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RF Accelerator Pressure Profile by Monte Carlo

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Vacuum pressure profile along a disc loaded waveguide accelerator structure is calculated by Monte Carlo modeling of molecular diffusion. For periodic geometries such as an RF accelerating structure, total pressure can be summed from individual cavity diffusion profiles. Results are compared with pressure profiles calculated using ordinary vacuum conductance concepts.

1 Introduction

Residual gas density along the beam trajectory is among the most important parameters in accelerator vacuum design. Over the past 100 years numerous formulas have been developed describing the transport of gas molecules through pipes at high vacuum. Once pressure is low enough that molecules collide only with walls and not with each other (molecular flow), transport is controlled only by geometry. Early calculations [1] were analytic solid angle integral sums of molecular reflections for a few simple geometries. By the 1960's computers were employed to calculate molecular transmission probabilities using Monte Carlo simulations[2]. Vacuum engineering texts imply that conductance of a system of pipes can be calculated by analogy with electrical circuits where resistances (conductance reciprocals) add in series. This assumption was proven generally false in a little-quoted paper by Oatley[3]. Nevertheless, many vacuum system computer codes such as VACCALC[4] and VAKTRAK[5] are built on this incorrect assumption. For accelerator geometries consisting of a series of many identical cavities, (Figure 1), summation of cavity resistances can lead to errors. This paper calculates density directly by Monte Carlo simulation of diffusion without resort to the concept of conductance or other ohm's law circuit analogies.

Thermal diffusion from a point source is a familiar image in science. Initially a substance is concentrated in a δ function at the source location. As time passes the concentration falls and spreads until after a long time it is uniform throughout the structure. If the source is continuously pumped, permanent outgasing will eventually stabilize in a density gradient over the whole structure which is unique to the source location and structure 'conductance'. This molecular density distribution can be simulated by Monte Carlo techniques. Complete Monte Carlo simulation of diffusion from all 50 cavities of an accelerator section is impractical and unnecessary. The present paper reduces this complexity by modeling only density distributions for a few selected outgas source locations along the structure. Because of symmetry and the smooth dependence of the distribution function on source location, intermediate distributions can be interpolated from the few actually simulated. Finally, total density profile can be added up as a superposition of all cavity outgas distributions.

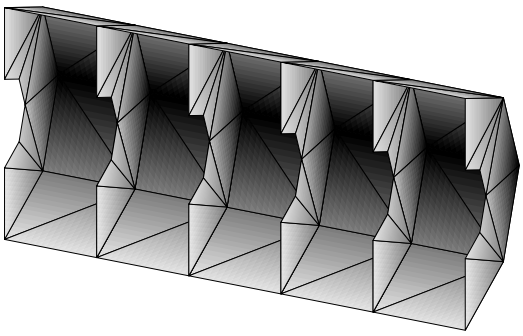

Figure 1: Accelerator cross section

2 Density Profile

2.1 Surface Outgassing Rate

Molecules continuously outgas from the surface of an accelerator structure. This outgassing, together with geometric conductance, controls molecule density along the accelerator. For copper at 45°C (318°K) operating temperature, with RF power on, an outgassing rate of $Cu_{gas} = 10^{-13}\text{torr} * \text{liter/sec} * \text{mm}^2$ has been used [†] for vacuum calculations. This is equivalent to a surface emission rate of about 3 molecules from each square millimeter every microsecond:

$$\dot{n} = \frac{Cu_{gas}}{(R/N_A)T} = \frac{(10^{-13}\text{torr} * \text{liter/sec} * \text{mm}^2)}{(1.0355 \times 10^{-22}\ \text{torr} * \text{liter}/^\circ\text{K}^{-1})(318^\circ\text{K})} = 3.04 \times 10^{-6}/\text{sec} * \text{mm}^2. \quad (1)$$

2.2 Molecular Residence Time

Monte Carlo simulations described later in section 3 allow us to follow molecules one at a time. The average path S of a typical molecule bounces back and forth from cavity to cavity in the accelerator structure until by chance it bounces into a pump . All molecules entering a pump are assumed captured and the structure is 'conductance limited'. Each molecule pursues its own diffusive path independent of all the rest. Not all molecules visit all cavities before they are captured by a pump but every cavity contains some of the molecules for parts of their life in the structure. The average molecule emitted in cavity i travels up and down the structure repeatedly visiting cavity j. S_{ij}(mm) is the path length accumulated in cavity j by the average molecule born in cavity i. Although calculated as a distance, S_{ij} can be converted to a cavity residence time using the average molecular speed $\bar{v}$. For air

[†]Numerous copper outgas measurements have been made. At 45°C their typical values are only 1/10 of the 10^{-13}torr*liter/sec*mm^2 suggested here for copper during exposure to high power RF electron/ion bombardment. See: The Stanford Two Mile Accelerator, R. B. Neal, p 889.

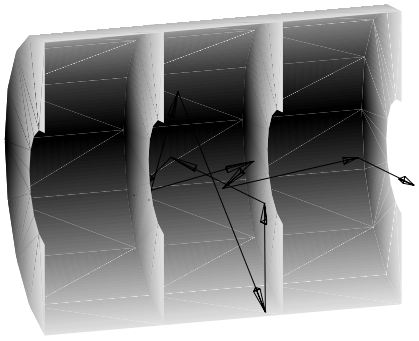

Figure 2: Molecular ray trajectory

(average molecular weight M = 29) at 45°C (318°K),

$$\bar{v} = \left[\frac{8}{\pi}\frac{kT}{M}\right]^{\frac{1}{2}} = \left[\frac{8}{\pi}\frac{(1.38\times10^{-23}\mathrm{J°K^{-1}})(318°\mathrm{K})}{29/(6.022\times10^{26}/\mathrm{kg})}\right]^{\frac{1}{2}} = 481.8\ \mathrm{m/sec} \tag{2}$$

For unsymmetrical distributions like the Maxwell-Boltzmann distribution of molecular speeds, the average reciprocal speed is not the reciprical of the the average speed. For Maxwell-Boltzmann, $< \frac{1}{v} >= \frac{4}{\pi}\frac{1}{\bar{v}}$. Thus the average residence time in cavity j for air molecules emitted in cavity i is:

$$< \tau_{ij} >= \frac{4}{\pi}\frac{1}{\bar{v}} < S_{ij} > \quad (\mathrm{sec}) \tag{3}$$

The τ distributions depend on cavity dimensions and where in the structure molecules originated. Monte Carlo simulations allow us to estimate these distributions by following a large number of molecules from their origin cavity i to the end of their trajectory in a pump.

2.3 Residence Distributions

How much time does the average molecule spend in each cavity? Consider a structure pumped at each end with the following dimensions typical of an NLC Xband accelerator structure.

No. of cavities	cavity dia $2b$	iris dia $2a$	cavity length l
50	22mm	8.4mm	8.75mm

Molecules wander aimlessly up and down the structure repeatedly visiting the same cavity. Molecules born in cavity #25 will repeatedly cross this midpoint cavity until a symmetric distribution of residence times accumulates. Molecules born near the ends of the structure where pumps are located have short lifetimes and skewed residence distributions. Figure 3 shows some of these residence distributions for outgas sources in cavities #5,#10,#15 & #25 from Monte Carlo simulations of 500 molecules each. Distribution averages $< S >$ are plotted in both milli seconds and equivalent meters of trajectory. Average total lifetimes and distances traveled are the areas under the distributions. For example, the average molecule born in #25 travels 55.8 meters and lives 147.5 ms. As the simulation accumulates histories of a large number of molecules, the distribution of their individual track lengths in a particular cavity can also be plotted. Figure 4 shows a distribution S_{23} of trajectory distance accumulated in cavity 2 for 10^4 molecules born in cavity 3 of a short 5 cavity structure. This distribution is not a simple gaussian. Cavity geometry imposes a pattern onto the distribution. How many molecules must be tracked before the variance in $< S >$ is sufficiently small? A measure of this is the variance width $\sigma_j = [\frac{1}{n}\Sigma_i^n(< S_j^2 > - < \bar{S}_j >^2)]^{\frac{1}{2}}$ which has been plotted as error bars on data in figure 3.

If we assume that residence distributions vary smoothly with source cavity, we can fill in the residence distributions for the rest of the cavities along the accelerator by interpolation

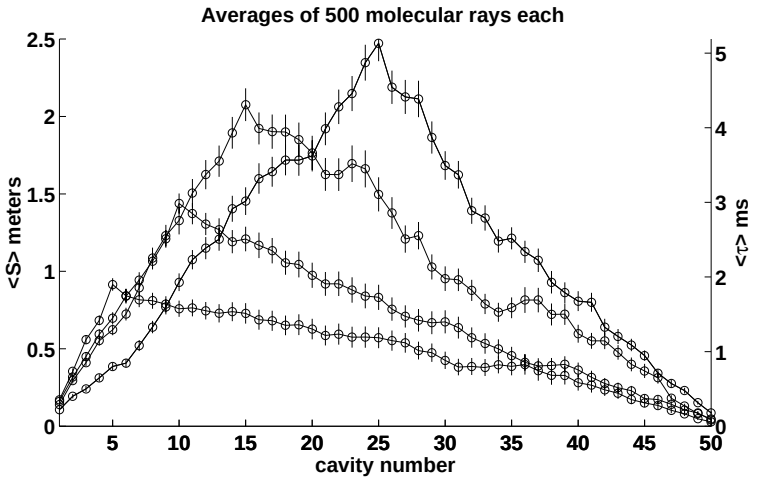

Figure 3: Residence distributions for outgas sources in cavities #5 #10 #15 & #25

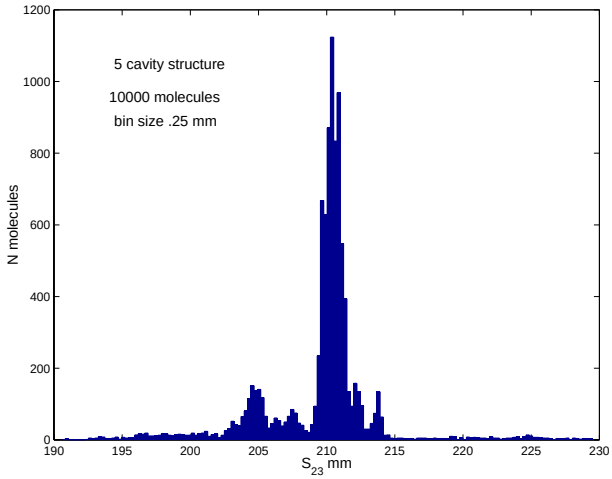

Figure 4: Distribution of residence in cavity #2 for 10000 molecules born in cavity #3 of a 5 cavity accelerating structure.

from the results of only a few Monte Carlo simulations. Runs of 500 molecules each were made for source cavities 5,10,15, & 25. Figure 3 shows that these distributions have simple triangular shapes for an accelerator structure with uniform cavity size. Symmetry implies that the distributions for cavity sources 26-50 would be reflections of the distributions already calculated for sources in cavities 1-25. To fill in distributions for sources in all cells, simple triangle approximations were generated using 2nd order polynomial fits to the peak of $< S >$ and its end values at cavities 1 and 50. Figure 5 shows this 2 dimensional distribution.

2.4 Molecular Density Distribution

Outgassing provides a steady source of fresh molecules in each cavity. The total number of molecules launched each second into cavity i with outgasing surface area A_i is

$$\dot{N}_i = A_i \dot{n} = (1253.8 \text{ mm}^2)(3.04 \times 10^6 \text{molecules/sec} * \text{mm}^2) = 3.812 \times 10^9 \text{molecules/sec} \quad (4)$$

The number of molecules resident in cavity j due to outgasing source $\dot{N}_i$ in cavity i is

$$N_{ij} = \dot{N}_i * \tau_{ij} \quad \text{(molecules)} \quad (5)$$

Since no molecule interacts with any other, the total density distribution is the superposition of residence distributions from all outgasing cavities. If cavity j has volume V_j (mm^3),

$$n(j) \equiv \frac{N_j}{V_j} = \frac{1}{V_j} \sum_i \dot{N}_i * \tau_{ij} \quad \text{(molecules/mm}^3\text{)} \quad (6)$$

This molecule density distribution $n(j)$ is plotted in figure 6 for the uniform 50 cavity accelerating structure. Equivalent pressure $P(j) = nkT$ [‡] is also plotted there. It should be pointed out that this result depends on the molecular weight of the gas. While distance traveled $< S >$ is a geometric property of the structure, the residence time depends also on molecular velocity. If the gas was hydrogen instead of air, the average velocity would go up by $\sqrt{29/2} = 3.8$. Residence time would be shortened by this amount and residual pressure would be correspondingly lower. In effect, hydrogen "pumps" faster than air.

3 Monte Carlo program

The physical assumptions necessary to formulate a Monte Carlo model of molecular diffusion are remarkably few.

1. Density of molecules is assumed sufficiently low that collisions between molecules can be neglected. Molecules travel straight paths between collisions with walls.

2. Molecule velocities are chosen at random from a Maxwell velocity distribution. (For simulation here, average velocity $\bar{v}$ was substituted for random selection from the Maxwell velocity distribution.) Direction of each trajectory is chosen at random from a cosine distribution with respect to the local wall surface normal.

[‡]Boltzmann constant $k = 1.38 \times 10^{-23}$Joules/°K $= 1.0351 \times 10^{-16}$ Torr $*$ mm^3/°K

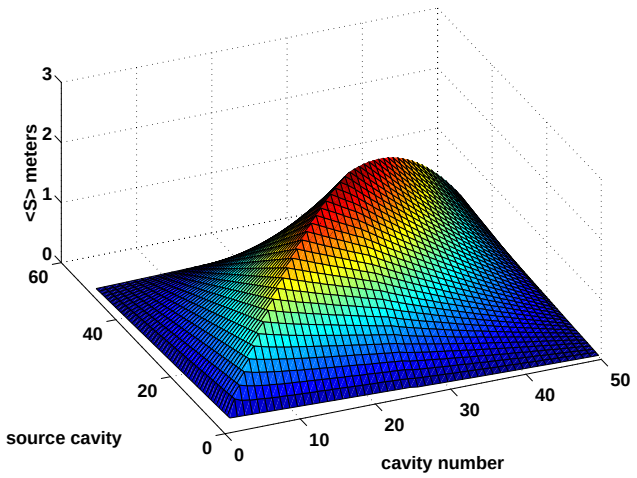

Figure 5: Average accumulated trajectory distributions $< S >$ (meters) for all cavity sources.

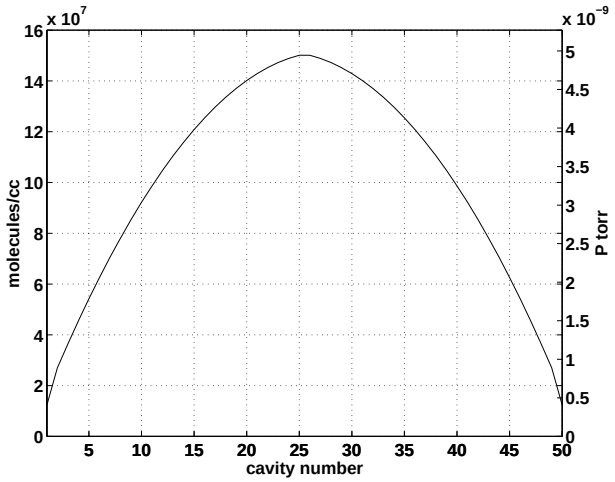

Figure 6: Density and pressure distribution for air outgas rate of 10^{-13} torr$*$liter/sec$*$mm^2.

Molecules are imagined not to bounce from wall to wall but rather to stick and reach thermal equilibrium before reemitting in a new direction uncorrelated to the original impact. To avoid storing the trajectories of thousands of molecules, trajectory contributions to cavity residence times are recursively averaged in as the simulation proceeds. To track each molecule through the structure, MATLAB Monte Carlo program *Accelflo.m* calls 4 subprograms to simulate diffusion:

$Accel =$	$Accelbuild$	Generates mesh geometry.
$ray =$	$outgas(sourcecell)$	launches initial random ray.
$hit =$	$impact(ray)$	locates hit coordinates on *Accel* mesh.
$ray =$	$bouncer(hit, ray)$	re-emits ray from surface until pump capture.

3.1 Mesh Geometry *Accelbuild.m*

Triangles are chosen as the simplest general 3D mesh element. An accelerating structure is naturally divided into cavities. *Accelbuild* intentionally closes each cavity by vacuum 'walls' across both iris openings so that tracking is confined to one cavity at a time. This 'particle in cell' approach greatly simplifies the trajectory search. Only the walls of the local cavity need be searched to find the next impact. Molecular impacts on vacuum walls are carried forward into the adjacent cell. Each cavity is an enclosure consisting of 5 surfaces shown in figure 7: inlet-disc, iris1, cylinder, iris2, and outlet-disc.

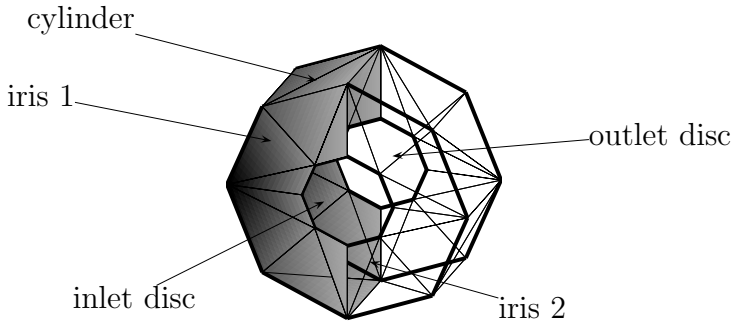

Figure 7: A Cavity mesh

The data array structure for cell geometry is:

Accel{surface,cavity}	.points(x,y,z)	node coordinates
	.faces(a,b,c)	triangle node point row indexes
	.normals(cosx,cosy,cosz)	triangle normal vectors
	.material('Cu', 'Vac', 'Pump')	impact surface

3.2 Generation of Molecular Rays *outgas.m*

To start a molecular ray from a chosen source cavity in the structure, *outgas.m* picks a random point on the copper surface of the source cavity. Selection is weighted for equal probability per unit area. The ray's direction is chosen from a cosine distribution with respect to the surface normal. Direction cosines [*cosx cosy cosz*] are first computed using 2 calls to a random number generator *rand* in equations 7. A rotation matrix then transforms [*cosx cosy cosz*] into the mesh coordinate system. Figure 8 shows the cosine distribution's probability density versus polar angle $\phi = \arccos(cosz)$ measured with respect to the surface normal. The algorithm (7) is:

$$\begin{aligned} r_1 &= rand \\ \rho &= \sqrt{1 - r_1} \\ \theta &= \pi(2 * rand - 1) \\ cosz &= \sqrt{r_1} \\ cosx &= \rho \cos(\theta) \\ cosy &= \rho \sin(\theta) \end{aligned} \qquad (7)$$

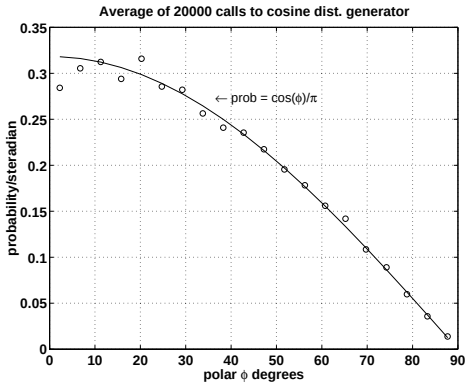

Figure 8: Cosine distribution density vs. polar angle ϕ

3.3 Finding impacts *impact.m*

Subroutine *impact(ray)* uses a geometric construction between unit vector **ray** and each candidate triangle to locate impact on mesh. Each mesh triangle's plane is extended to ∞ in all directions. Intersect point **P** in this plane is computed from equations 8 illustrated in figure 10. To determine if **P** hits mesh triangle, triangle's area is computed from the vector cross product of its sides $\mathbf{r_{12}} \times \mathbf{r_{13}}$. If **P** lies inside triangle the 3 subtriangles [1,2,p], [1,3,p] and [2,3,p] sum to the area of the enclosing mesh triangle. If **P** misses, their sum exceeds it as illustrated in figure 9.

4 Pressure Profile by conductance calculation

This final section calculates pressure profile by normal conductance methods for comparison with the Monte Carlo result of figure 6. Conductance is defined by $F \equiv Q/\Delta P$ (liters/sec) where Q is mass flow (torr∗liters/sec) and ΔP is pressure drop (torr). The conductance of each iris and cavity in the accelerator can be calculated in isolation by considering them as short tubes or apertures connecting 2 infinite vacuum vessels. Engineering formulas exist for the conductance of many simple geometries. The underlying assumption of conductance

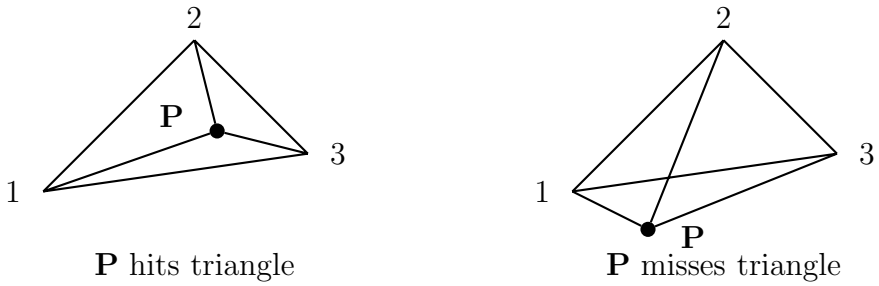

Figure 9: Criterion for ray impact on mesh triangle

$$
\begin{aligned}
\mathbf{C} &= \mathbf{r_{12}} \times \mathbf{r_{13}} \\
s &= \frac{\mathbf{d} \cdot \mathbf{C}}{\mathbf{ray} \cdot \mathbf{C}} \\
\mathbf{P} &= \mathbf{R} + s * \mathbf{ray}
\end{aligned}
\qquad (8)
$$

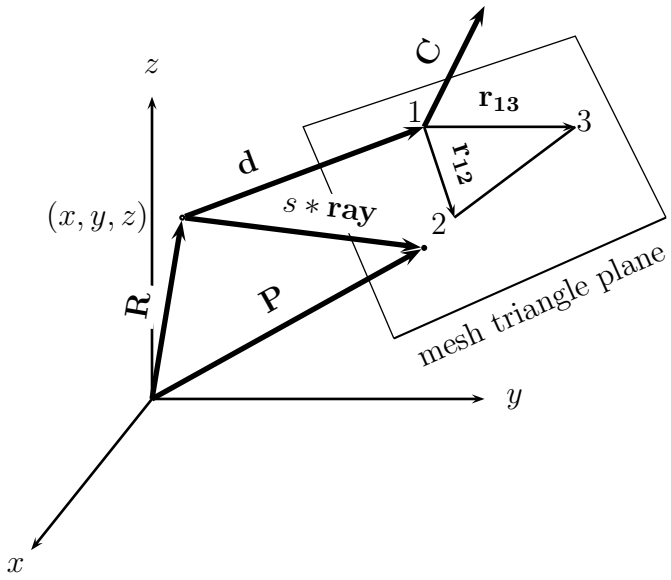

Figure 10: Mesh triangle impact point vector geometry

calculations is that F is a unique property of the element independent of its surroundings. The conductance of a composite structure is assumed not to depend on the order of elements. Like electrical resistors, conductance reciprocals are supposed to be addable in series. Oatley[3] showed this assumption to be generally false.

4.1 Conductances

The conductance of a circular aperture with radius a (mm) connecting two large vessels can be used to calculate the iris conductance F_a[6]:

$$F_a = \frac{\bar{v}}{4}(\pi a^2) = (\frac{481800 \text{ mm/sec}}{4})\pi(4.2 \text{ mm})^2 = 6.675 \text{ liters/sec} \qquad (9)$$

Conductance of short circular tubes of radius b (mm) and length l can be calculated by the same circular aperture formula modified by Clausing' factor $K(l/b)$ shown in figure 11. Each

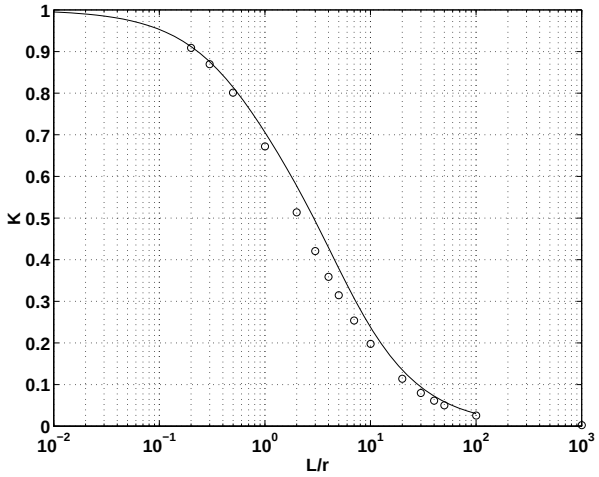

Figure 11: Conductance correction factor K vs length to radius ratio l/b

accelerator cavity of diameter $2b = 22$ mm can be considered as a a short tube of length $l = 8.75$ mm with an l/b ratio $8.75/11 = .7955$ for which Clausing's correction $K = .715$. The conductance of each short cavity tube in the accelerator structure is then

$$F_b = K\frac{\bar{v}}{4}(\pi b^2) = .715(\frac{481800 \text{ mm/sec}}{4})\pi(11.0 \text{ mm})^2 = 32.7 \text{ liters/sec} \tag{10}$$

4.2 Accelerator conductance model

To calculate the pressure profile, the accelerator section can be seen as 50 composit iris/cavity conductances $F = F_a F_b/(F_a + F_b)$ in series with outgassing flows $Q_{cu} = A_{cavity} C u_{gas}$ injected into each cavity. Pumping at each end is represented by fixed zero pressures. By assuming a flow $Q = F\Delta P$ between cavities, a system of algebraic equations can be assembled for all the cavity pressures, eq (11).

$$\begin{bmatrix} Q_{cu} \\ Q_{cu} \\ \vdots \\ Q_{cu} \\ Q_{cu} \end{bmatrix} = \begin{bmatrix} F_a + F & -F & & & \\ -F & 2F & & 0 & \\ & & \ddots & & \\ & 0 & & 2F & -F \\ & & & -F & F_a + F \end{bmatrix} * \begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_{49} \\ P_{50} \end{bmatrix} \tag{11}$$

This equation is readily solved by inverting the conductance matrix: $P = \mathcal{F}^{-1} Q_{cu}$. The results of this calculation are compared with the Monte Carlo simulation in figure 12.

Peak pressure calculated from a chain of conductances is about 15% higher than Monte Carlo calculations. For engineering purposes the simpler conductance approach may often be good enough since it is a conservative over-estimate and the basic outgassing rate Cu_{gas} is

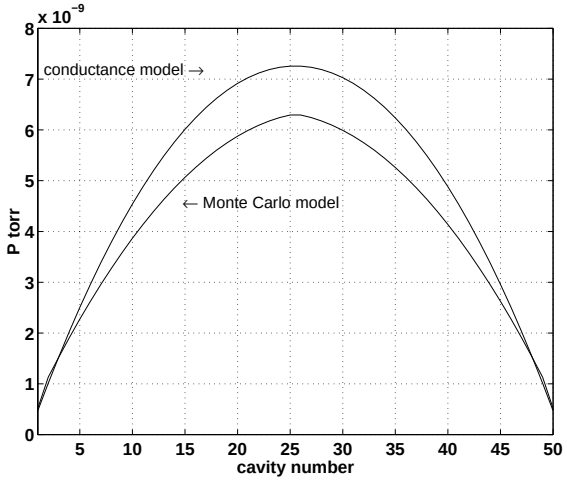

Figure 12: Pressure distribution by conductance calculation compared with pressure distribution by Monte Carlo.

probably not well known in the first place. In fact, pressure profile calculated by conductance methods is remarkably close to the direct Monte Carlo approach. Never the less, these results confirm Oatley's examples [3] showing that short geometric conductances such as accelerator cavities can not be chained together for exact calculation of overall conductance or pressure profile. The conductance formulas found in texts are only exact in isolation where the conductance interconnects two large volumes. Models based on direct interconnection of conductances are only approximate.

Acknowledgement

This paper was read critically by Hobey DeStaebler who contributed substative corrections and improvements.

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[2] D.H. Davis, 'Monte Carlo Calculation of Molecular Flow Rates through a Cylindrical Elbow and Pipes of Other Shapes', *Journal of Applied Physics*, vol.21 p.1169, 1960. This paper is a concise description of Monte Carlo methods applied to conductance calculation of relatively simple geometries.

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[5] VAKTRAK, SLAC-Pub-5962, V.Ziemann, 1992.

[6] Saul Dushman,'Scientific Foundations of Vaccuum Technique', 2nd Edition,1962. Although modern ion pumping and gettering technology came later, "Dushman" has remained a scientific reference on vacuum technology for 50 years. *Section 2.4 Molecular Flow* covers conductance formulas used in this paper.