

# SIMULATION OF GAS SCATTERING LIFETIME USING POSITION-AND SPECIES-DEPENDENT PRESSURE AND APERTURE PROFILES \*

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## Abstract

When computing gas scattering lifetime for storage rings, it is common to use the average pressure, even though it is known that the pressure varies with location in the ring and varies differently for different gas species. In addition, other simplifications are commonly made, such as assuming that the apertures in the horizontal and vertical planes are independent and assuming that the momentum acceptance can be characterized by a single value. In this paper, we describe computation of the elastic and bremsstrahlung scattering lifetimes that includes species-specific gas pressure profiles computed with Synrad+ and Molflow+. The computations make use of the detailed shape of the dynamic acceptance and the position-dependent momentum acceptance computed with `elegant`. Comparisons are made to simpler methods for the multi-bend achromat upgrade lattice for the Advanced Photon Source.

## INTRODUCTION

Particles in storage rings undergo scattering from residual gas atoms, which may result in particle loss when the scattering places a particle outside the physical or dynamical acceptance of the ring. In this paper, we outline an elaboration of lifetime calculations for elastic and inelastic gas scattering that removes common assumptions. E.g., it is common to assume that the elastic gas scattering lifetime is limited in the vertical plane only, that the momentum acceptance is constant around the ring, and that the vacuum pressure is constant around the ring. The present calculations use results from Molflow+ and Synrad+ [1,2], which allow computing species-specific pressure profiles. They also use dynamic acceptance (DA) and local momentum acceptance (LMA) [3,4], results from `elegant` [5].

A general form for the lifetime is (compare [6])

$$\frac{1}{\tau} = \frac{c}{L} \sum_{g=1}^G \sum_{a=1}^{C_g} \int_0^L \sigma_{g,a}(s) S_{g,a} n_g(s) ds, \quad (1)$$

where  $L$  is the length of the ring (or a periodic unit),  $G$  is the number of molecular gas constituents,  $C_g$  is the number of atomic components of gas  $g$ ,  $\sigma_{g,a}(s)$  is the out-scattering cross section for atomic component  $a$  of gas  $g$  at location  $s$ ,  $S_{g,a}$  is the number of atoms of type  $a$  in a molecule of gas  $g$ , and  $n_g(s)$  is the number density of gas  $g$  at location  $s$ , which is related to the partial pressure  $p_g(s)$  by  $n_g(s) = \frac{p_g(s)}{k_b T}$ .

The out-scattering cross section is given by

$$\sigma_{g,a}(s) = \int_{q_1(s)}^{q_2(s)} \frac{d\sigma_{g,a}}{dq} dq \quad (2)$$

where  $q$  is the scattering coordinate,  $q_1$  is the maximum surviving value of  $q$ , and  $q_2$  is the physically-limiting value of  $q$ . E.g., for elastic scattering,  $q$  is the change in slope of the particle trajectory,  $q_1$  is the maximum change that will keep the particle within the acceptance, and  $q_2 = \infty$ . For gas bremsstrahlung,  $q$  is the change in fractional momentum deviation  $\delta$ ,  $q_1$  is the momentum acceptance, and  $q_2 = 1$ .

## ELASTIC NUCLEAR SCATTERING

Elastic scattering from atomic nuclei is described by the Rutherford cross section [7]

$$\frac{d\sigma_{g,a}}{d\Omega} = \frac{Z_{g,a}^2 r_e^2}{4\gamma^2} \frac{1}{\sin^4 \frac{\theta}{2}} \equiv \frac{E_{g,a}}{\sin^4 \frac{\theta}{2}}, \quad (3)$$

where  $Z_{g,a}$  is the atomic number,  $r_e$  is the classical electron radius, and  $\gamma$  is the relativistic factor. The scattering angle  $\theta$  is assumed to be large compared to the angular divergence of the particle beam. While the cross section does not depend on azimuthal angle  $\phi$ , the out-scattering cross section may, because the maximum surviving angle  $\hat{\theta}$  depends on the position in the ring, whether the scattering occurs mostly in the horizontal or vertical plane, and on the beta functions at the scattering location. The local value of the out-scattering cross section may thus be written

$$\sigma_{g,a}(s) = \int_0^{2\pi} \int_{\hat{\theta}(s,\phi)}^{\pi} \frac{d\sigma_{g,a}}{d\Omega} d\theta \sin \theta d\phi. \quad (4)$$

Performing the integral over  $\theta$  gives

$$\sigma_{g,a}(s) = E_{g,a} I_e(s), \quad (5)$$

where

$$I_e(s) = \int_0^{2\pi} \frac{2}{\tan^2 \frac{1}{2} \hat{\theta}(\phi, s)} d\phi. \quad (6)$$

In low emittance storage rings, the transverse aperture is determined by some combination of beam dynamics and physical aperture limits, i.e., by the “dynamic acceptance” or DA. Typically the DA is determined by tracking particles for many turns starting at  $s = 0$ , giving a set of  $(x, y)$  pairs at the aperture limit that trace out the DA contour. If  $(x_0(\phi), y_0(\phi))$  for  $\phi : [0, 2\pi]$  gives the DA contour at  $s = 0$ , then the beta functions  $\beta_x$  and  $\beta_y$  may be used to write

$$\hat{\theta}(s, \phi) = \left[ \frac{x_0^2(\phi)}{\beta_x(s)\beta_x(0)} + \frac{y_0^2(\phi)}{\beta_y(s)\beta_y(0)} \right]^{\frac{1}{2}}, \quad (7)$$

## 5: Beam Dynamics and EM Fields

### D11 - Code Developments and Simulation Techniques

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where we assume angles are  $\ll 1$ . In a practical application, this equation is inserted into Eq. (6) and the integral over  $\phi$  is computed numerically for each value of  $s$ , using the corresponding values of the beta functions as obtained from an optics code.

Using Equation 1, we can write the lifetime as

$$\frac{1}{\tau} = \sum_{g=1}^G \frac{c}{L} \left( \sum_{a=1}^{C_g} E_{g,a} S_{g,a} \right) \int_0^L I_e(s) n_g(s) ds. \quad (8)$$

This has the form of a sum over the scattering rates, or inverse lifetimes, for each gas species. The integrals over  $s$  are again to be computed numerically, ideally using species- and position-dependent pressure profiles from simulation with programs like Molflow+.

Returning to Eq. (7), we see that the acceptance is expected to be smaller when the beta functions are larger. Ideally, the vacuum pressure should be minimized at locations where one or both of the beta functions are large. This could be accomplished through enlarging the aperture at such locations, placing pumping near such locations, and avoiding placing absorbers near such locations. Particular care should be taken for gases that have high Z constituents, such as CO and CO<sub>2</sub>.

## BREMSSTRAHLUNG SCATTERING LIFETIME

The differential bremsstrahlung cross-section for atomic number  $Z$  is [8, 9]

$$\frac{d\sigma}{dk} = 4\alpha r_e^2 \left\{ \left( \frac{4}{3k} - \frac{4}{3} + k \right) T_1(Z) + \frac{T_2(Z)}{9} \left( \frac{1}{k} - 1 \right) \right\}, \quad (9)$$

where  $k$  is the energy of the emitted photon as a fraction of the electron energy,

$$T_1(Z) = Z^2(L_{rad}(Z) - f(Z)) + ZL'_{rad}(Z), \quad (10)$$

and  $T_2(Z) = (Z^2 + Z)$ . The functions  $L_{rad}(Z)$ ,  $f(Z)$ , and  $L'_{rad}(Z)$  are described in [9]. The fractional change in energy of the electron is  $u = -k$ .

The limiting energy aperture  $k_{ap}$  is a function of  $s$ . Integrating from  $k_{ap}(s) = -u_{ap}(s)$  to 1, we find

$$\sigma_{g,a}(s) = \frac{16\alpha r_e^2}{3} S_{g,a} \left( T_1(Z_{g,a}) A(k_{ap}) + T_2(Z_{g,a}) B(k_{ap}) \right) \quad (11)$$

where

$$A(k) = \frac{-5 + 8k - 3k^2 - 8 \ln k}{6} \quad (12)$$

and

$$B(k) = \frac{-1 + k + \ln k}{9}. \quad (13)$$

Using Equation 1, the bremsstrahlung lifetime is

$$\frac{1}{\tau} = \sum_{g=1}^G \frac{16\alpha r_e^2}{3L} \left\{ \left( \sum_{a=1}^{C_g} S_{g,a} T_1(Z_{g,a}) \right) \int_0^L n_g(s) A(k_{ap}(s)) ds + \left( \sum_{a=1}^{C_g} S_{g,a} T_2(Z_{g,a}) \right) \int_0^L n_g(s) B(k_{ap}(s)) ds \right\}. \quad (14)$$

This again has the form of a sum over scattering rates from the individual gas species. In a practical application, the two integrals can be carried out numerically using pressure profile data from a simulation of the vacuum system and local momentum aperture data from a tracking program, such as elegant [5].

The guidance for vacuum design inherent in these results is fairly clear. In particular, one should endeavor to reduce the pressure for high-Z gases at locations with small local momentum aperture on the negative side.

## APPLICATION

The APS upgrade project is investigating the possible replacement of the existing double-bend lattice with a hybrid multi-bend achromat lattice [10] having much lower emittance [11]. The lattice functions for the most recent version of this design are shown in [12]. A simulated commissioning procedure [13] is used to generate 100 corrected error ensembles for the design, from which 100 instances of the DA and LMA are obtained by tracking [12]. Each DA result is used for computation of the elastic scattering lifetime, while each LMA result is used for computation of the bremsstrahlung scattering lifetime.

The program Molflow+ has been used to model the notional small-bore vacuum system, which includes sputter ion pumps, non-evaporable getter (NEG) cartridge pumps, NEG strips, and NEG coatings. These pumping methods are not equally effective for all gas species. For example, NEG pumps are ineffective in pumping CH<sub>4</sub> and noble gases (e.g., Ar, which makes up 1% of air). The simulations include the photo-desorption of gas molecules that results from synchrotron radiation striking the chamber and discrete absorbers, assuming exposure to 1000 ampere-hours of beam. Fig. 1 shows the resultant pressure profiles from Synrad+/Molflow+ for the five gas species included in the analysis. The figure also shows the variation in the scattering rates as a function of position and species. We see that these generally follow the corresponding pressure profiles, but not exactly.

Figures 2 and 3 show histograms of the elastic scattering and bremsstrahlung lifetimes. For each figure, two results are shown, one with variable pressure vs position as computed with Synrad+/Molflow+, and another for which the pressure for each species is averaged over position. The differences are on the order of 10 to 20 %, as can also be seen in Table 1. The total gas scattering lifetime for 1000 A-h is 26 h, which is shorter than desired. Improvements to the vacuum system design are in progress that are expected to significantly improve this.

## CONCLUSIONS

We have presented a methodology and results for a more accurate computation of gas scattering lifetimes, based on vacuum system modeling and accelerator acceptance modeling. The vacuum simulations are very sensitive to a set of assumptions that are difficult to pin down precisely

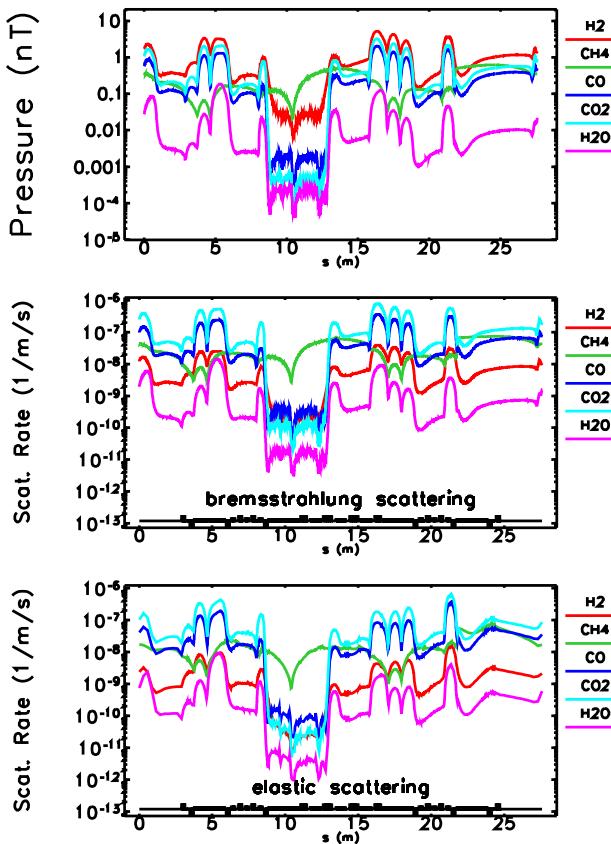


Figure 1: Species-specific pressure and mean gas scattering rates.

(surface chemistry, surface roughness, thermal and photon-stimulated outgassing rates, pumping speeds). For this reason, we plan to compare simulation results with measured pressures on real systems, including existing APS accelerator systems, which have much in common with what is planned for the MBA upgrade. This will help refine the inputs and establish error bars on the results. We also plan to use these simulation tools to predict how quickly the new ring can be brought to full beam current.

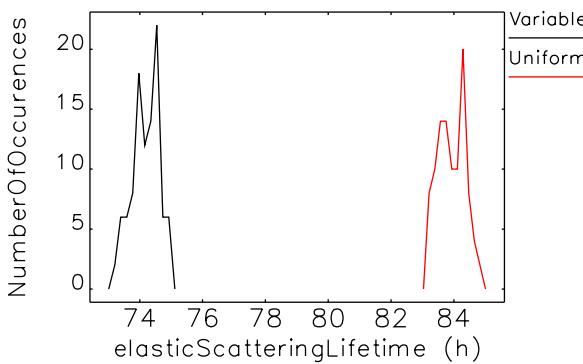


Figure 2: Distribution of elastic scattering lifetimes for variable and uniform pressure assumptions.

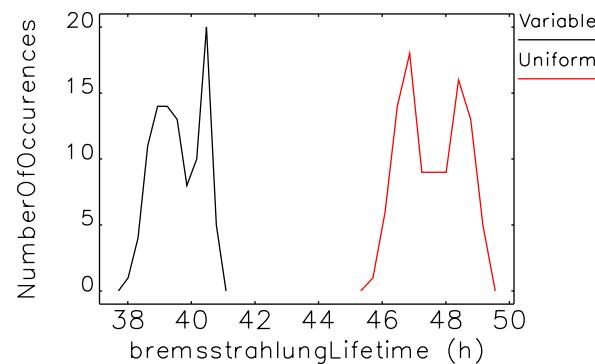


Figure 3: Distribution of bremsstrahlung scattering lifetimes for variable and uniform pressure assumptions.

Table 1: Elastic Scattering ('e') and Bremsstrahlung ('b') Lifetime Results from Calculations Using s-variable Pressure ('v') and Uniform Pressure ('u')

$\int I dt$	$\tau_{e,v}$	$\tau_{e,u}$	$\tau_{b,v}$	$\tau_{b,u}$
A-h	h	h	h	h
100	15.2	17.4	8.2	9.8
1000	74.2	83.9	39.6	47.6

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