

# BENCHMARKING AND CALIBRATION OF MONTE CARLO VACUUM SIMULATIONS WITH SYNRAD AND MOLFLOW+

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## Abstract

The APS-Upgrade project is using SynRad and MolFlow+ to evaluate the vacuum system design for the future 6 GeV, 200 mA APS-Upgrade storage ring. The goal of this work is to explore PSD outgassing predictions from the two programs in order to build confidence in pressure calculations for the APS-U storage ring vacuum system. A study is performed on calibrating PSD measurements for aluminum vacuum chambers and then applying them to APS-U vacuum system calculations. The study reveals that a PSD measurement may not reveal a single unique behavior for a vacuum material and that multiple sources should be considered for vacuum calculations.

## INTRODUCTION

SynRad and MolFlow+ [1] are Monte Carlo based programs created by R. Kersevan and M. Ady of CERN for vacuum system analysis. SynRad calculates photon flux distributions from magnetic sources. MolFlow+ calculates complex conductances and pressures in the molecular flow regime. The programs can be coupled to predict dynamic outgassing and pressures and conditioning times for accelerator vacuum systems. The APS-Upgrade project is using SynRad and MolFlow+ to evaluate the vacuum system design for the future 6 GeV, 200 mA APS-Upgrade storage ring.

Predicting dynamic outgassing requires the incorporation of photon stimulated desorption (PSD) measurements to connect the distribution of photon fluxes calculated in SynRad to outgassing in MolFlow+. The goal of a typical PSD measurement is to expose an angled chamber to a collimated photon source and measure the released gas load. The PSD yield data in units of molecules/photon is plotted as a function of linear photon dose in units of photons/meter and can be used to predict accelerator vacuum system gas loads.

The goal of this work is to explore PSD outgassing predictions from the two programs in order to build confidence in pressure calculations for the APS-U storage ring vacuum system.

## CALCULATING PSD OUTGASSING WITH MOLFLOW+

The goal of a coupled SynRad and MolFlow+ analysis is to predict PSD gas loads based on beam conditioning and then calculate resultant pressure profiles in MolFlow+. Predicting PSD gas loads requires the calibration of a function which connects the linear distribution of photon flux from the x-axis of a PSD measurement to the spatial distribution of photon flux calculated from the same experiment

recreated in SynRad. The function is calibrated to produce outgassing loads in MolFlow+ equivalent to the y-axis of the original PSD measurement.

A diagram for the calibration process is shown in Fig. 2. The three step calibration process goes as follows:

1. Recreate the vacuum chamber interior geometry and ray trace from a PSD measurement experiment in SynRad with a model that includes photon scattering and calculate photon flux densities on all chamber surfaces, see Figure 1.
2. Use a first guess for a power law function to map the flux computed on all meshed surfaces as outgassing in a MolFlow model. A good first guess is using a power law function plotted through the original experimental data. Perform the computation for multiple time points which are equivalent to flux accumulation points on the x-axis.
3. Verify total computed gas loads in MolFlow+ at multiple time points versus the original measurement. If the points aren't equal then iterate by 'shifting' the x-axis of the power law function left or right and restart at step 2 until the new function maps gas loads equivalent to the original experiment. When the computed gas loads are close enough to the original experiment at multiple time points then the new power law function has been appropriately calibrated for use in MolFlow+ models.

The final calibration converts the linear photon flux from the experimental data, with units of photons/meter, to spatial photon flux calculations from SynRad with units of photons/cm<sup>2</sup>.

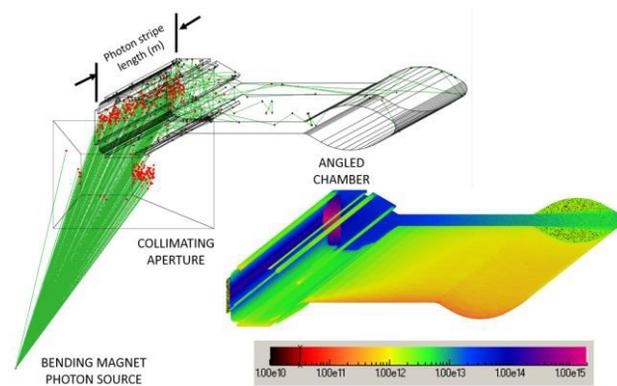


Figure 1: PSD measurement ray trace created in SynRad (left) with calculated spatial photon flux densities in log scale and units of photons/cm<sup>2</sup>/s (right).

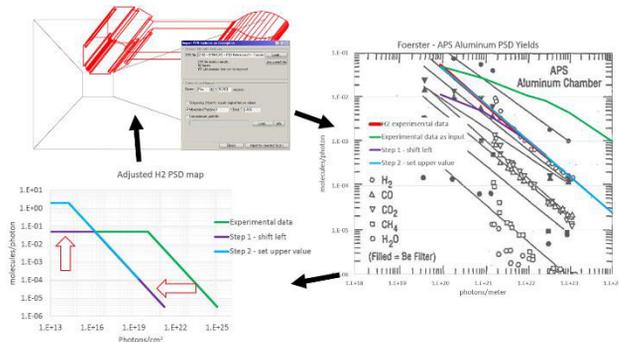


Figure 2: Diagram of PSD measurement calibration for use in MolFlow+.

### MOLFLOW+ MODEL OF APS-U STORAGE RING VACUUM SYSTEM

A SynRad and MolFlow+ model of one sector of the APS-U storage ring vacuum system has been created as shown in Figure 3 with a shared geometry for both programs. Photon flux distributions are calculated in SynRad from upstream bending magnets sources. Local and distributed pumping are defined in the MolFlow model. PSD gas loads are mapped into MolFlow+ and then pressure profiles are computed from the center of the beam aperture.

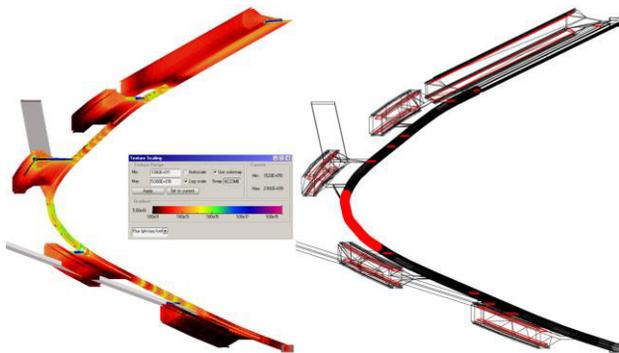


Figure 3: SynRad ray trace with photon scattering shown in log scale (left) and MolFlow+ pumping elements (right) highlighted in red.

### ALUMINUM PSD MEASUREMENT STUDY FOR APS-U MODEL

Aluminum vacuum chambers account for about 90% of vacuum surfaces within the APS-U storage ring vacuum system design therefore its outgassing behaviour is a key parameter for APS-U vacuum system calculations. The following study compares four PSD measurements [2-5] on aluminum vacuum chambers. Figure 4 compares cross sections of extruded aluminum vacuum chambers used in past and existing accelerators including three from this study [6]. Figure 5 shows the four models recreated for use in SynRad and MolFlow+ [6].

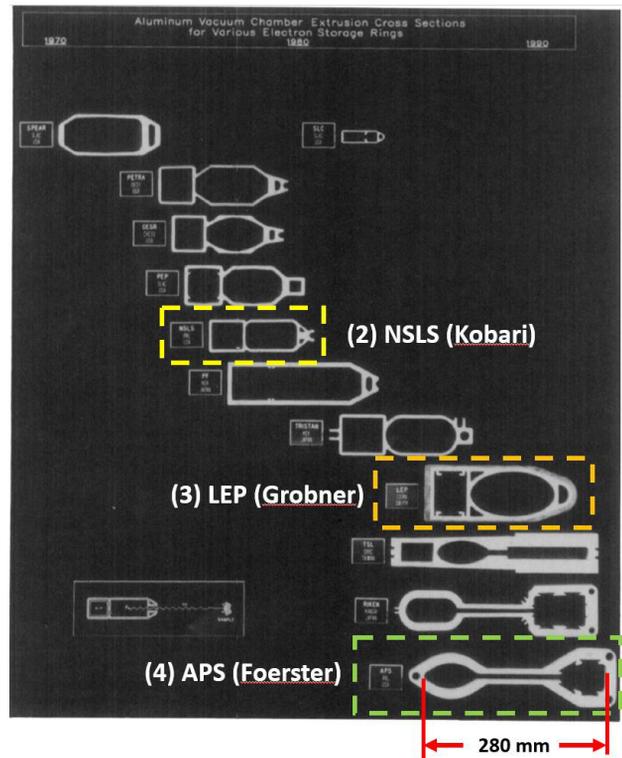


Figure 4: Comparison of aluminum vacuum chambers from the PSD measurement study.

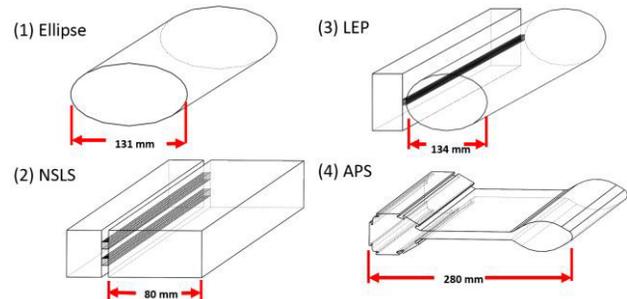


Figure 5: Simplified 3D models of the interior volumes of four aluminum vacuum chambers for use in MolFlow+.

Figure 6 compares the H<sub>2</sub> portion of the PSD measurements including extended power law curves fit to the data. The magnitude and cleanup slope are similar but not equal. The differences between the magnitudes and clean-up slopes of the PSD yields lead to variations in the MolFlow+ calculations. Average photon doses within the APS-U model at 1000 A\*hrs are ~1E24 photons/meter. Pressure profiles for the APS-U model are shown in Figure 7 calculated at the 200 mA max beam current and at 1000 A\*hrs conditioning time. An APS-U design requirement is to reach 2 nTorr average pressures by 1000 A\*hrs in order to achieve suitable beam lifetimes.

The study reveals that the calibration of the PSD measurements will not necessarily reveal one unique outgassing function for a given material. The reasons for the variation could come from experimental differences including the varying chamber geometries and bakeout conditions, limits

to the amount of data measured for each experiment, and also error in the power law curve fit. The range of calculated pressures varies by a factor of 18. A more narrow pressure margin may be established by taking new PSD measurements from an aluminum chamber with the same design and bakeout as planned for the APS-U storage ring vacuum system.

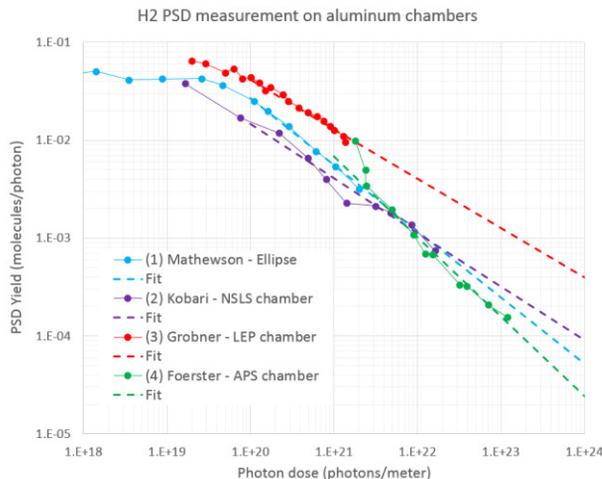


Figure 6: Comparison of H<sub>2</sub> PSD measurements and power law curves fit to the data for the four aluminum vacuum chambers in the study.

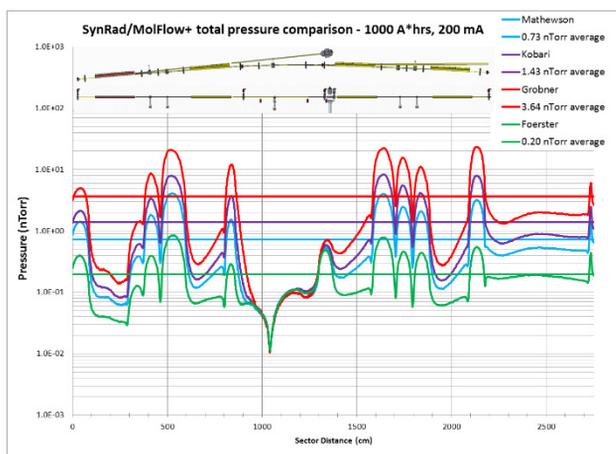


Figure 7: Comparison of pressure profiles calculated from the APS-U vacuum system model in MolFlow+ using four separate aluminum PSD measurements.

## CONCLUSION

The variation in results from the aluminum PSD study indicates that one PSD measurement will not necessarily reveal the universal behavior of a certain material. The study helps establish a range of expectations for MolFlow+ pressure predictions. It also suggests that a new PSD measurement from the APS-U aluminum vacuum chamber designs could help build confidence in vacuum calculations and vacuum system performance.

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