yield rate of particles out of the target surfaces and,  $d$  is the target thickness.

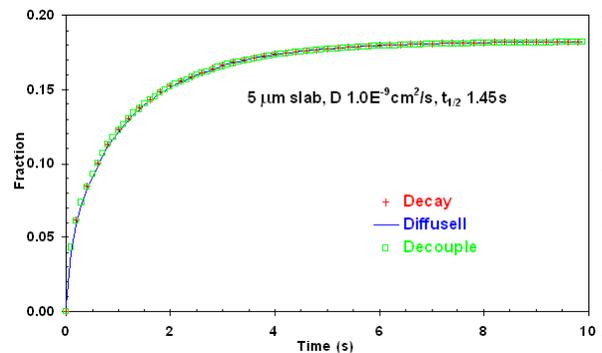


Figure 1: Yield of  $^{133}\text{Sn}$  calculated with 3 different solutions.

It is also possible to use analytic solutions to Eq.1 without the decay term ( $\lambda=0$ , for stable isotopes) and then apply radioactive decay [3]. However, in most cases, analytic solutions to Eq.1 do not exist or in a few cases

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where they do exist, are too complicated. Fortunately, numerical approximation techniques are widely applicable to most practical diffusion problems. We developed a finite-difference code, *Diffuse II*, which solves the PDE of diffusion with radioactive decay - for planar geometry thin films and slabs, cylindrical and spherical geometry targets [1]. To verify the accuracy of the *Diffuse II* code, we compare the results with analytic solutions for simple geometry targets. Fig.1 compares the results obtained with analytic solutions from Eq.3 (Decay) for  $^{133}\text{Sn}$  diffusion yield from a thin slab  $\text{UC}_2$  target with the results obtained from *Diffuse II* (decay included), and the results by first calculating stable element diffusion and then adding the radioactive decay (Decouple). The maximum difference between all the 3 solutions is less than 1%. Similar agreements are also achieved for thin film calculations.

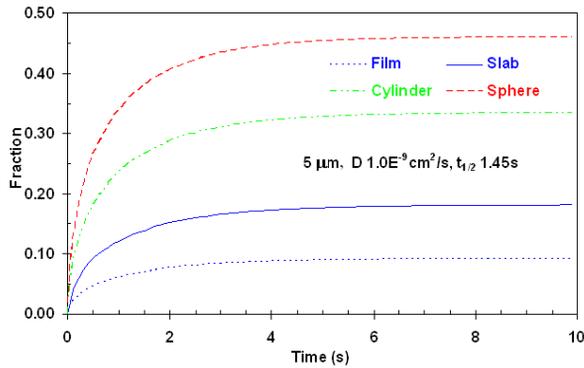


Figure 2: Fractional release of  $^{133}\text{Sn}$  from 4 different targets.

Diffusion release also depends on geometry, as shown in Fig.2 – the fractional yields of  $^{133}\text{Sn}$  from 4 different geometry  $\text{UC}_2$  targets simulated with *Diffuse II* (sphere and cylinder, diameter 5  $\mu\text{m}$ ; slab and film, 5  $\mu\text{m}$  thick).

### EFFUSIVE FLOW

Under molecular flow conditions, the characteristic evacuation time for particles passing through a tube with one end closed is [4]:

$$t_c = \frac{4V}{\pi^2 C} \quad (4)$$

where,  $V$  is the volume, and  $C$  is the conductance of the straight tube when both ends open.

A more generalized formula including particle sticking times on the surfaces, is [5]:

$$t_c = N_b \tau_0 \cdot e^{\frac{H_{ad}}{k \cdot T}} + \frac{3}{4} \cdot \frac{l}{v} \quad (5)$$

where,  $H_{ad}$  is the enthalpy of adsorption for the particle on a given surface;  $N_b$  is the characteristic number of surface collisions with the walls of the vacuum system during transport,  $l$  is the average distance traveled by a particle in the transport system;  $v$  is the average Maxwell velocity;  $T$  is the absolute temperature;  $k$  is the Boltzmann constant, and  $\tau_0$  is a time constant.

For complicated vapor transport systems, applications of vacuum conductance theory are generally compromised

as its accuracy deteriorates significantly. However, Monte Carlo simulations offer accurate solutions for complicated systems, as well as for simpler systems. We developed a code *Effusion* to simulate effusive-flow of particles through complicated vacuum systems. *Effusion* has been used to study a novel concept of vapor transport systems with approximately two orders of magnitude shorter effusive-flow distances than conventional vapor transport systems [6]. Recently, the code was parallelized to simulate effusive-flow in a proposed two-step target [7].

Because of the porous nature of ISOL target materials as required for fast particle diffusion release and effusive-flow transport, the thermal conductivity is usually poor and consequently, heat removal is very inefficient in a direct target. In a two-step target, however, the first step target is made of a high density material with high thermal conductivity such as W or Hg in which high power light ion beams produce neutrons via spallation reactions. The neutrons generate radioactive species through fission reactions in the second step target made of actinide material. In this conception, the second step target and vapor transport system temperatures are insulated from that of the first step, therefore, efficient heat removal, and optimum diffusion and vapor transport are achievable.

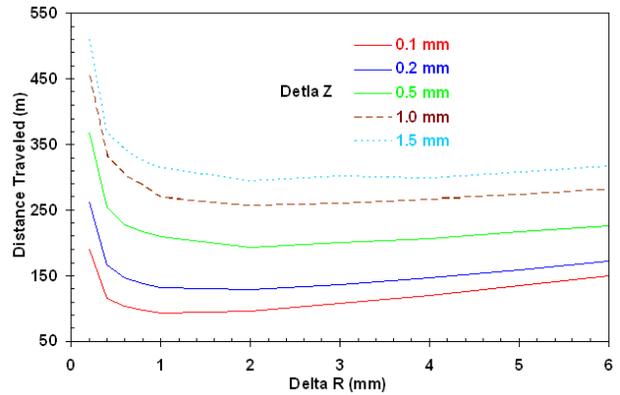


Figure 3: Average distance traveled versus matrix spacing.

Compared with a direct ISOL target, a two-step target is more complicated, and the size of the second step target is much larger because it surrounds the first step target and sufficient target thickness is necessary to provide high neutron-induced fission rates. The target material and matrix design also need to meet the requirements for fast diffusion release, similar to a conventional direct ISOL target. However, the effusive-flow of particles becomes a concern - because of the increased size of the second step target. In the simulations, the target is assumed to be composed of an inner cylindrical first step W target surrounded by an annular second step  $\text{UC}_2$  target of inner diameter 5 cm, outer diameter 15 cm and length 25 cm. The second step target is made up of stacked disks of sintered  $\text{UC}_2$  fine powders deposited on both sides of thin annular graphite disks (the overall thickness of a disk is approximately 0.4 mm). The annular gap between the disks and the outer chamber walls (Delta R) as well as the axial spacing between the disks (Delta Z) significantly affects the number of particle collisions with the surfaces

and the average distance a particle travels during the effusive-flow transport.

As shown in Fig.3, the average distance traveled by a particle is reduced when the spacing between disks, Delta Z, is decreased. It reaches a minimum at the annular gap Delta R of ~1 to 2 mm. The number of collisions with surfaces rapidly decreases with increasing Delta Z up to ~2 mm, after which the decrease is slower, as shown in Fig.4. The optimum Delta R is ~1 to 2 mm and an optimum Delta Z is approximately 0.1 mm that minimize the vapor transport time. In the studies, particle effusive-flow times were also simulated for different target lengths with Delta Z 0.1 mm and Delta R 2 mm, as shown in Fig.5. The average distance a particle travels and the average numbers of surface collisions increase linearly with the target lengths, similar as the simulation results for conventional ISOL targets. In the simulations, uniform particle generation rate inside the target is assumed.

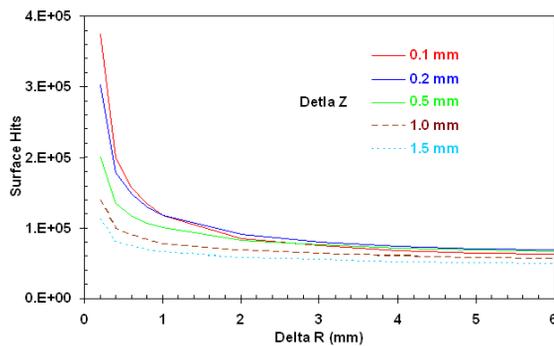


Figure 4: Average surface collisions versus matrix spacing.

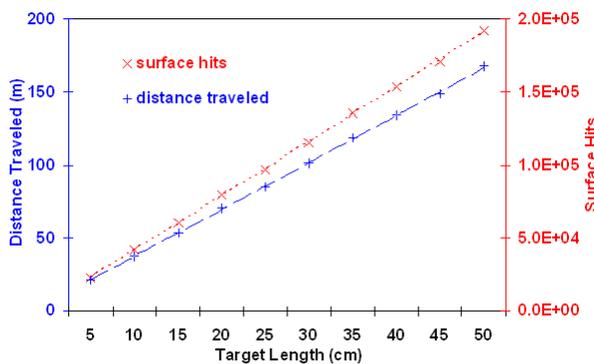


Figure 5: Average distance traveled and average number of surface collisions versus the target length.

### COMBINED EFFECTS OF DIFFUSION AND EFFUSIVE FLOW

The production rate of an isotope with an ISOL facility is mainly limited by: radioactive decay, cross section of nuclear reaction, primary beam intensity and energy, effective target thickness, leakage of the target-vapor transport systems, ionization efficiency of the ion source, acceleration and transport efficiency of the accelerator and beam transport systems. Most decay losses of short-lived particles are dominated by the time required for diffusion and effusive-flow, while decay losses due to all

other processes such as - ionization in the ion source and acceleration to higher energies can usually be ignored.

An approximation of the maximum yield rate involving decay losses in effusive-flow for the steady state (constant diffusion release rate), may also apply for the transient:

$$Y(t) \approx \frac{J(t)}{1 + t_C \cdot \lambda} \cdot [1 - e^{-(\lambda + \frac{1}{t_C})t}] \quad (6)$$

where,  $J$  is diffusion release rate from the target surfaces, calculated with *Diffuse II* or an analytic solution to Eq.1 including decay;  $t_C$  is the characteristic time for particle transport through the vapor transport systems calculated with *Effusion* or from vacuum conduction theory.

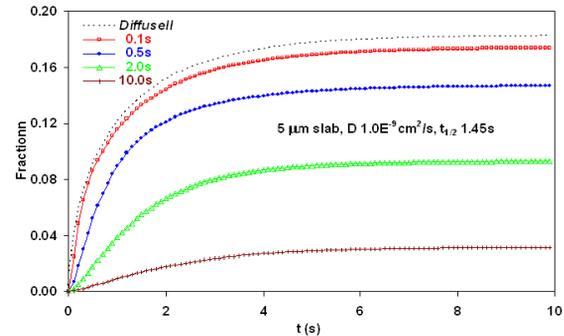


Figure 6: Fractional release rate of  $^{133}\text{Sn}$  versus effusion time.

Fig.6 shows the fractional release rate of  $^{133}\text{Sn}$  from a slab  $\text{UC}_2$  target and at different effusive-flow delays. For short-lived species, delays in the diffusion release and the effusive-flow are critical, therefore, highly refractory, low density matrixes and elevated temperatures are important.

### CONCLUSIONS

The ISOL target-vapor transport system simulations described in this paper were performed with the codes developed at ORNL as a cost effective means for design and optimization of target/vapor transport systems for present and next generation ISOL facilities.

### ACKNOWLEDGEMENTS

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