CAS

THE CERN ACCELERATOR SCHOOL

Vacuum in Accelerators – CERN Accelerator School

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Analytical and Numerical Tools for Vacuum Systems

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Program of the course:

1. Why do we need to calculate pressure profiles in an accelerator in the first place?
   - Beam lifetime, emittance blow-up, beam-losses, radiation damage, personal safety issues, etc…
2. How can it be done?

   The old way…

   Analytical methods: Diffusion equation, parabolic profiles, etc…

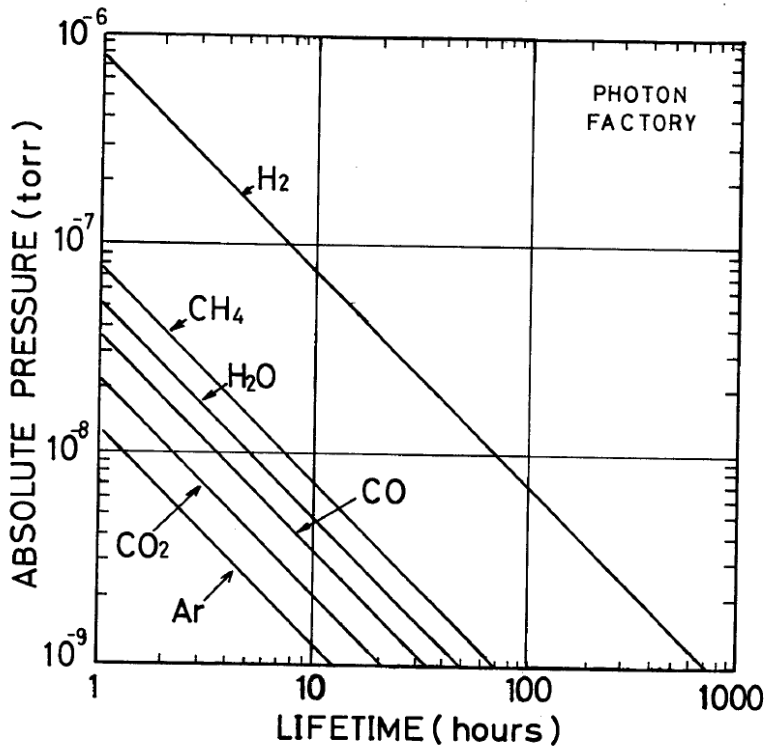
   The modern way, using computers

   Analytical methods: symbolic solution of differential equations

   Numerical methods: Finite-Element Method, Montecarlo, commercial codes, etc…
3. It's all about the conductance… and the gas load!
4. Conclusions
5. References

1. Why do we need to calculate pressure profiles in an accelerator in the first place?

- Fact: Energetic particles, charged or neutral, interact with matter;
- In particular, inside the vacuum system of an accelerator, they interact with the residual-gas, which may be detrimental to the correct operation of the machine;
- The degree of sensitivity to the level (total pressure) and quality (gas composition) of the vacuum is a function of the accelerator type;
- Few examples to clarify. The vacuum level and quality of…:



Substance	Molecular Weight	Radiation Length (g cm^{-2})
H	1	58
C	12	42.5
O	16	34.2
CH_4	16	45.5
H_2O	18	35.9
CO	28	37.3
Ar	40	19.4
CO_2	44	36.1

- …description of the interaction between charged beams …ng, on leptons and hadrons (in most cases on e⁻ and …

From: "Some notes on the photoelectron induced gas desorption problems in the Photon Factory and TRISTAN", A.G.Mathewson et al., KEK Laboratory Note KEK-78-9, 1978

Th… …to knowing what the pressure profile will be, in …her accelerator: <u>beam lifetime, ion trapping, …vel, material activation, and more</u>.

2. How can it be done? The old way…

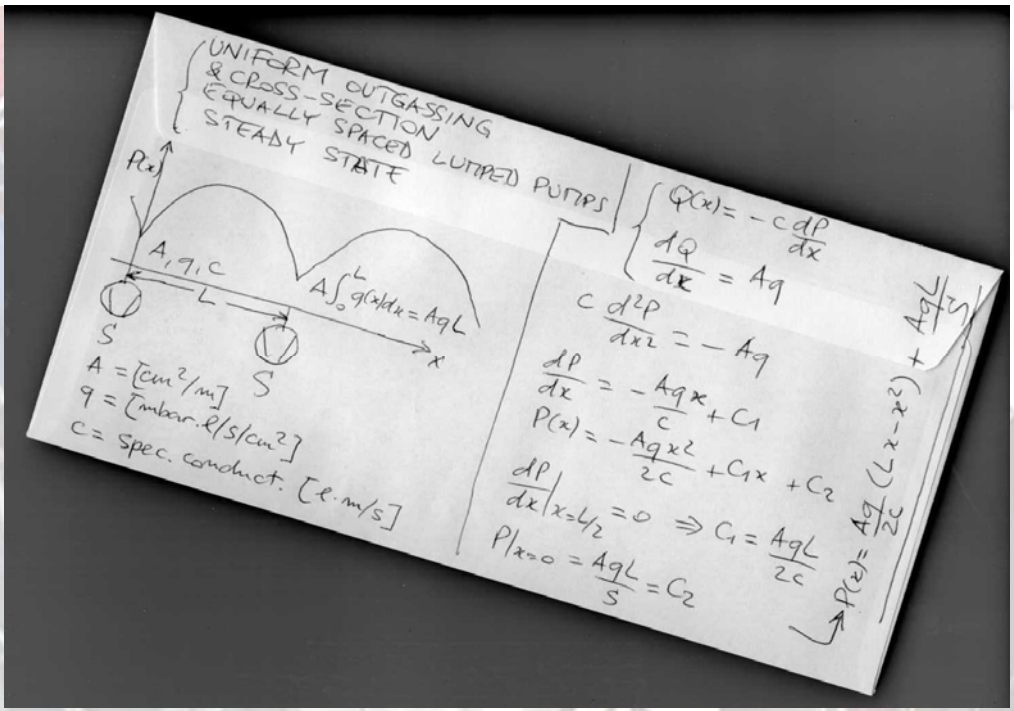
Analytical methods:

Paper and pencil

$$P = Q / S$$

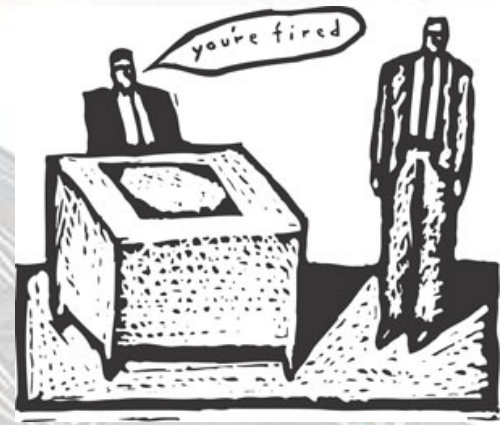
Estimate Q, determine the needed pressure P, get S, the number of pumps to buy. Good **starting point**, but can't we be a little bit more specific?

More advanced calculations: back-of-the-envelope…



Not bad either, but can we design a multi-million (billion) dollar/€ machine around this?

Your average boss will fire you if you do that!!!



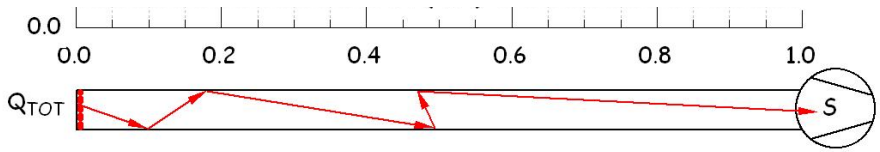
2 How can it be done?

Analytic formulae:

- Simplest case: a straight tube, with uniform cross-section and outgassing from one end (be it thermal or other), pumped by one pump at the far end:

At the pump: $P = Q_{TOT}/S$

$$P(x) = Q_{TOT}\left(\frac{1}{S} + \frac{L-x}{c}\right)$$



$$\begin{cases} P_{AVERAGE} = \frac{1}{L}\int_0^L P(x)dx = Q_{TOT}\left(\frac{L}{2c} + \frac{1}{S}\right) = \frac{Q_{TOT}}{S_{EFF}} \\ P_{MAX} = Q_{TOT} \cdot \mathrm{L/c} \qquad S_{EFF} = \left(\frac{L}{2c} + \frac{1}{S}\right)^{-1} \end{cases}$$

2 How can it be done?

Analytic formulae:

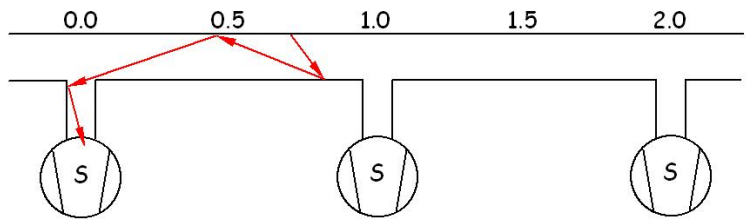
- Another simple case: assume that the vacuum chamber of your circular accelerator is a straight tube, with uniform cross-section and outgassing (be it thermal or other), pumped by equally spaced lumped pumps (L=1m):

$$\begin{cases} Q(x) = -c\dfrac{dP(x)}{dx} \\ \dfrac{dQ(x)}{dx} = Aq \end{cases}$$

$$c\frac{d^2P}{dx^2} = -Aq$$

$$\begin{cases} \dfrac{dP}{dx}(x = L/2) = 0 \\ P(x=0) = AqL/S \end{cases}$$

$$P(x) = \frac{AqL}{2c}\left(Lx - x^2\right) + \frac{AqL}{S}$$



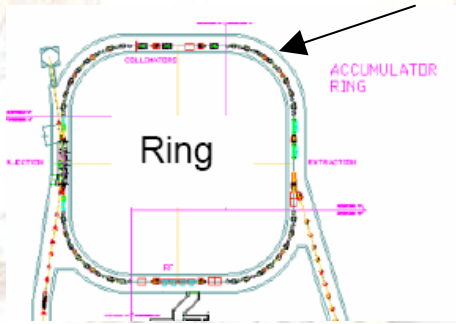
$$\begin{cases} P_{AVERAGE} = \dfrac{1}{L}\displaystyle\int_0^L P(x)dx = AqL\left(\frac{L}{12c} + \frac{1}{S}\right) = AqL(1/S_{EFF}) \\ P_{MAX} = AqL\left(\dfrac{1}{8c} + \dfrac{1}{S}\right) \qquad S_{EFF} = \left(\dfrac{L}{12c} + \dfrac{1}{S}\right)^{-1} \end{cases}$$

2 How can it be done?

Analytic formulae:

- The following example shows an analytic estimate of the pressure profile for the **SNS accumulator ring**

$$P(x) = Q\left(\frac{L}{S} + \frac{L^2 - x^2}{2C'}\right)$$



which is valid because the cross-section (i.e. the conductances) are **very large** and the outgassing uniformly distributed

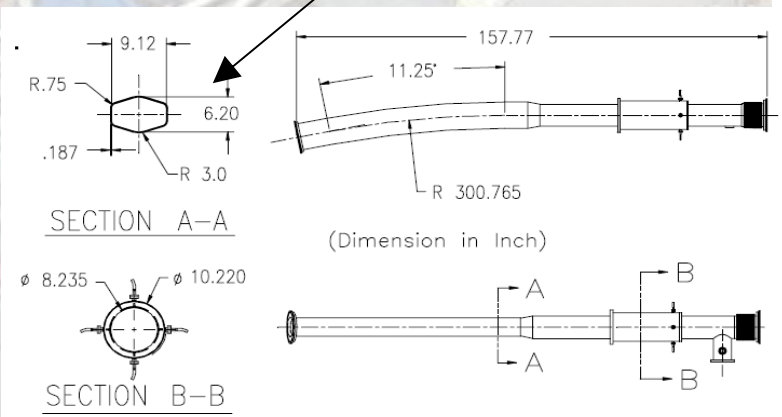


Fig.1 Design of Arc Halfcell Chamber

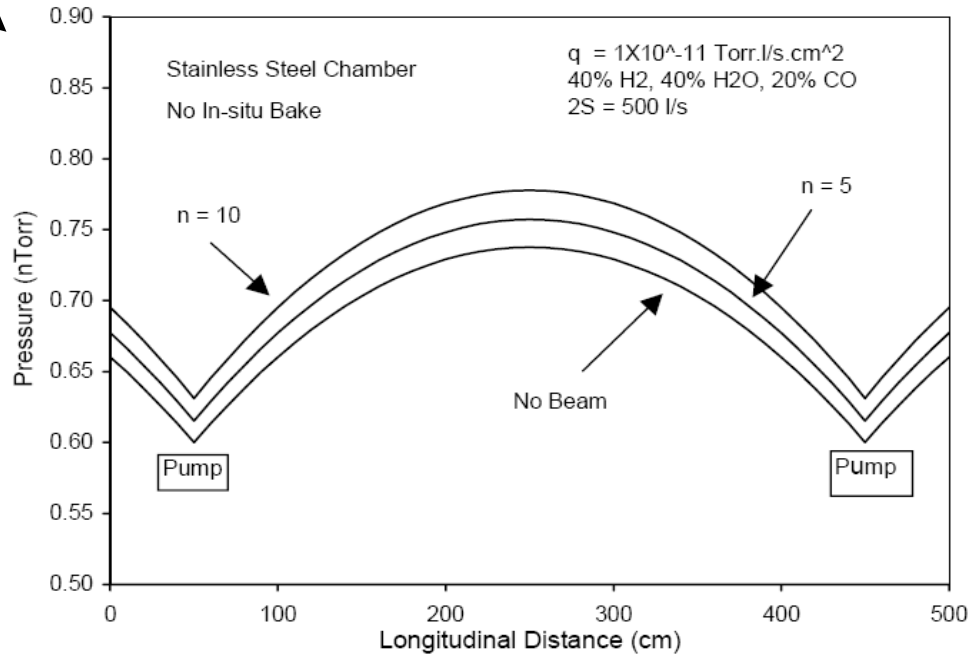


Fig. 3. Pressure in Ring Arc Sectors without beam and with beam using different ion desorption coefficients

From "Design of the SNS accumulator ring vacuum systems", H.C. Hseuh et al, Proc. PAC 1999, NY

2 How can it be done?

Analytic formulae: Diffusion model

- The dynamic gas balance inside a vacuum chamber can be written as :
  (n=gas density; s=distrib.pumping speed; c=spec.conductance)

$$V\frac{dn}{dt} = q - s\cdot n + c\frac{d^2n}{dx^2}$$

→ In quasi-equilibrium conditions:

$$\begin{cases} V\dfrac{dn}{dt} \approx 0 \\ V\dfrac{dn}{dt} << q \quad \text{or} \quad V\dfrac{dn}{dt} << s\cdot n \quad \text{or} \quad V\dfrac{dn}{dt} << c\dfrac{d^2n}{dt^2} \end{cases}$$

$$c\frac{d^2n}{dx^2} - s\cdot n + q = 0$$

2nd-order differential equation with 2 solutions:

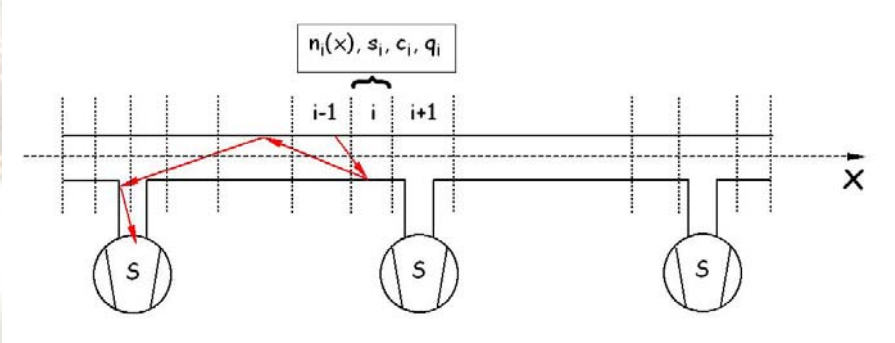
$$\begin{cases} n(x) = -\dfrac{q}{2c}x^2 + C_{1A}z + C_{2A} & \text{for } s = 0 \\ n(x) = -\dfrac{q}{c} + C_{1B}e^{\sqrt{s/c}\,x} + C_{2B}e^{-\sqrt{s/c}\,x} & \text{for } s > 0 \end{cases}$$

where the C_1's and C_2's are set by the **boundary conditions**

2 How can it be done?

- **Analytic formulae: Diffusion model**

In an accelerator, the chamber is often "a tube", and can therefore be reasonably segmented into N elements, with $s_i=0$ or $s_i>0$



Let the i-th element at $x_{i-1} < x < x_i$, described by the equation above, with the C_{1i} and C_{2i} defined by

$$n_i(x_i) = n_{i+1}(x_i)$$
$$\partial n_i(x_i)/\partial x = \partial n_{i+1}(x_i)/\partial x$$

This is a system of 2N-2 equations with 2N-2 unknowns, which can be easily solved.

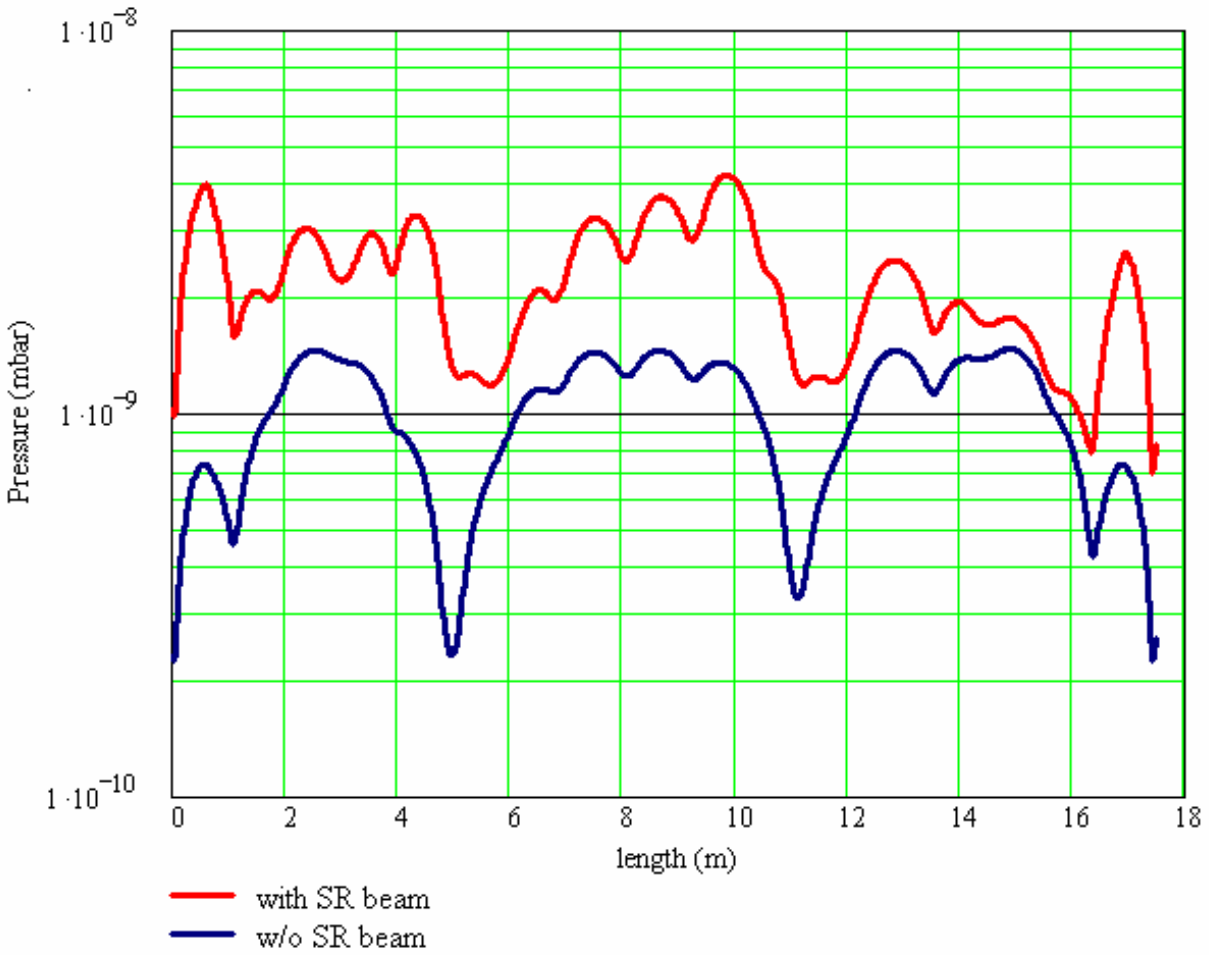
The pressure along the vacuum chamber is given by the analytical formula

$$\begin{cases} n_i(x) = -\dfrac{q_i}{2c_i}x^2 + C_{1i}z + C_{2i} & \text{for } s_i = 0 \\ n_i(x) = -\dfrac{q_i}{c_i} + C_{1i}e^{\sqrt{s_i/c_i}\,x} + C_{2i}e^{-\sqrt{s_i/c_i}\,x} & \text{for } s_i > 0 \end{cases}$$

2 How can it be done?

- **Analytic formulae: Diffusion model**

Example: calculation of the pressure profile for the arc section of Diamond **(courtesy of O.B.Malyshev, ASTeC, Daresbury, UK)**



Average pressure:

without a beam:

$\langle P_t \rangle = 1 \cdot 10^{-9}$ mbar

due to SR photons only:

$\langle P_\gamma \rangle = 1 \cdot 10^{-9}$ mbar

Sum (i.e with a beam):

$\langle P_{din} \rangle = \langle P_t \rangle + \langle P_\gamma \rangle =$

$= 2 \cdot 10^{-9}$ mbar

2 How can it be done?

- **Analytic formulae: time-dependent analytic profile (*)**

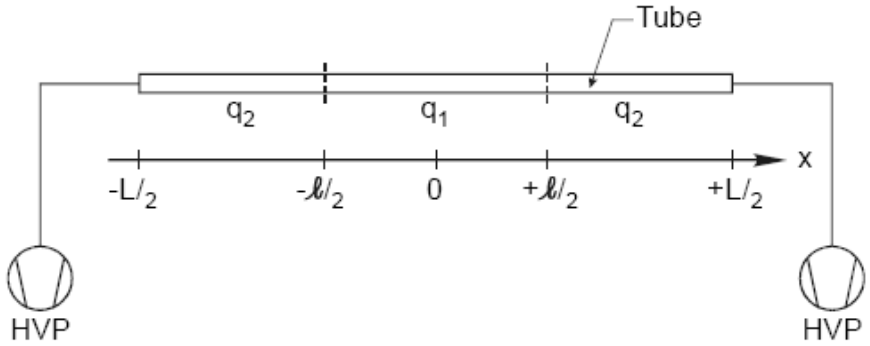


Figure 1: Schematic drawing of the geometry studied. HVP represents a generic high-vacuum pump.

The differential equation is:

$$c\frac{\partial^2 p(x,t)}{\partial x^2} = -q(x,t) + v\frac{\partial p(x,t)}{\partial t} \quad (4)$$

where $q(x,t)$ includes both the steady state degassing from the walls, q_s, and the impulsive source, q_i, and v is the volume per unit length of the tube. A product of two delta functions will represent the impulsive source:

$$q_i(x,t) = q'\delta(x)\delta(t) \quad (5)$$

where q' is a constant proportional to the amount of gas liberated at $x = 0$ in $t = 0$. The solution is:

$$p(x,t) = -\frac{q_s}{2c}x^2 + \frac{Q_T}{2}\left(\frac{1}{S} + \frac{L}{4c}\right) + \frac{q'}{(4\pi cvt)^{\frac{1}{2}}}\exp\left(-\frac{v}{4ct}x^2\right) \quad (6)$$

One can see that this solution corresponds to the combination of the usual parabolic steady state result plus a transient solution represented by a Gauss function with a time-varying standard deviation. This result was obtained considering the following boundary conditions:

- there is a maximum of the pressure at $x = 0$;
- for the steady-state solution, the pressure at the end of the tube, $x = L/2$, is the total throughput, Q_T, divided by the total pumping speed, $2S$.
- for the transient solution, all the gas reaching the pumps is pumped.

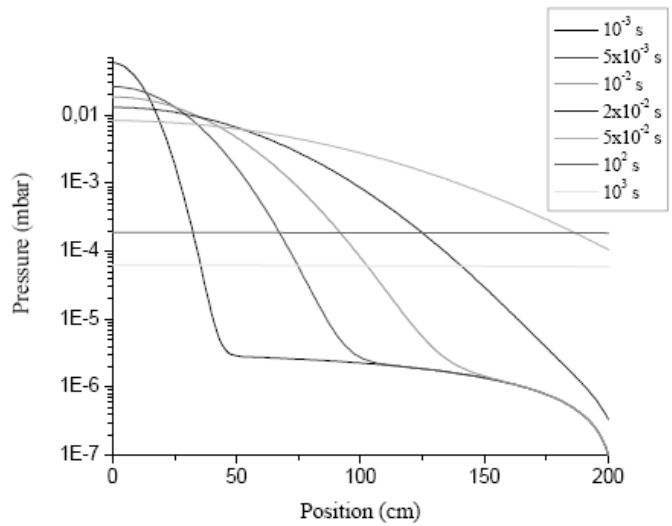
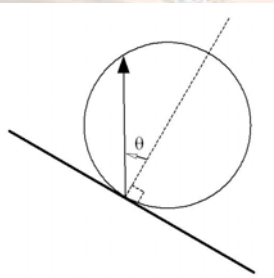


Figure 4: Pressure profile along the tube at different times, for $x \geq 0$ cm.

From "Time dependence of the pressure profile in a tube with axially-dependent degassing", F.T.Degasaperi et al., Proc. PAC-01, Chicago, 2001

2 How can it be done?



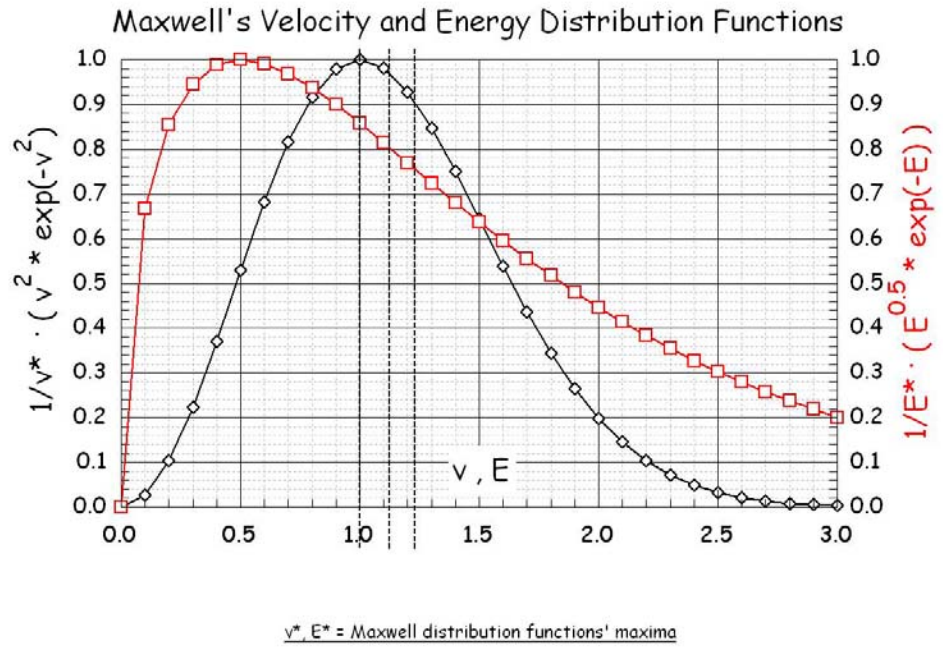
Montecarlo (MC) method #1:

Under UHV conditions the following assumptions can be made:

- Each molecule is independent, i.e. it collides only with the walls of the vacuum chamber
- The reflection of molecules from the chamber walls is diffuse (Lambert's Law)
- The accomodation coefficient is equal to one, i.e. the molecules are thermalized to the wall temperature. The Maxwell distribution of molecular speeds is valid
- The gas obeys the ideal-gas law: PV=RT
- The <u>average</u> velocity, <u>most probable</u> velocity, <u>root mean square</u> velocity of the molecules, and the inpingement rate are given by:

$$\frac{1}{N}\frac{dn}{d\omega} = \frac{\cos\theta}{\pi} \qquad d\omega = \sin\theta\, d\theta\, d\varphi$$

$$\theta = \sin^{-1}\sqrt{\beta} \quad \text{with } \beta \text{ uniformly distributed in } [0,1]$$



$$Z_a = \text{impingement rate} = \frac{n \cdot v_a}{4}$$

$$v_a = \text{average speed} = \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot M}}$$

$$v_{mp} = \text{most probable speed} = \sqrt{\frac{2 \cdot R \cdot T}{M}}$$

$$v_{rms} = \sqrt{< v^2 >} = \sqrt{\frac{3 \cdot R \cdot T}{M}}$$

2 How can it be done?

Montecarlo (MC) method #2:

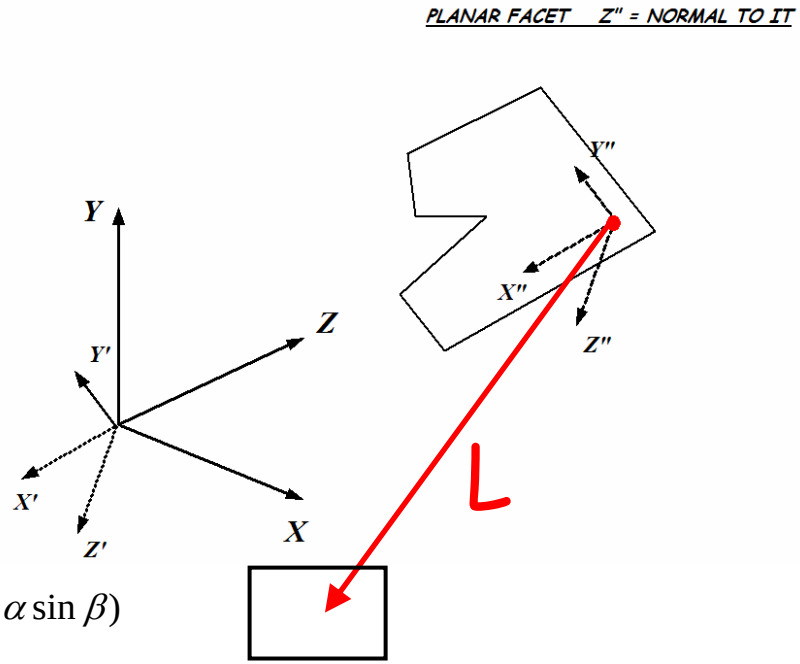
- Let's assume, without loss of generality, that a vacuum system be modeled using polygonal planar facets;
- Let XYZ be an arbitrary cartesian frame of reference;
- Let X"Y"Z" be the frame of reference whose origin corresponds to the location of a molecule located on the facet, with Z" perpendicular to the facet;
- Let X'Y'Z' a frame of reference parallel to X"Y"Z", whose origin is the same as XYZ;
- Let α and β be defined as such: β is the rotation about the Y axis which takes X onto X'; α is the rotation about X (X') which makes Y become Y';
- With such definitions, the following transformations can be written:

$$\begin{pmatrix} X'' \\ Y'' \\ Z'' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} X' \\ Y' \\ Z' \end{pmatrix}$$

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} X'' \\ Y'' \\ Z'' \end{pmatrix}$$

- Upon desorption of the molecule from the source facet s, let L be the generic length of the trajectory to the next target facet t;

$$X'' = L\sin\theta\cos\varphi$$
$$Y'' = L\sin\theta\sin\varphi$$
$$Z'' = L\cos\theta$$



- Combining the two relations, one gets

$$X_t = X_s + L_t(\sin\theta\cos\varphi\cos\beta - \sin\theta\sin\varphi\sin\alpha\sin\beta - \cos\theta\cos\alpha\sin\beta)$$
$$Y_t = Y_s + L_t(\sin\theta\sin\varphi\cos\alpha - \cos\theta\sin\alpha)$$
$$Z_t = Z_s + L_t(\sin\theta\cos\varphi\sin\beta + \sin\theta\sin\varphi\sin\alpha\cos\beta + \cos\theta\cos\alpha\cos\beta)$$

- where the value for L, L_t, i.e. the length of the trajectory to the next facet encountered, is a function of the geometric description of facet t, and it is not given here (see (*) and references therein)

(*) "Molflow User's Guide, R. Kersevan, Note ST/M-91/17, Sincrotrone Trieste

2 How can it be done?

Montecarlo (MC) method #3:

- **Averaging over a large number of molecular traces yields estimates of the pressure, inpingement rate, conductance, pumping speed, etc…:**

- Let N be the number of molecules entering, for instance, a tube from one end;
- Let m be the number of molecules leaving the tube at the other end:

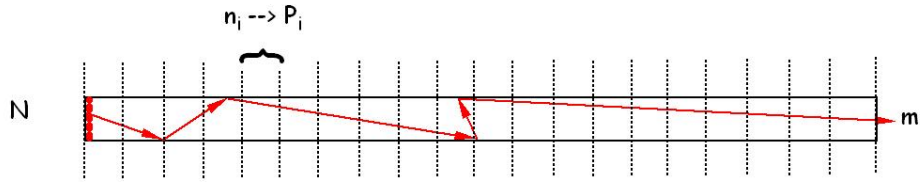
  w = m/N is the **transmission probability**;

- The values for w follow a **binomial distribution**, which has a standard deviation

$$\sigma = \sqrt{\frac{w \cdot (1-w)}{N}}$$

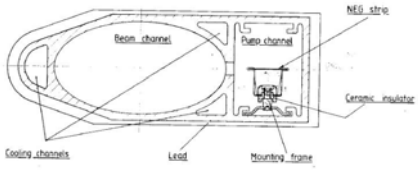
- If n_i is the number of molecular hits in the i-th segment of the tube, and P_i the associated pressure, then the normalized standard deviation for the pressure P_i is:

$$\sigma_{n_i}(\%) = \sqrt{\frac{1}{n_i}\left(1 - \frac{n_i}{N}\right)} \cdot 100$$



From Y. Suetsugu, JVST A14(1), 1996 p.245-250

2 How can it be done?



Montecarlo (MC) method #4: how to convert from molecular hits to pressures

- If n_i is the number of collisions on one segment of the vacuum chamber (A cm^2), and Q is the outgassing (in mbar·l/s), then Q/kT is the number of molecules/s. If N is the number of molecules traced, then, the mean number of collisions/cm^2 in that segment is

$$Z_i = {n_i}/{AN}$$

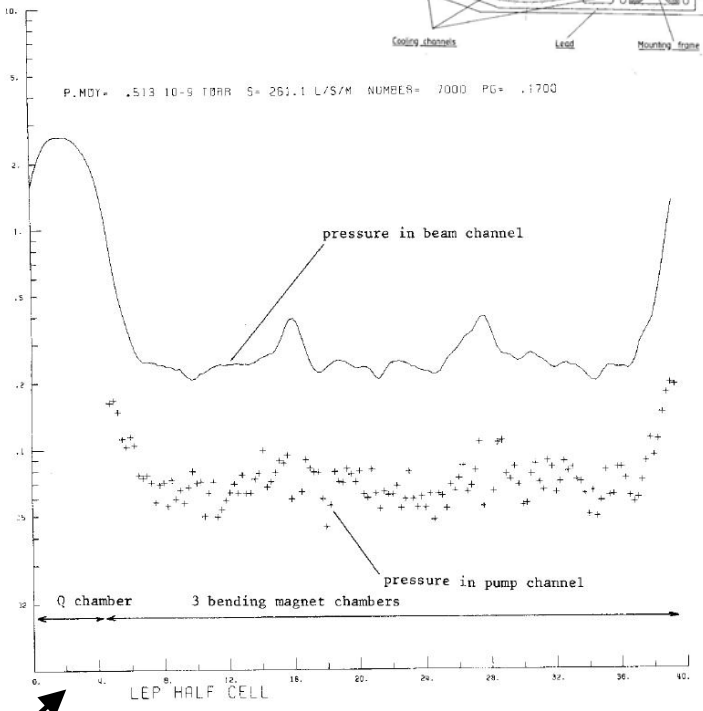
- The estimate of the impingement rate is

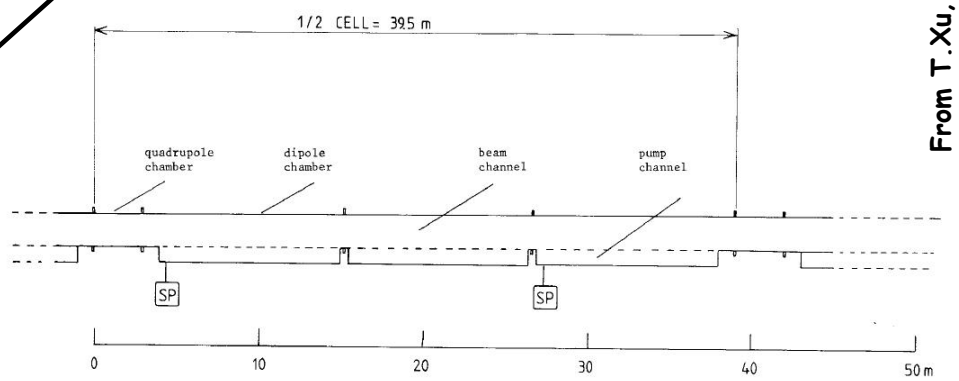
$$Z_i = \frac{n_i Q}{ANkT}$$

- At equilibrium, the relation between the pressure P_i (on segment i) and the corresponding inpingement rate Z_i is

$$P_i = {4kTZ_i}/{v_a} = \frac{4Qn_i}{v_a AN}$$

$$P_{avg} = \frac{4Q}{v_a AN}\sum n_i$$



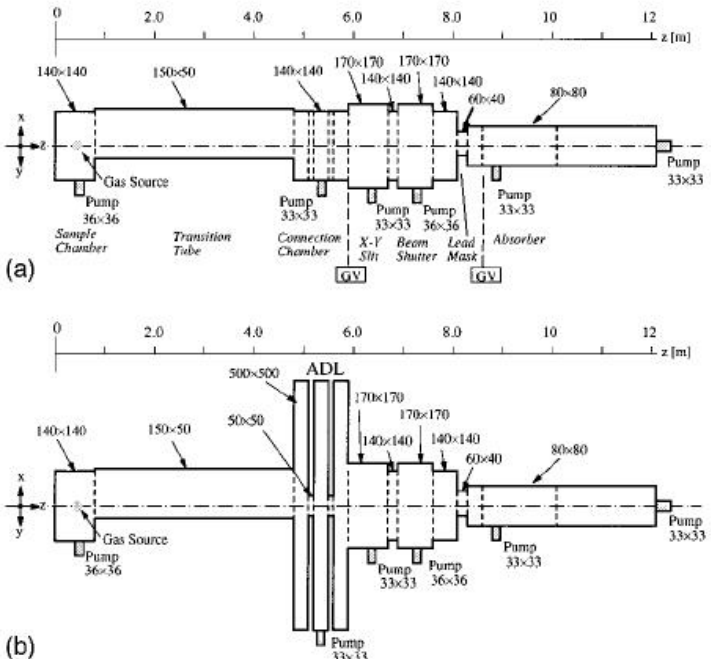


From T.Xu, JM. Laurent, O. Groebner CERN-LEPVA/86-02

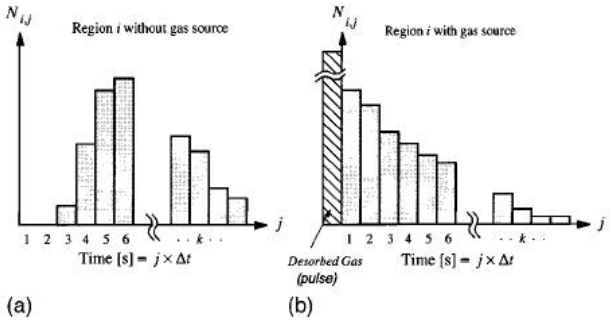
2 How can it be done?

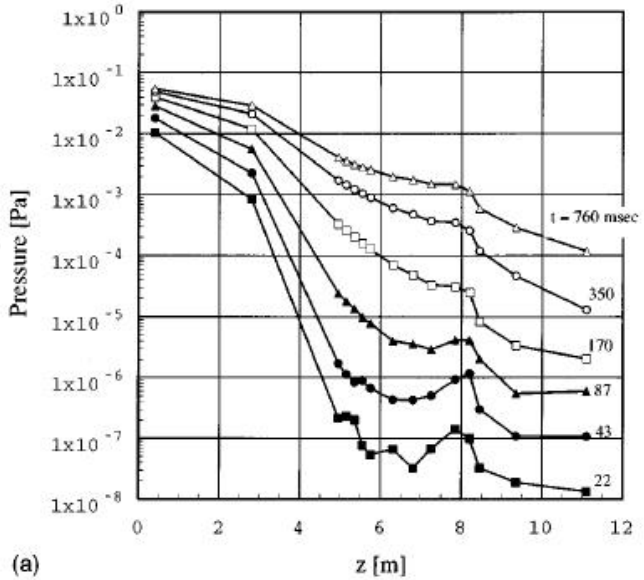
Montecarlo (MC) method #5:

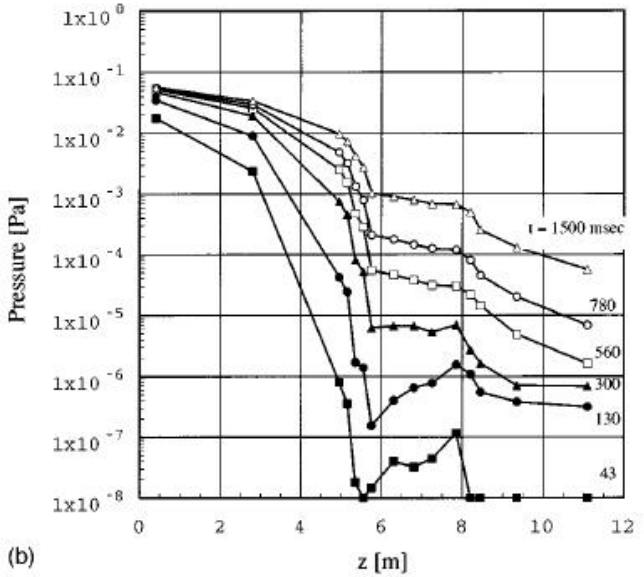
- **Time-dependent case**: acoustic delay line at Tristan synchrotron



- **The length of all trajectories is translated into time intervals by means of the average molecular speed**







From Y. Suetsugu, JVST A14(1), 1996 p.245-250

2 How can it be done?

Montecarlo (MC) method #6:

Optimization of the pumping/trapping efficiency of a pump-out box in order to minimize the pollution of the SC RF cavity of CESR (Cornell Electron-Positron Storage Ring): (*)

A small excerpt from the paper abstract:

riods are compared. Gas species are analyzed. A Monte-Carlo computer code is used to simulate the gas condensation/adsorption profile along the waveguide. The warm-up desorption curve is extracted, which might help us to understand the interaction between gas molecules and substrates. The pumping speed of the window pump-out box was evaluated by using the same code and was compared with the speed due to cryo-pumping. New designs of the pump-out box were explored to improve its pumping speed.

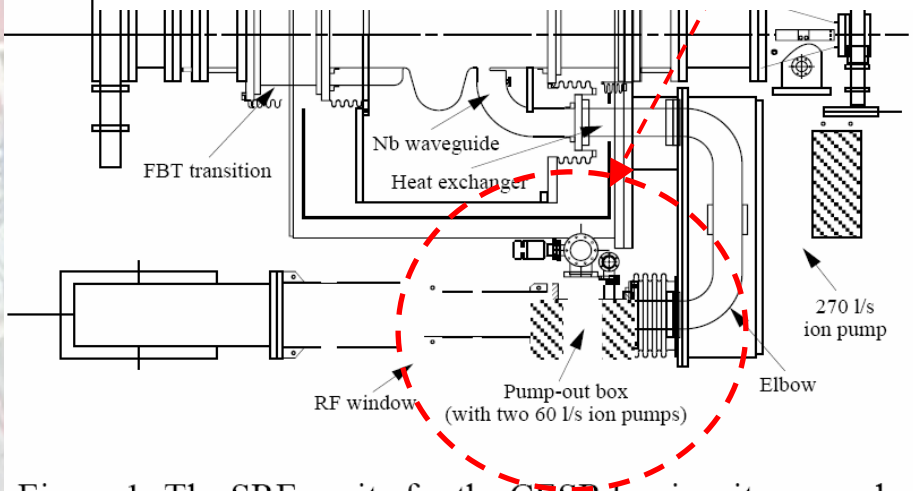


Figure 1: The SRF cavity for the CESR luminosity upgrade

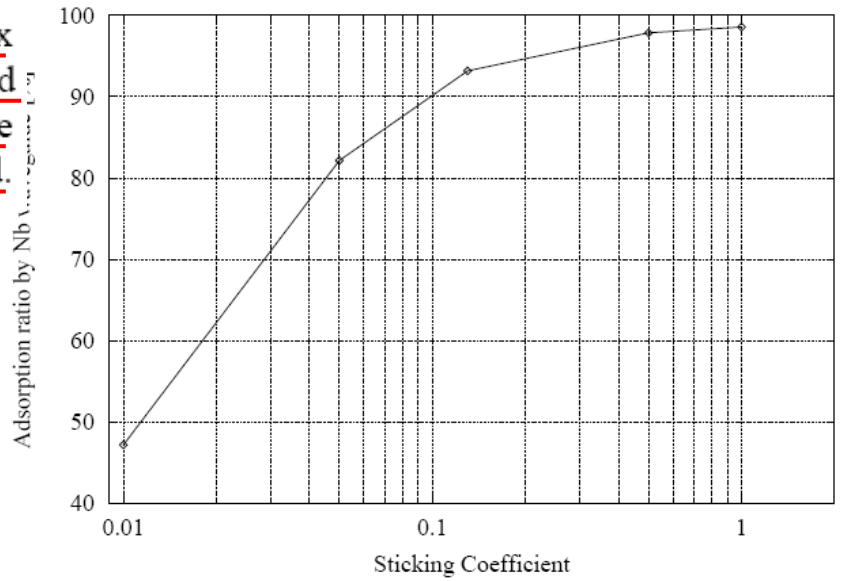


Figure 4: Ratio of the H_2 adsorbed by the Nb waveguide to that enters the cell of the cavity as a function of s

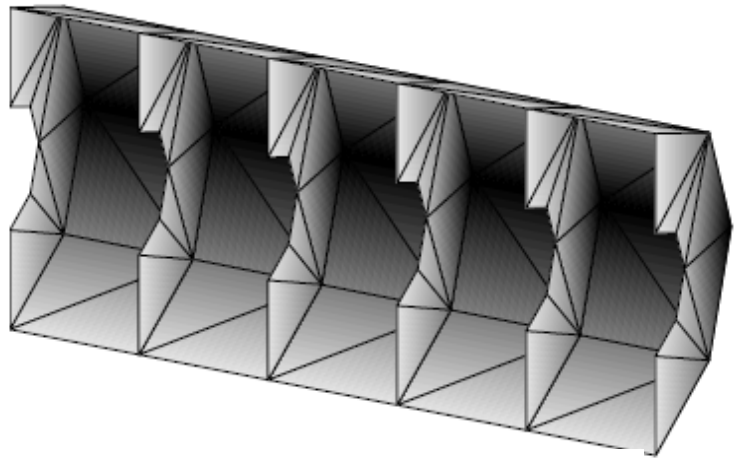
(*) "Condensation\adsorption and evacuation of residual gases in the SRF system for the CESR luminosity upgrade", R.L.Geng et al., Proc. PAC-99, p983, 1999

2 How can it be done?

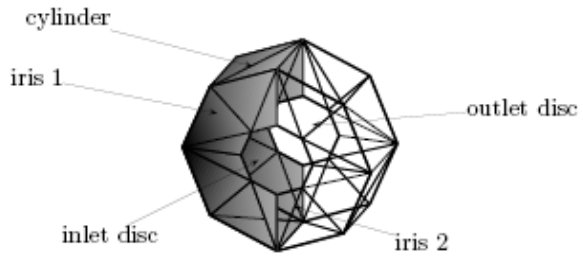
Using Matlab, an implementation of the Montecarlo method
Example: multi-cavity (50) RF accelerator pressure profile (*)

- A series of Matlab programs are written

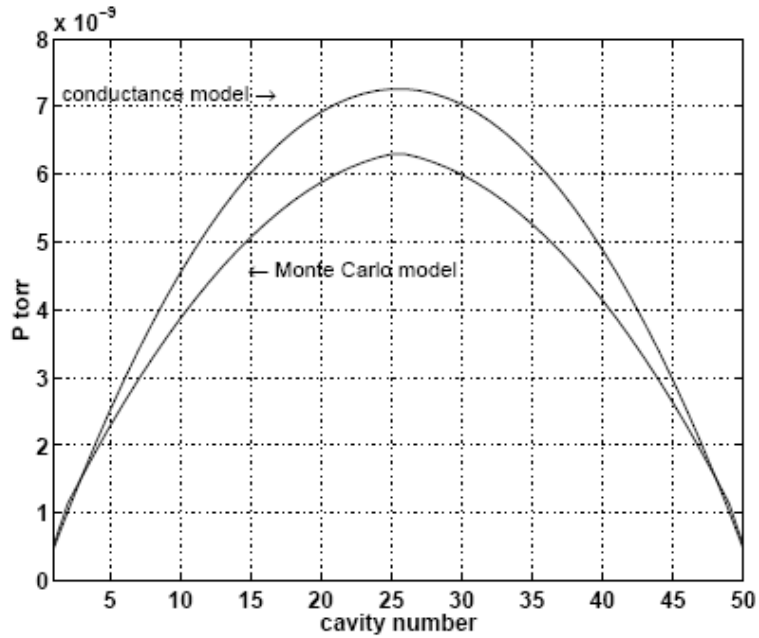
$Accel =$	$Accelbuild$	Generates mesh geometry.
$ray =$	$outgas(sourcecell)$	launches initial random ray.
$hit =$	$impact(ray)$	locates hit coordinates on $Accel$ mesh.
$ray =$	$bouncer(hit, ray)$	re-emits ray from surface until pump capture.



- The first one does the meshing



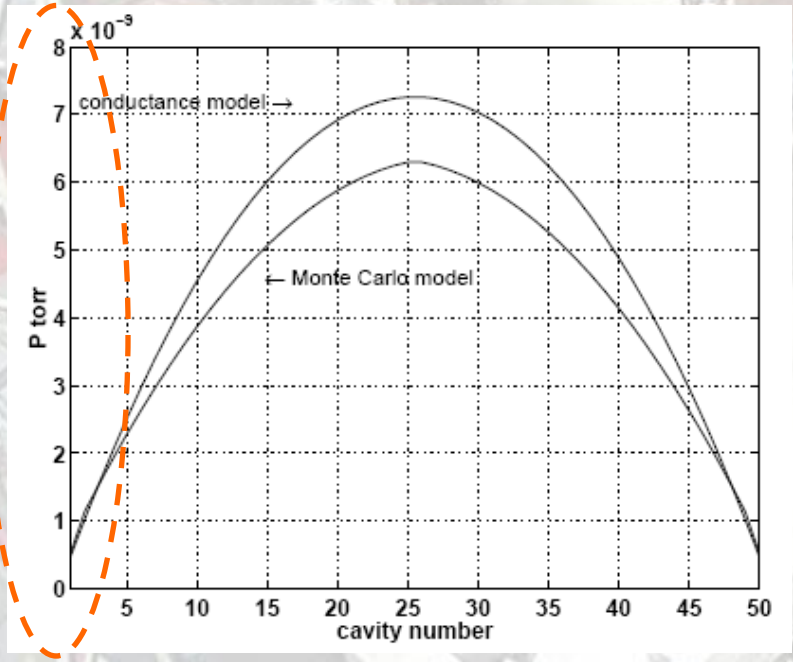
- while the others generate molecules according to the cosine law, find the impact with the next element in the model, and then iterates until the first "pump" is found
- The result is compared to a conductance calculation based on adding the reciprocal of the conductances of each of the 50 cells...

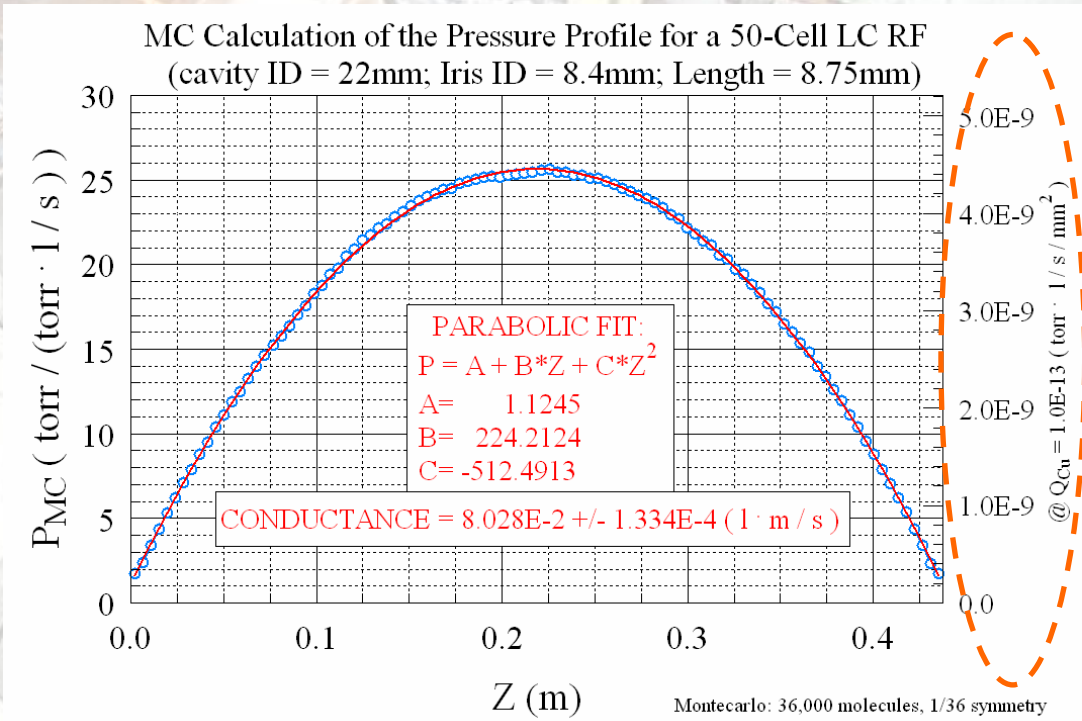


(*) "RF accelerator pressure profile", G.B.Bowden, Linear Collider Collaboration tech note LCC-078, Stanford, 2002

2 How can it be done?

Example: comparison of Matlab implementation of MC and full MC for multi-cavity (50) RF accelerator pressure profile (*)





(*) "RF accelerator pressure profile", G.B.Bowden, Linear Collider Collaboration tech note LCC-078, Stanford, 2002

2 How can it be done?

Transfer-Matrix method:
Program: **VAKTRAK**

• Starting from the equation $$c\frac{d^2P}{dx^2} - sP = -q$$

where s is the linear pumping speed (l/s/m), c the specific conductance (l•m/s), and q the specific outgassing yield (mbar•l/s), we get a solution of the type

$$P(x) = C_1 e^{\alpha x} + C_2 e^{-\alpha x} + \frac{q}{s}$$

with $$\alpha = \sqrt{s/c}$$

• By analogy with machine lattice programs (e.g.TRANSPORT), where the particle beam is tracked through the magnetic lattice, the transfer matrix **for the pressure** through the "vacuum lattice" is given by:

$$\begin{pmatrix} P(L) \\ dP/dx(L) \\ 1 \end{pmatrix} = \begin{pmatrix} \cosh(\alpha L) & \frac{\sinh(\alpha L)}{\alpha} & -\frac{q}{c}\frac{\cosh(\alpha L)-1}{\alpha^2} \\ \alpha\sinh(\alpha L) & \cosh(\alpha L) & -\frac{q}{c}\frac{\sinh(\alpha L)}{\alpha} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} P_0 \\ dP_0/dx \\ 1 \end{pmatrix}$$

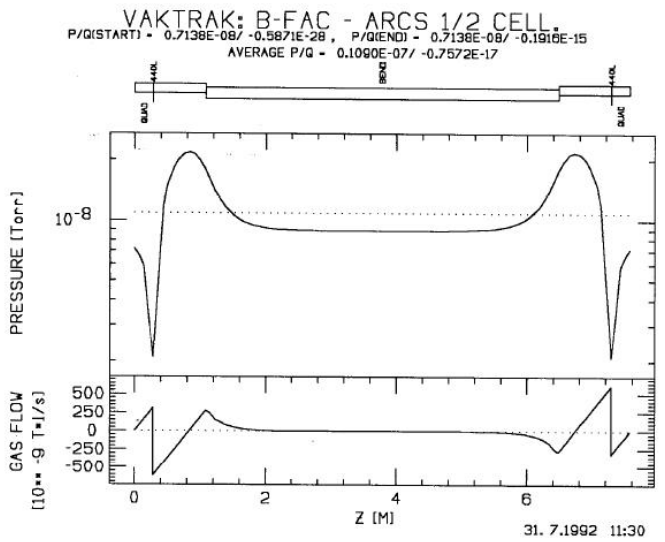


Figure 1: *Longitudinal Pressure Profile*

```
'B-FAC - ARCS 1/2 CELL.'
25  0.28  8.64  0    1.113E-6  'QUAD'
 2  0     0     440  0         '440L'
25  0.80  8.64  0    1.113E-6  '    '
26  5.4   8     119  1.063E-6  'BEND'
25  0.80  8.64  0    1.113E-6  '    '
 2  0     0     440  0         '440L'
25  0.28  8.64  0    1.113E-6  'QUAD'
```

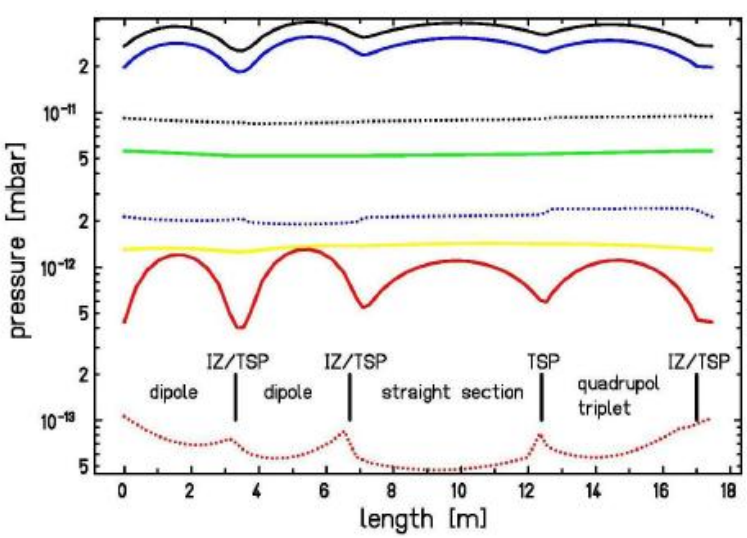
From "Vacuum Tracking", V. Ziemann, SLAC-PUB-5962 (1992)

2 How can it be done?

Transfer-Matrix method:
Program: **VAKTRAK**

- Another example using **VAKTRAK**: analysis of the SIS18 machine at GSI, Darmstadt;
- Multi-component analysis of partial pressure evolution

Simulation with VAKTRAK



The calculation fits to the partial and total pressure recorded in the period S03 of the SIS 18.

Advantages of NEG-coated vacuum chambers:

- Distributed pumping speed for some the residual gases
- Solution to the problem of limited conductance
- Lower desorption yields for ions, photons and electrons than stainless steel

VAKTRAK Code by V. Ziemann:
http://www3.tsl.uu.se/~ziemann/vakdyn/

J. Kurdal GSI Accelerator Facility VBE-UHV 6

From: J. Kurdal, Proc. IUVSTA NEG-coating Workshop, Catania, Apr 2006

2 How can it be done?

Transfer-Matrix method:

Program: **VACCALC(*)**

- Starting from the equation as before we get a solution of the type

$$c\frac{d^2P}{dx^2} - sP = -q \qquad \{ \ldots \text{discretization} \ldots \} \rightarrow$$

- A technique based on the **finite differences** is used to solve the differential equation

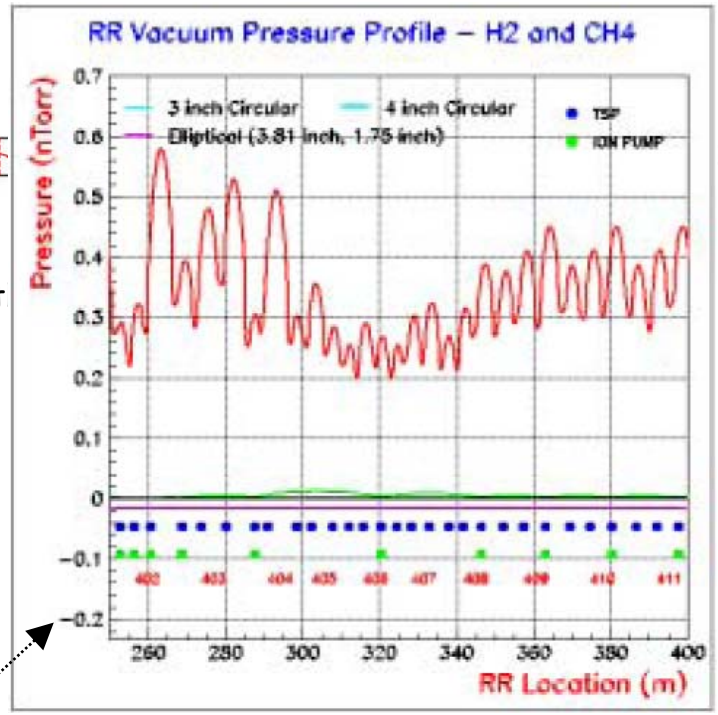
$$\frac{d}{dx}\left(c\frac{dP}{dx}\right) - sP + q = 0$$

$$\frac{d}{dx}\left(c_i\frac{dP}{dx}\right) = \frac{(c_{i+1} - c_i)P_{i+1} + (c_i - c_{i-1})P_{i-1}}{2\Delta x^2} - \frac{(c_{i+1} - c_{i-1} + 2c_i)P_i}{2\Delta x^2}$$

- which becomes in matrix form

$$\begin{Bmatrix} -\frac{c_2+3c_1}{2} - s_1\Delta z^2 & \frac{c_2+3c_1}{2} & & & \\ \cdot & \cdot & & & \\ & \frac{c_i+c_{i-1}}{2} & -\frac{c_{i+1}+c_{i-1}+2c_i}{2} - s_i\Delta z^2 & \frac{c_{i+1}+c_i}{2} & \frac{c_{i+1}+c_i}{2} \\ & & \cdot & \cdot & \\ & & \frac{c_{n-1}+3c_n}{2} & -\frac{c_{n-1}+3c_n}{2} - s_n\Delta z^2 & \end{Bmatrix} \begin{Bmatrix} P_1 \\ \cdot \\ P_i \\ \cdot \\ P_n \end{Bmatrix} = \begin{Bmatrix} -q_1\Delta z^2 - 2Q_1\Delta z \\ \cdot \\ -q_i\Delta z^2 \\ \cdot \\ -q_n\Delta z^2 - 2Q_n\Delta z \end{Bmatrix}$$

- and can be solved to obtain the pressures P_i



From: ""Residual gas pressure profile in the recycler ring", M. Gounder et al, Proc. PAC 2003

(*) "A method for calculating pressure profiles in vacuum pipes", M.K. Sullivan, SLAC, 1993

2 How can it be done?

Another implementation of discretization and matrix description:
Program: **VASCO**(*)

- The 1D-diffusion equation for steady state conditions, where the surface coverage is assumed to vary with a time constant much longer than the gas density

$$V\frac{\partial n_g(x,t)}{\partial t} = a\,D_g\cdot\frac{\partial^2 n_g(x,t)}{\partial x^2} + \frac{I}{e}\sum_j\left\{\eta_{i,\,j^+\to g}\,\sigma_j^b\cdot n_j\right\} - \left(\frac{A\cdot v_g}{4}\cdot\alpha_g + C_g\right)\cdot n_g + \eta_{ph,g}\cdot\Gamma_{ph} + \eta_{e,g}\cdot\Gamma_e + A\cdot q_g \quad (1)$$

Where V = volume of the chamber per unit length [m^2]; A = surface area per unit length [m]; a = chamber cross section area [m^2]. On the right hand side the following terms are found, in the order:

1. Molecular diffusion due to pressure gradient: $a\cdot D_g$ = specific conductance per unit length [$m^4\cdot s^{-1}$], and $D_g = \frac{2}{3}v_g\cdot r(x)$ diffusion coefficient [$m^2\cdot s^{-1}$] for a section of radius = $r(x)$.
2. Ion induced desorption: I = beam current [A]; e = electron charge [C]; $\eta_{i,\,j^+\to g}$ ion induced desorption yield in number molecules g per incident ion j^+; σ_j^b = ionisation cross-section of the gas-beam particle interaction [m^2].
3. Distributed pumping due to either a surface with a sticking probability α_g or linear pumping along the wall chamber C_g [$m^2\cdot s^{-1}$] per unit length: $v_g = \sqrt{\frac{8k_B\cdot T}{\pi\cdot m_g}}$, Maxwell-Boltzmann distribution average molecular velocity [$m\cdot s^{-1}$], with temperature T [K], molecular mass m_g [kg] and the Boltzmann constant k_B [$kg\cdot m^2\cdot K^{-1}\cdot s^2$].
4. Photon induced gas desorption: $\eta_{ph,g}$ photon induced desorption yield in number molecules g per incident photon; Γ_{ph} = photon flux to the wall per unit length [$m^{-1}\cdot s^{-1}$].
5. Electron induced gas desorption: $\eta_{e,g}$ electron induced desorption yield in number molecules g per incident electron; Γ_e = electron flux to the wall per unit length [$m^{-1}\cdot s^{-1}$].
6. q_{ph} = thermal outgassing per unit area [$m^{-2}\cdot s^{-1}$].

(*) "VASCO (VAcuum Stability Code): multi-gas code to calculate gas density profile in a UHV system", A. Rossi, CERN, unpublished.

2 How can it be done?

Another implementation of discretization and matrix description:
Program: **VASCO**(*) **#2**

- It can be assumed that the ions accelerated to the wall can be implanted or have a long sojourn time.
- In this case the ionized molecule is **lost** from the particle balance, and the term

$$-\frac{I}{e}\sigma_g^b \cdot n_g$$

should be added on the right side of the equation.

- The set of equations seen above can be expressed more concisely in matrix form:

$$\bar{n} = \begin{bmatrix} n_{H_2} & n_{CH_4} & n_{CO} & n_{CO_2} \end{bmatrix}'$$

$$\bar{\bar{A}} = a \cdot \begin{bmatrix} D_{H_2} & 0 & 0 & 0 \\ 0 & D_{CH_4} & 0 & 0 \\ 0 & 0 & D_{CO} & 0 \\ 0 & 0 & 0 & D_{CO_2} \end{bmatrix}$$

$$\bar{\bar{\sigma}} = \begin{bmatrix} \sigma_{H_2} & 0 & 0 & 0 \\ 0 & \sigma_{CH_4} & 0 & 0 \\ 0 & 0 & \sigma_{CO} & 0 \\ 0 & 0 & 0 & \sigma_{CO_2} \end{bmatrix}$$

(*) VASCO (Vacuum Stability Code): multi-gas code to calculate gas density profile in a UHV system", A. Rossi, CERN, unpublished,

2 How can it be done?

Another implementation of discretization and matrix description:

Program: **VASCO**(*) **#3**

$$\overline{\overline{\eta}}_i = \begin{bmatrix} \eta_{H_2^+-H_2} & \eta_{CH_4^+-H_2} & \eta_{CO^+-H_2} & \eta_{CO_2^+-H_2} \\ \eta_{H_2^+-CH_4} & \eta_{CH_4^+-CH_4} & \eta_{CO^+-CH_4} & \eta_{CO_2^+-CH_4} \\ \eta_{H_2^+-CO} & \eta_{CH_4^+-CO} & \eta_{CO^+-CO} & \eta_{CO_2^+-CO} \\ \eta_{H_2^+-CO_2} & \eta_{CH_4^+-CO_2} & \eta_{CO^+-CO_2} & \eta_{CO_2^+-CO_2} \end{bmatrix}$$

$$\overline{\eta}_e = \begin{bmatrix} \eta_{e-H_2} & \eta_{e-CH_4} & \eta_{e-CO} & \eta_{e-CO_2} \end{bmatrix}'$$

$$\overline{\eta}_{ph} = \begin{bmatrix} \eta_{ph-H_2} & \eta_{ph-CH_4} & \eta_{ph-CO} & \eta_{ph-CO_2} \end{bmatrix}'$$

$$\overline{v} = \sqrt{8k_BT/\pi} \begin{bmatrix} \sqrt{1/m_{H_2}} & 0 & 0 & 0 \\ 0 & \sqrt{1/m_{CH_4}} & 0 & 0 \\ 0 & 0 & \sqrt{1/m_{CO}} & 0 \\ 0 & 0 & 0 & \sqrt{1/m_{CO_2}} \end{bmatrix}$$

$$\overline{\overline{C}}_{bs} = \begin{bmatrix} C_{H_2} & 0 & 0 & 0 \\ 0 & C_{CH_4} & 0 & 0 \\ 0 & 0 & C_{CO} & 0 \\ 0 & 0 & 0 & C_{CO_2} \end{bmatrix}$$

$$\overline{\overline{\alpha}} = \begin{bmatrix} \alpha_{H_2} & 0 & 0 & 0 \\ 0 & \alpha_{CH_4} & 0 & 0 \\ 0 & 0 & \alpha_{CO} & 0 \\ 0 & 0 & 0 & \alpha_{CO_2} \end{bmatrix}$$

The thermal outgassing rate Q in (molecules/s/m^2) (where q_{gas} is in Torr·l/s/cm^2) is

$$Q = \frac{1.33 \cdot 10^{-5}}{kT} \begin{bmatrix} q_{H_2} & q_{CH_4} & q_{CO} & q_{CO_2} \end{bmatrix}$$

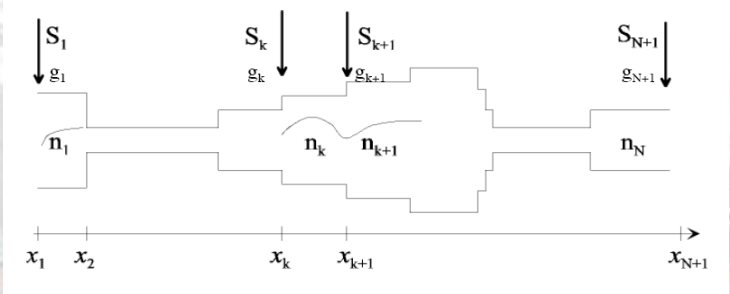
(*) 'VASCO (VAcuum Stability Code): multi-gas code to calculate gas density profile in a UHV system", A. Rossi, CERN, unpublished,

2 How can it be done?

Another implementation of discretization and matrix description:

Program: **VASCO**(*) **#4**

- The vacuum system under study is then discretized and all quantities and parameters of the N sections are defined



The geometry considered by VASCO is always radially-symmetric (cylindrical), in order to allow a one-dimensional approximation (1D-diffusion equation)

- This algorithm has been checked against a MC calculation, for obtaining the pressure profile for ALBA

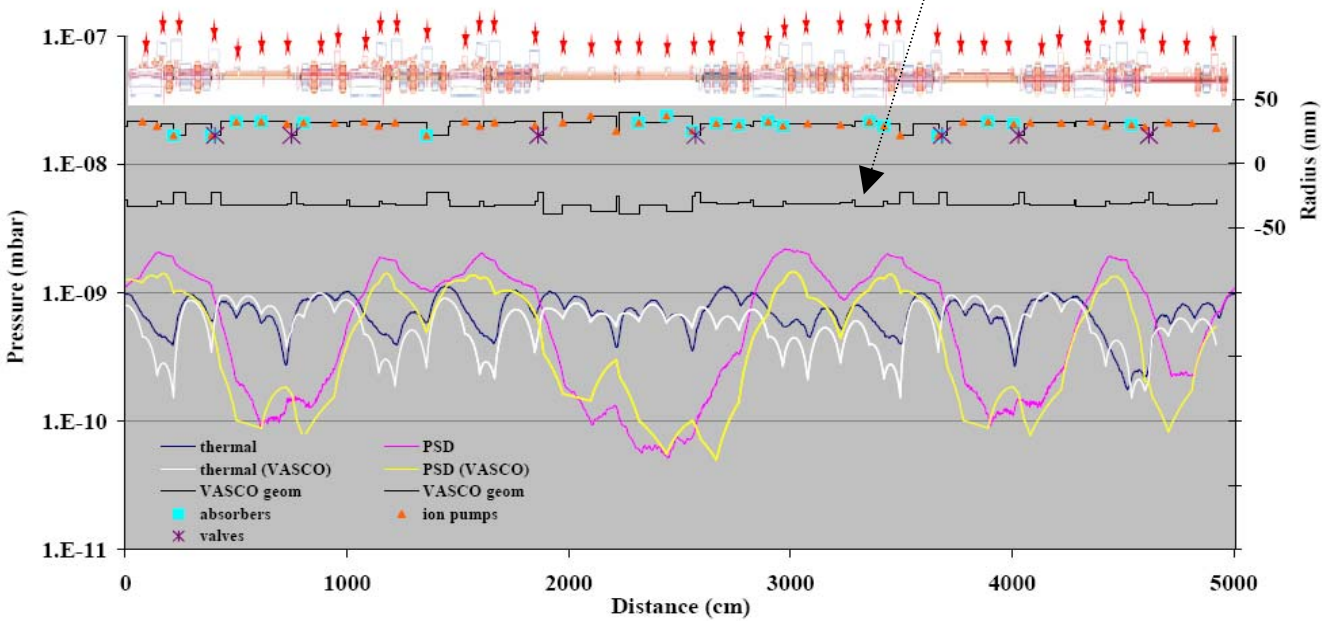


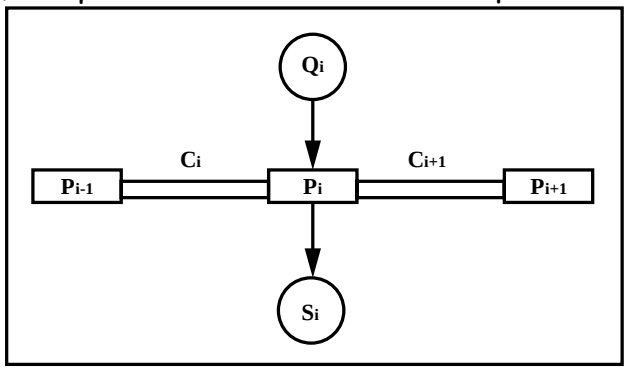
Figure 1: Comparison between VASCO and MOLFLOW results for the case with in situ bake-out, at 400mA, after 1000Ah

(*) "Report on calculations of pressure profile for the ALBA synchrotron light source", A. Rossi, CERN AT-VAC Tech.Note, May 2006, unpublished,

2 How can it be done?

Another one-dimensional algorithm: Application of the Continuity Principle of Gas Flow (CPoGF)#1

The CPoGF algorithm is, basically, a reproduction of the balance equation for a 1D discretized system:



based on the equation $$c_i\left(P_{i-1}-P_i\right)+c_{i+1}\left(P_{i+1}-P_i\right)+Q_i=S_iP_i$$

Different boundary conditions (BC) can be considered:

1) **Periodic BC:**

$$\begin{cases}P_0=P_n\\P_{n+1}=P_0\end{cases}$$

The pressure equation (1) becomes

$$\begin{cases}C_1\left(P_n-P_1\right)+C_2\left(P_2-P_1\right)+Q_1=S_1P_1\\C_i\left(P_{i-1}-P_i\right)+C_{i+1}\left(P_{i+1}-P_i\right)+Q_i=S_iP_i\\C_n\left(P_{n-1}-P_n\right)+C_1\left(P_1-P_n\right)+Q_n=S_nP_n\end{cases}$$

with i=2, 3, …, n-1.

2) **"Smooth"BC:**

$$\begin{cases}P_0=P_1\\P_{n+1}=P_n\end{cases}$$

The pressure equation (1) becomes

$$\begin{cases}C_2\left(P_2-P_1\right)+Q_1=S_1P_1\\C_i\left(P_{i-1}-P_i\right)+C_{i+1}\left(P_{i+1}-P_i\right)+Q_i=S_iP_i\\C_n\left(P_{n-1}-P_n\right)+Q_n=S_nP_n\end{cases}$$

with i=2, 3, …, n-1.

(*) "Calculation of pressure profiles in the CESR hardbend and IR regions", Y. Li et al., Proc. Int'l Workshop on Performance Improvement of e-e+ Colider Particle Factories", Tsukuba, 1999

2 How can it be done?

Another one-dimensional algorithm: Application of the Continuity Principle of Gas Flow (CPoGF):#2

3) **Fixed-Pressure BC:**

$$\begin{cases} -C_1 P_1 + C_2 (P_2 - P_1) + (Q_1 + C_1 P_0) = S_1 P_1 \\ C_i (P_{i-1} - P_i) + C_{i+1} (P_{i+1} - P_i) + Q_i = S_i P_i \\ C_n (P_{n-1} - P_n) - C_1 P_n + (C_{n+1} P_{n+1} + Q_n) = S_n P_n \end{cases}$$

with i=2, 3, …, n-1.

Implementation of the algorithm:

Smooth and fixed-pressure cases:

$$a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \quad (i=1, 2, \ldots, n)$$

where, for (***i*= 2,3,…, n-1**)

$$\begin{cases} a_i = -C_i / (C_i + C_{i+1} + S_i) \\ b_i = -C_{i+1} / (C_i + C_{i+1} + S_i) \\ d_i = Q_i / (C_i + C_{i+1} + S_i) \end{cases}$$

Coefficients for elements #1 and n, for the smooth boundary condition are

$$\begin{cases} a_1 = 0 \\ b_1 = -C_2 / (C_2 + S_1) \\ d_1 = Q_1 / (C_2 + S_1) \end{cases}$$

$$\begin{cases} a_n = -C_n / (C_n + S_n) \\ b_n = 0 \\ d_n = Q_n / (C_n + S_n) \end{cases}$$

while for the fixed pressure boundary condition

$$\begin{cases} a_1 = 0 \\ b_1 = -C_2 / (C_1 + C_2 + S_1) \\ d_1 = (Q_1 + C_1 P_0) / (C_1 + C_2 + S_1) \end{cases}$$

$$\begin{cases} a_n = -C_n / (C_n + C_{n+1} + S_n) \\ b_n = 0 \\ d_n = (Q_n + C_{n+1} P_{n+1}) / (C_n + C_{n+1} + S_n) \end{cases}$$

One can proceed solving for P_i in the i-th equation and then substituting it into the (i+1)-th, and so forth for all i's. With this **FORWARD SUBSTITUTION** technique the equations become

$$\begin{cases} P_i = d_i^* - b_i^* P_{i+1} \\ P_n = d_n^* \end{cases} \qquad (i=1, 2, \ldots, n-1)$$

with

$$\begin{cases} b_1^* = b_1 \\ d_1^* = d_1 \end{cases}$$

$$\begin{cases} b_i^* = b_i / (1 - a_i b_{i-1}^*) \\ d_i^* = (d_i - a_i d_{i-1}^*) / (1 - a_i b_{i-1}^*) \end{cases} \qquad (i=2, 3, \ldots, n-1)$$

$$d_n^* = (d_n - a_n d_{n-1}^*) / (1 - a_n b_{n-1})$$

(*) "Calculation of pressure profiles in the CESR hardbend and IR regions", Y. Li et al., Proc. Int'l Workshop on Performance Improvement of e-e+ Colider Particle Factories", Tsukuba, 1999

2 How can it be done?

Another one-dimensional algorithm: Application of the Continuity Principle of Gas Flow (CPoGF): #3

Now the pressure profile can be easily calculated by **CHASING BACK**, i.e. calculating P_n and then substituting it into the (n-1)-th equation, to calculate P_{n-1}, and so on till i=1

Implementation of the algorithm:

Periodic BC case:

$$\begin{cases} a_1 P_n + P_1 + b_1 P_2 = d_1 \\ a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \quad (i=2, 3, \ldots, n-1) \\ a_n P_{n-1} + P_n + b_n P_1 = d_n \end{cases}$$

for $i=1,2,\ldots,n-1$

$$\begin{cases} a_i = -C_i / (C_i + C_{i+1} + S_i) \\ b_i = -C_{i+1} / (C_i + C_{i+1} + S_i) \quad (i=1,2,\ldots,n-1) \\ d_i = Q_i / (C_i + C_{i+1} + S_i) \end{cases}$$

and

$$\begin{cases} a_n = -C_n / (C_n + C_1 + S_n) \\ b_n = -C_1 / (C_n + C_1 + S_n) \\ d_n = Q_n / (C_n + C_1 + S_n) \end{cases}$$

The equations can be re-formatted to the form of

$$a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \quad (i=1, 2, \ldots, n)$$

By solving for P_i (i=1, … n-1) as a function of Pi+1 and Pn, the equations for the periodic BC case become

$$P_i = d_i^* - b_i^* P_{i+1} + a_i^* P_n \quad (i=1, 2, \ldots, n-1)$$

and

$$P_n = d_n^* - b_n^* P_1$$

or

$$P_1 = d_n^* / b_n^* - P_n / b_n^*$$

with

$$a_1^* = -a_1, \quad b_1^* = b_1, \quad d_1^* = d_1$$

and for $i=2, 3, \ldots, n-1$

$$\begin{cases} a_i^* = -a_{i-1}^* a_i / (1 - a_i b_{i-1}^*) \\ b_i^* = b_i / (1 - a_i b_{i-1}^*) \\ d_i^* = (d_i - a_i d_{i-1}^*) / (1 - a_i b_{i-1}^*) \end{cases}$$

and

$$\begin{cases} d_n^* = (d_n - a_n d_{n-1}^*) / (1 - a_n a_{n-1}^* - a_n b_{n-1}^*) \\ b_n^* = b_n / (1 - a_n a_{n-1}^* - a_n b_{n-1}^*) \end{cases}$$

(*) "Calculation of pressure profiles in the CESR hardbend and IR regions", Y. Li et al., Proc. Int'l Workshop on Performance Improvement of e-e+ Colider Particle Factories", Tsukuba, 1999

2 How can it be done?

Another one-dimensional algorithm: Application of the Continuity Principle of Gas Flow (CPoGF): #4

Substituting $P_n = d_n^* - b_n^* P_1$

into $a_1 P_n + P_1 + b_1 P_2 = d_1$

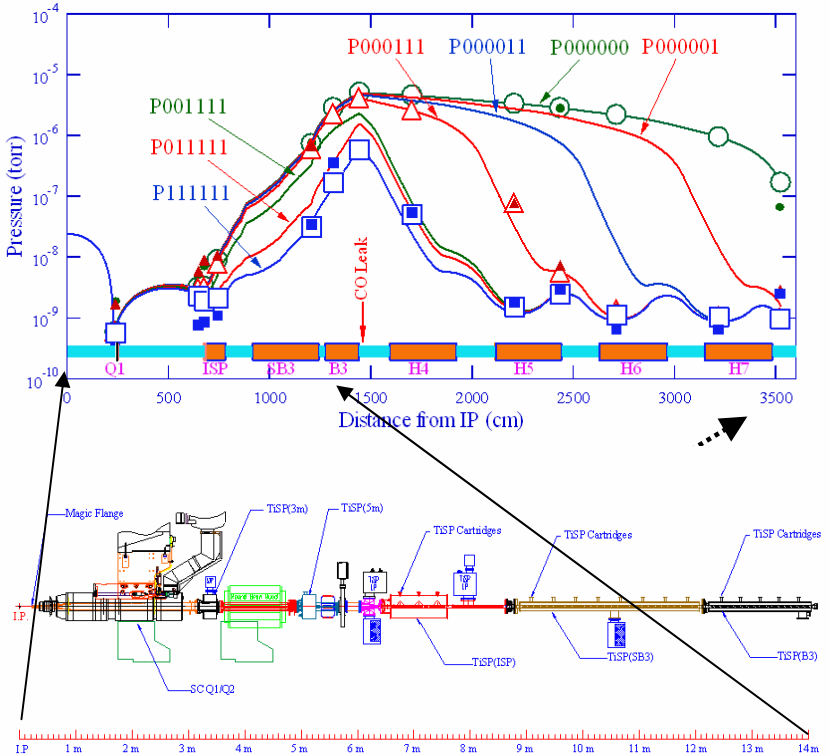
to eliminate P_1, one obtains

$$\begin{cases} P_1 + b_1^{**} P_2 = d_1^{**} \\ a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \quad (\mathbf{i=2, 3, \ldots, n-1}) \\ a_n^{**} P_{n-1} + P_n = d_n^{**} \end{cases}$$

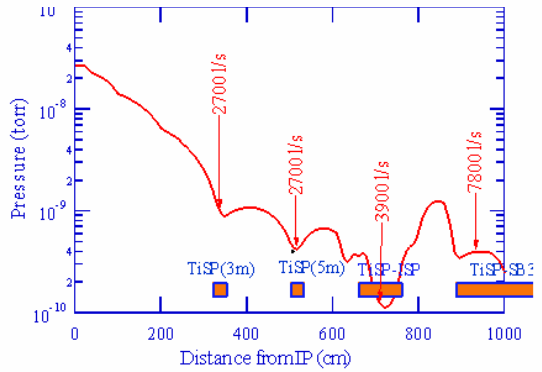
This equation is exactly the same as

$$a_i P_{i-1} + P_i + b_i P_{i+1} = d_i \quad (i=1, 2, \ldots, n)$$

and therefore the pressure profile can be calculated by solving the equation using the same method of **FORWARD SUBSTITUTION** and **CHASING BACK**, as described for the other two BC cases.



Example: the CESR ID region, +/- 35m from the interaction point of the CLEO detector (*)



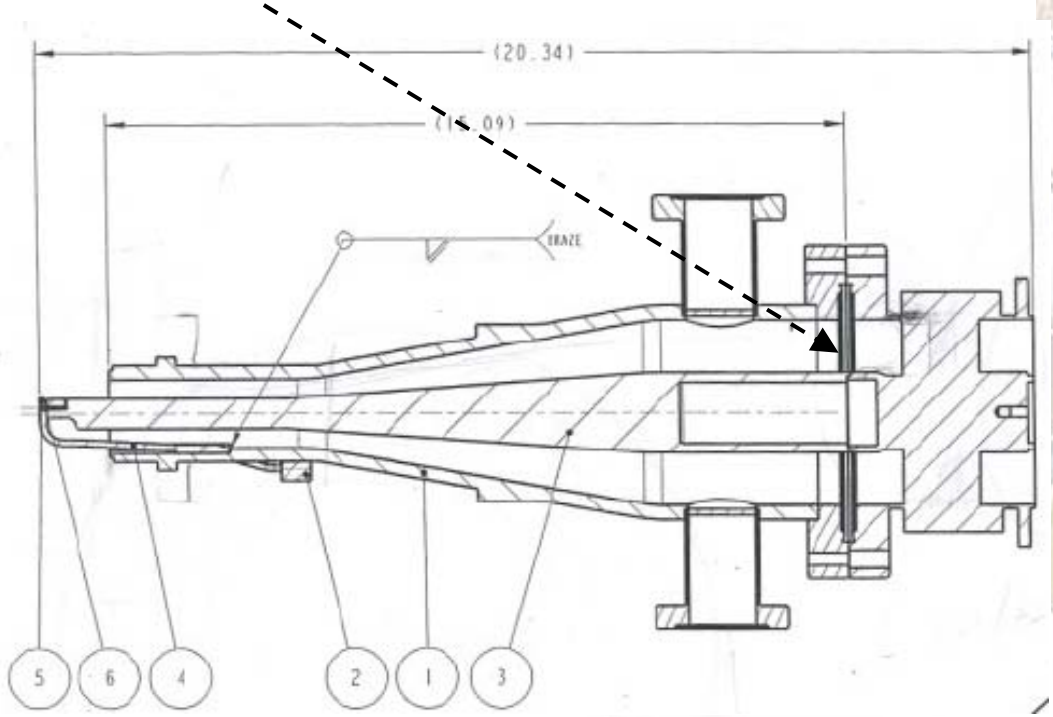
Predicted pressure profile in the IR for CESR Phase III operation at 500mA×500mA beam currents.

(*) "Calculation of pressure profiles in the CESR hardbend and IR regions", Y. Li et al., Proc. Int'l Workshop on Performance Improvement of e-e+ Colider Particle Factories", Tsukuba, 1999

2 How can it be done?

Another application of the Continuity Principle of Gas Flow (CPoGF) using commercially available software (MathCAD #1)

RF coupler pressure distribution, RFQ H^+ accelerator, at the SNS: the aim was to predict the pressure rise in front of the ceramic window, and avoid damaging it



Example of Flow balance at several nodes: MathCAD script

$$C_{2a\_3a}\cdot\left(P_{3a}-P_{2a}\right)-C_{3a\_4a}\cdot\left(P_{4a}-P_{3a}\right)-Q_{3\_4}=0\times 10^{0}\,W$$

$$C_{3a\_4a}\cdot\left(P_{4a}-P_{3a}\right)-C_{4a\_5a}\cdot\left(P_{5a}-P_{4a}\right)-Q_{4\_5}=0\times 10^{0}\,W$$

$$C_{4a\_5a}\cdot\left(P_{5a}-P_{4a}\right)-C_{5a\_6a}\cdot\left(P_{6a}-P_{5a}\right)-Q_{5\_6}=0\times 10^{0}\,W$$

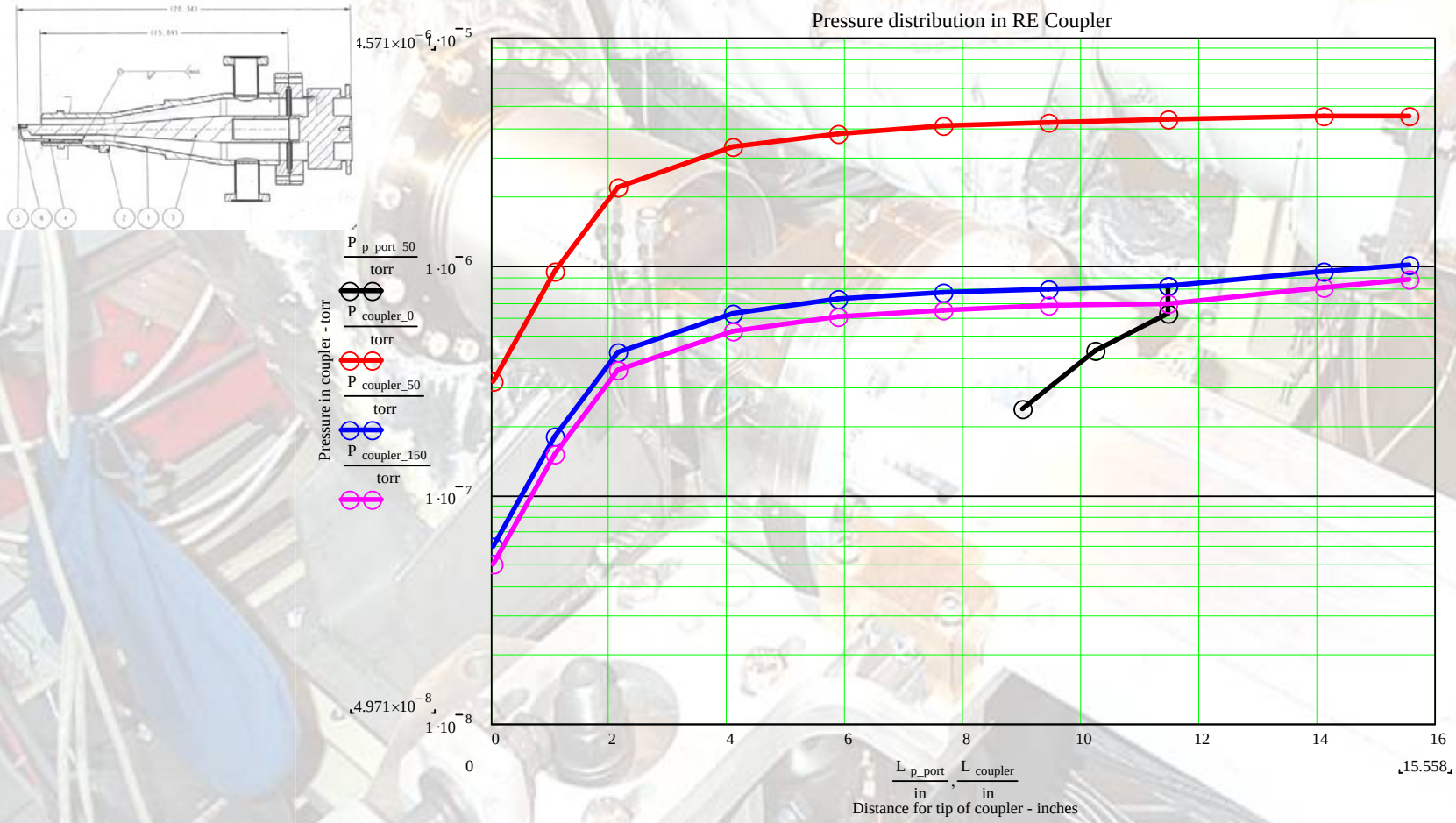
$$C_{5a\_6a}\cdot\left(P_{6a}-P_{5a}\right)-C_{6a\_7a}\cdot\left(P_{7a}-P_{6a}\right)-Q_{6\_7}+C_{6a\_9}\cdot\left(P_{6a}-P_{9}\right)-Q_{6a\_9}+C_{6a\_11}\cdot\left(P_{6a}-P_{11}\right)-Q_{6a\_11}=0\times 10^{0}\,W$$

(*) Courtesy of P. Ladd, SNS, ORNL, Oak Ridge, USA, private communication

2 How can it be done?

Another application of the Continuity Principle of Gas Flow (CPoGF) using commercially available software (MathCAD #2)

•RF Coupler Pressure



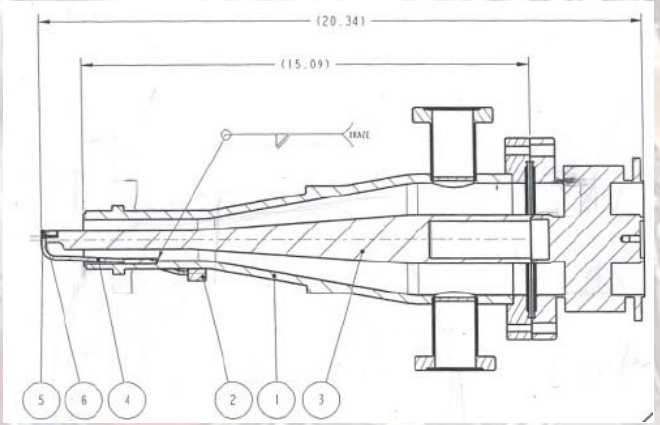
(*) Courtesy of P. Ladd, SNS, ORNL, Oak Ridge, USA, private communication

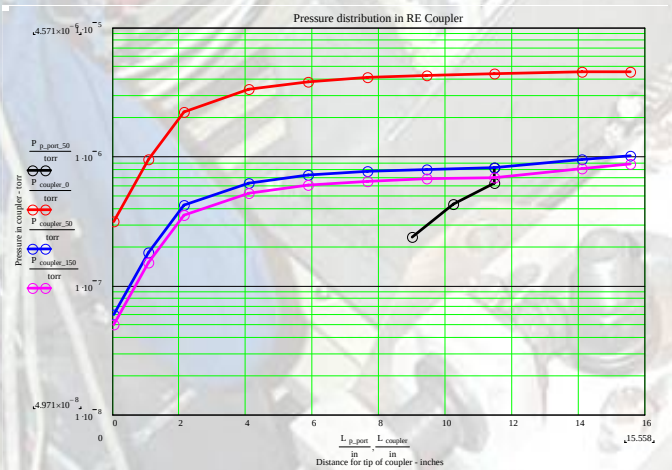
2 How can it be done?

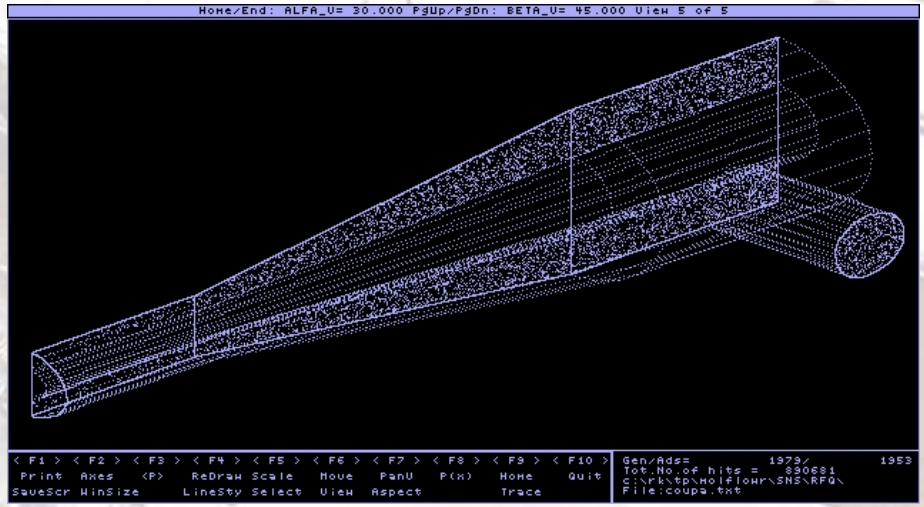
Comparison with 3D Montecarlo simulation (Molflow), same geometry:

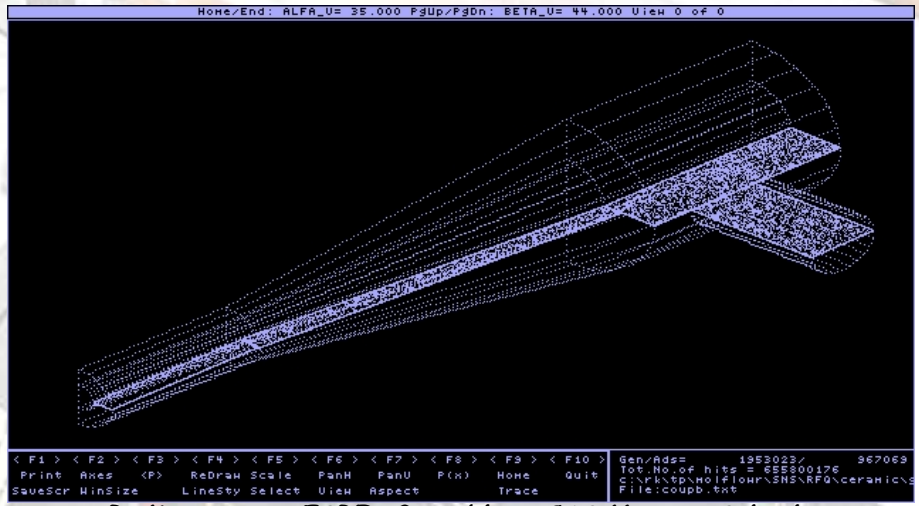
RF Coupler Pressure:

MathCAD vs Molflow









(*) Courtesy of P. Ladd, SNS, ORNL, Oak Ridge, USA, private communication

2 How can it be done?

Finite-Element Method (proprietary codes and commercial programs)

- The **angular coefficients method** (ACM) or **view-factor method** (VF) is based on th
- The total surface (in 3D space) is divided into n elementary surfaces;

- On the i-th surface, the following equation holds

$$\nu_{inc} = \sum_{j=1}^{n} \varphi_{i->j} \cdot \nu_j$$

which leads to a system of algebraic equations

$$\nu_i = \nu_{0i} + (1 - \varepsilon_i) \sum_{j=1}^{n} \varphi_{i->j} \cdot \nu_j$$

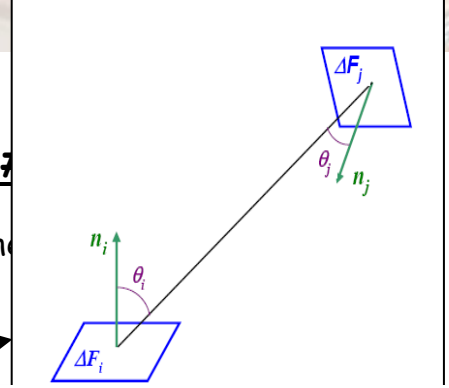
where $\nu_i = \nu_{0i} + (1 - \varepsilon_i) \nu_{inc,i}$

ε_i can be taken as the sticking probability

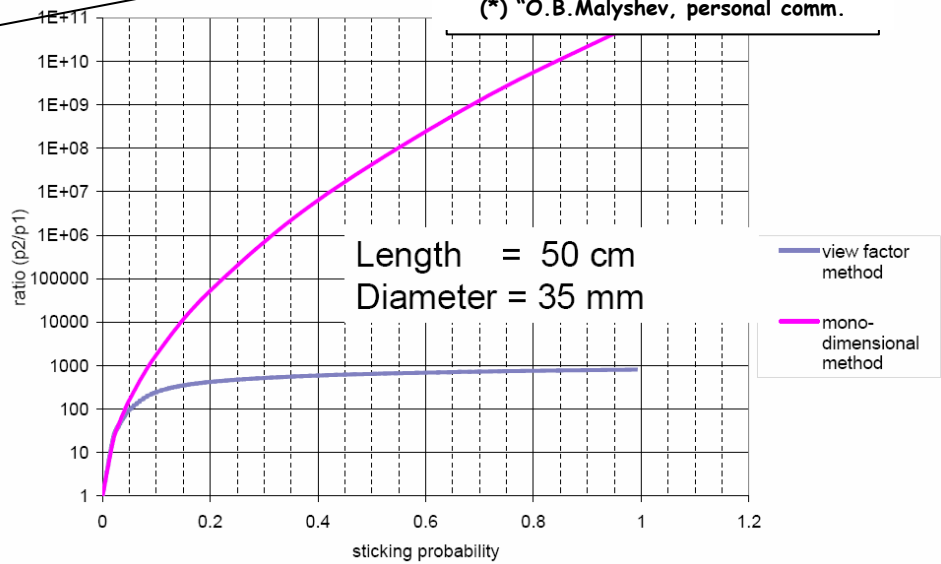
$\phi_{i->j}$ is the angular coefficient, and

$\nu_{ads} = \varepsilon_i \sum_{j=1}^{n} \varphi_{i->j} \cdot \nu_j$ is the adsorbed flux

EXAMPLE: comparison of a **continuos model** (see next slide, 1D discretization) vs. ACM



(*) "O.B.Malyshev, personal comm.



From: "In-situ characterization of NEG pipe coatings: the transmission factor method", A. Bonucci, proc. IUVSTA workshop on NEG-coatings, Catania, Apr 2006

It is clear that the 1D analytic method overestimates by orders of magnitude the ratio of the pressures at the two ends of a circular tube, as soon as the sticking coefficient of the side-wall exceeds ~5%

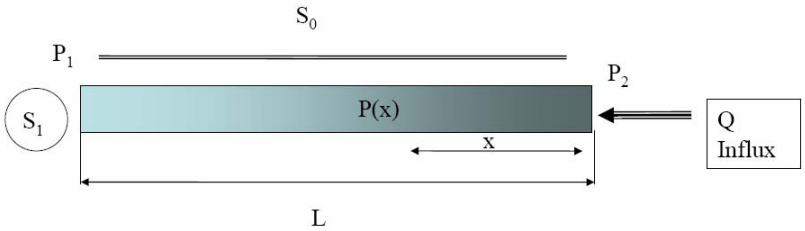
(*) "Molecular flow in complex vacuum systems", G.L.Saksaganskii, Gordon&Breach, NY 1988

2 How can it be done?

Finite-Element Method (proprietary codes and commercial programs) #2:

The angular coefficients method (ACM) or view-factor (VF) method is based on the mass flux balance(*);

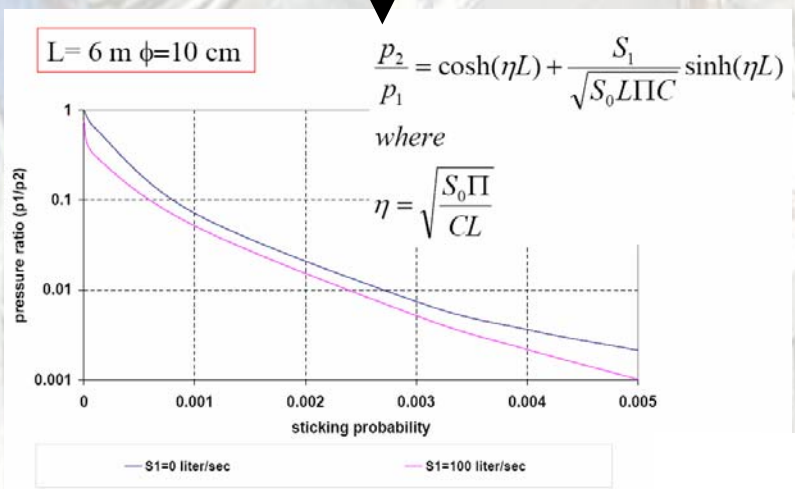
CONTINUOS MODEL **vs** **ANGULAR COEFFICIENT METHOD (ANSYS #1)**



$$CL\left.\frac{dp}{dx}\right|_{x=l} = S_1 p_1$$

$$\frac{d^2 p(x)}{dx^2} + \frac{S_0 \Pi}{CL} p(x) = 0$$

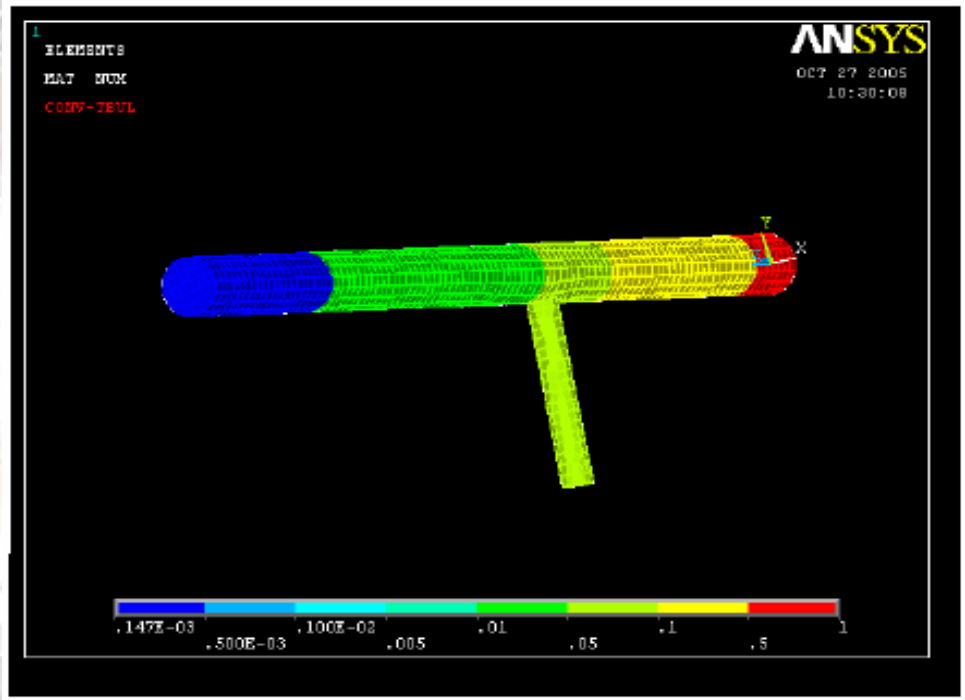
$$p(x=0) = p_2$$



$$\frac{p_2}{p_1} = \cosh(\eta L) + \frac{S_1}{\sqrt{S_0 L \Pi C}} \sinh(\eta L)$$

where

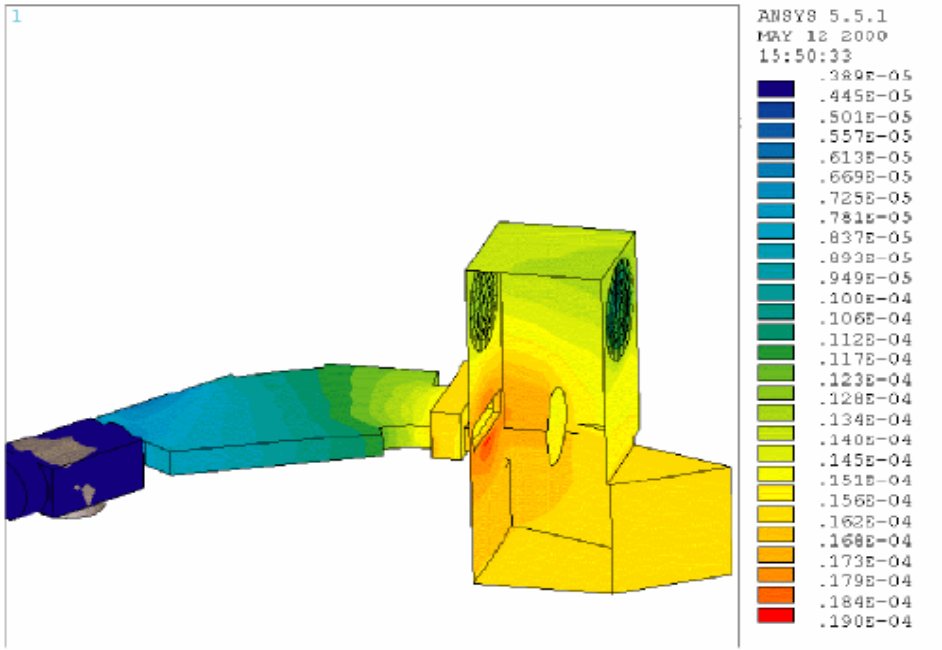
$$\eta = \sqrt{\frac{S_0 \Pi}{CL}}$$



(*) "In-situ characterization of NEG pipe coatings: the transmission factor method", A. Bonucci, proc. IUVSTA workshop on NEG-coatings, Catania, Apr 2006

2 How can it be done?

Finite-Element Method (ANSYS #2):



Wafer deposition ion-implanter, Varian Semiconductor Equipment Ass., Newburyport, MA, USA

(*) "Modeling photoresist outgassing pressure distribution using the FEM method", M.R. Lafontaine et al, ANSYS conference

- In the analogy, **pressure P** is equivalent to **radiation temperature T^4**; the **gas flow** ϕ to **radiation heat-flow q**.
- The following transformations are done

$$\begin{cases} \dfrac{P}{k}\sqrt{\dfrac{R}{2\pi MT}} \Leftarrow \sigma T^4 \\ \phi \Leftarrow q \end{cases}$$

- The pressure is then given by:

$$1.621\cdot 10^{-34}\sqrt{MT}\cdot T^4 \quad \text{P in Torr}$$

- A pumps is simulated by transforming the pumping speed S of a pump of effective area A_p to the "emissivity" of the surface simulating the pump, as follows:

$$\frac{S}{A_p}\sqrt{\frac{R}{2\pi MT}} \Leftarrow \varepsilon_p$$

- In the radiation model, the ambient radiation "temperature" is absolute zero, and therefore the previous assignment becomes

$$0.2749\sqrt{\frac{R}{2\pi MT}} \Leftarrow \varepsilon_p \quad \text{in cgs units}$$

where S is in l/s, A_p in cm^2, ε_p dimensionless.

$$p = \frac{Q}{S}$$

2 How can it be done?

Commercially available FEM programs can be used to analyse a vacuum system(*):

Example (ANSYS) #3:

$$q = C(p_2 - p_1)$$

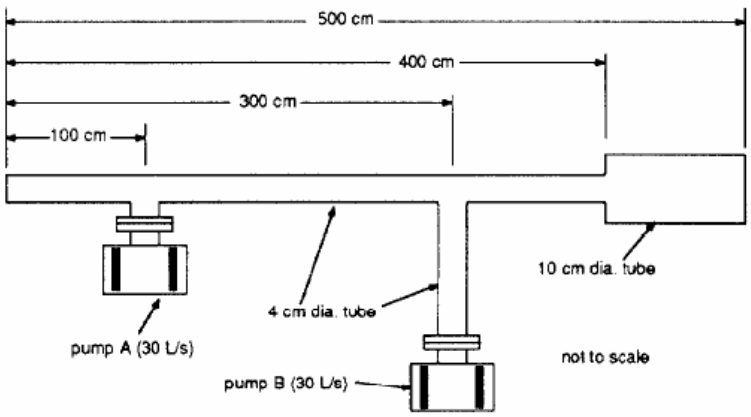
B. Thermal Analogy

For each quantity and relationship expressed in equations (3) and (4), a thermal conduction analogy exists. These vacuum/thermal analogies are summarized in Table 1.

Table 1 Vacuum - Thermal Relationships

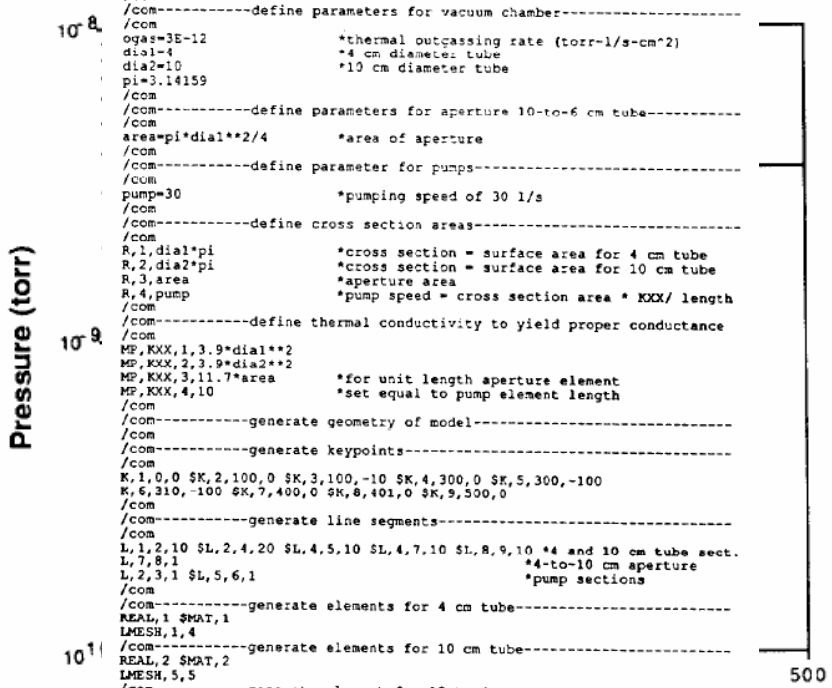
p	Pressure	Torr	T	Temperature	°C
Q	Gas Sources	Torr x l / s x cm²	$\dot{q}$	Heat Sources	W/cm³
C	Gas Conductance	l/s	kA/l	Thermal Conductance	W/°C

The analogy for a pump with a pumping speed S is a conduction element with a thermal conductance equal to S and with a temperature boundary condition, T = 0, at the free end.



Input data script:

```
/TITLE,Example: Vacuum Calculation Using a Thermal Conduction Model
/com
KAN,-1                  *thermal analysis
ET,1,32                 *2-D thermal conduction link
/com
/com-----------define parameters for vacuum chamber----------------------
/com
ogas=3E-12              *thermal outgassing rate (torr-l/s-cm^2)
dia1=4                  *4 cm diameter tube
dia2=10                 *10 cm diameter tube
pi=3.14159
/com
/com-----------define parameters for aperture 10-to-6 cm tube-----------
/com
area=pi*dia1**2/4       *area of aperture
/com
/com-----------define parameter for pumps----------------------------
/com
pump=30                 *pumping speed of 30 l/s
/com
/com-----------define cross section areas----------------------------
/com
R,1,dia1*pi             *cross section = surface area for 4 cm tube
R,2,dia2*pi             *cross section = surface area for 10 cm tube
R,3,area                *aperture area
R,4,pump                *pump speed = cross section area * KXX/ length
/com
/com-----------define thermal conductivity to yield proper conductance
/com
MP,KXX,1,3.9*dia1**2
MP,KXX,2,3.9*dia2**2
MP,KXX,3,11.7*area      *for unit length aperture element
MP,KXX,4,10             *set equal to pump element length
/com
/com-----------generate geometry of model----------------------------
/com
/com-----------generate keypoints-----------------------------------
/com
K,1,0,0 $K,2,100,0 $K,3,100,-10 $K,4,300,0 $K,5,300,-100
K,6,310,-100 $K,7,400,0 $K,8,401,0 $K,9,500,0
/com
/com-----------generate line segments-------------------------------
/com
L,1,2,10 $L,2,4,20 $L,4,5,10 $L,4,7,10 $L,8,9,10 *4 and 10 cm tube sect.
L,7,8,1                                  *4-to-10 cm aperture
L,2,3,1 $L,5,6,1                         *pump sections
/com
/com-----------generate elements for 4 cm tube-----------------------
REAL,1 $MAT,1
LMESH,1,4
/com-----------generate elements for 10 cm tube----------------------
REAL,2 $MAT,2
LMESH,5,5
/com-----------generate element for 10-to-4 cm aperture---------------
REAL,3 $MAT,3
LMESH,6,6
/com-----------generate elements for 30 l/s pumps--------------------
REAL,4 $MAT,4
LMESH,7,8
/com
/com-------define heat generation (outgassing rate) for tube sections--
/com
ERSEL,REAL,1,2                *select only 4 and 10 cm tube sections
QE,ALL,ogas
KTEMP,-1
EALL
/com
/com----------define temperature (pressure) = 0 at end of pumps--------
/com
KNT,3,TEMP,0 $KNT,6,TEMP,0
/com
/com-------------------------------------------------------------------
iter,1,1,1
afwrite,,1
fini
```



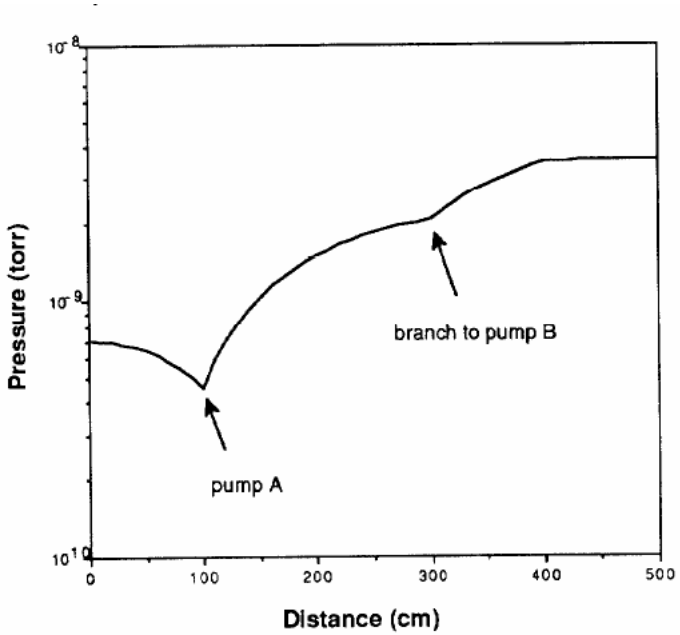
(*) "Calculation of pressure distribution in vacuum systems using a commercial FEM program – J Howell et al., "Proc. PAC 1991, p 2297

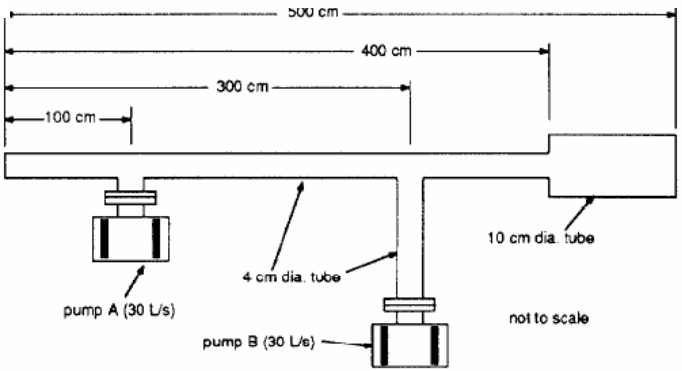
2 How can it be done?

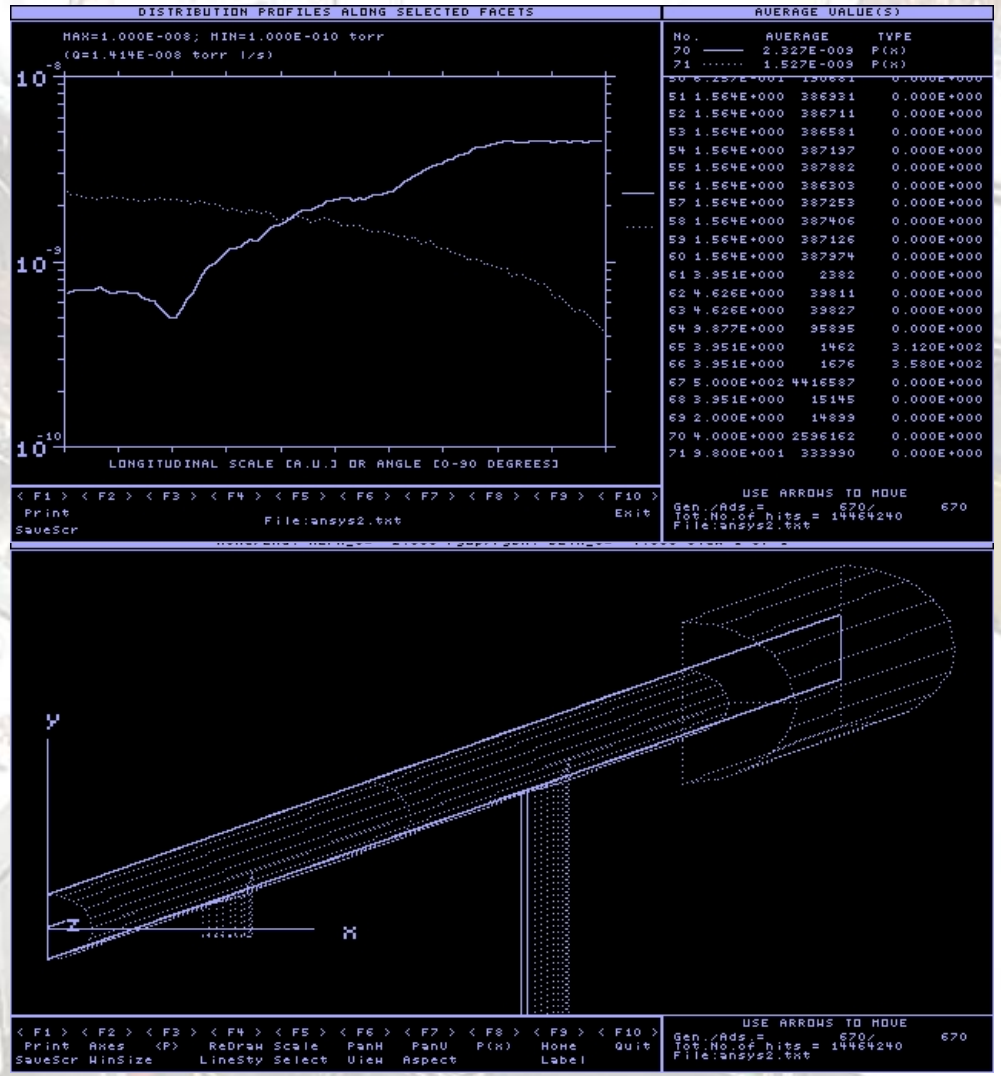
Comparison with 3D Montecarlo simulation (Molflow), same geometry:

ANSYS vs **Molflow**

(*) "Calculation of pressure distribution in vacuum systems using a commercial FEM program - J Howell et al., "Proc. PAC 1991, p 2297



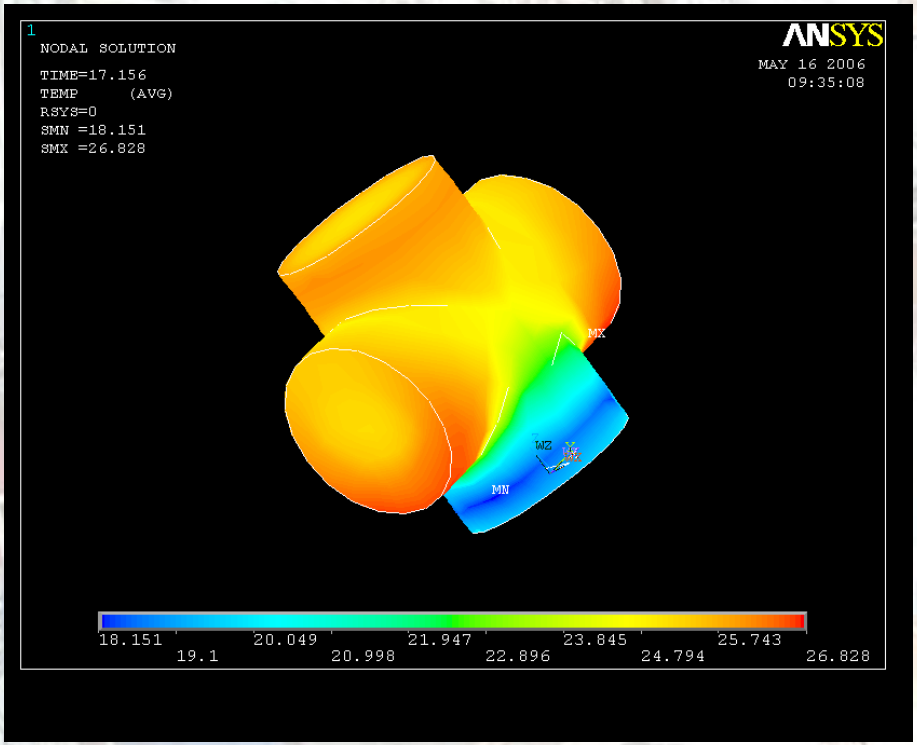


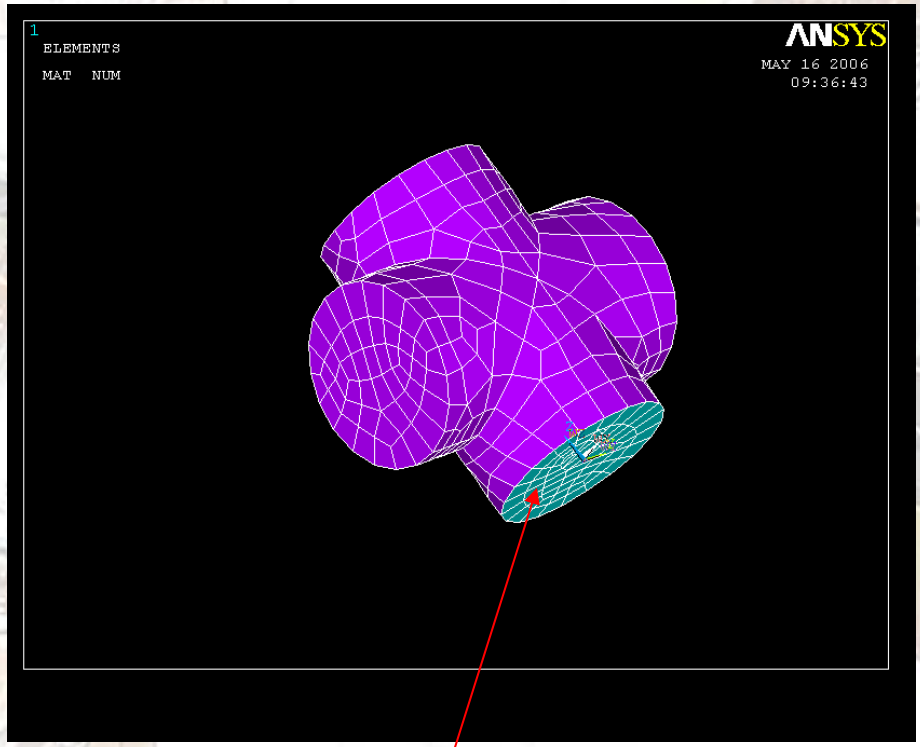


2 How can it be done?

Another example of pressure calculation using ANSYS (*)

4-way cross with uniform desorption and one pump:





Pressure field distribution

Sticking coefficient=0.5

(*) Courtesy of A. Bonucci, SAES Getters, Milan, personal communication, 2006

3 It´s all about the conductance… and the gas load!

NUMERICAL METHODS:

- It is clear by now that all numerical calculational methods we have seen so far, except the MC and the one based on the view-factor (VF) algorithm, need the preliminary calculation of the conductance of all the elements;
- This conductance calculations have to rely either on MC and/or VF, or on analytical calculations. The latter ones, as we have seen, are strictly correct only when round(ish) cross-sections are concerned. In particular they fail very badly when complex 3D shapes are concerned, which is often the case in accelerators;
- The conductance, in l/s, of a tube of length L and uniform cross-section is given by the well known formula of Clausing, which corrected one incorrectly set by Knudsen (missed the correction factor k):

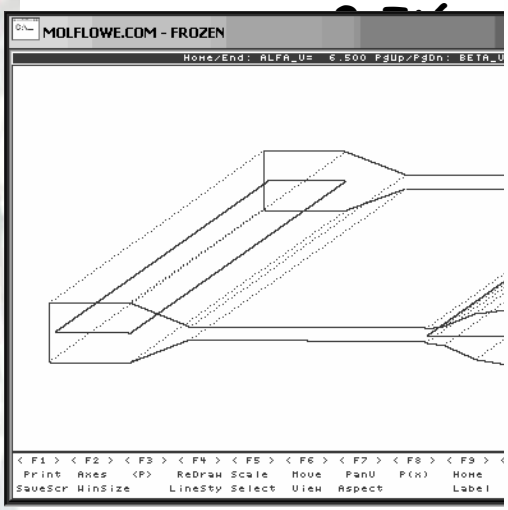
$$C = k\frac{4}{3}v_a\int_0^L \frac{A^2}{H}dx$$

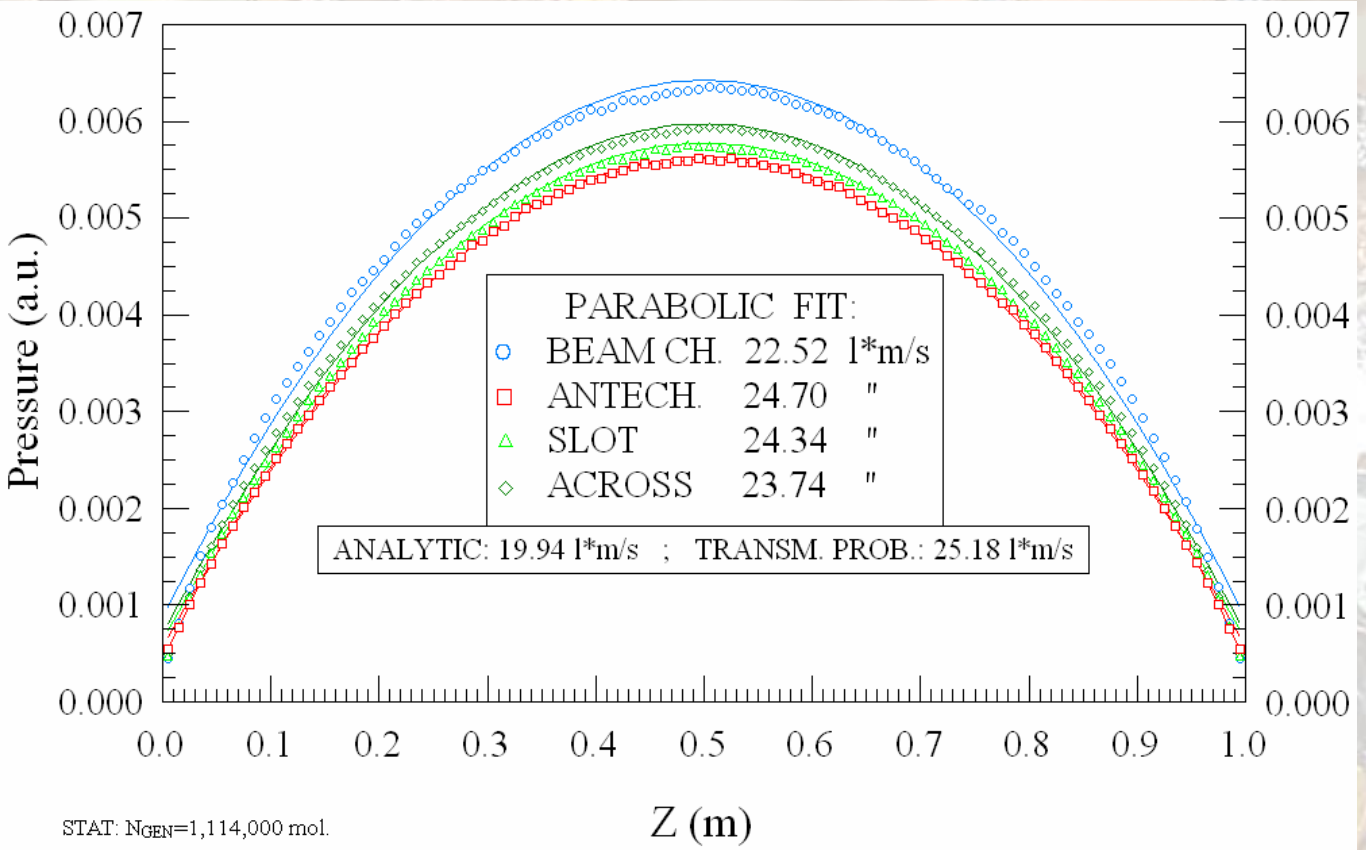
- Where A is the cross-sectional area in cm^2, H the perimeter in cm, v_a the average gas velocity in m/s
- For an arbitrary cross-section, the calculation of the correction factor k is, against what one could think, quite a formidable task, which has been the subject of many papers throughout the last 70+ years
- Considered how many of the algorithms that have been described so far work, it is easy to understand that the under(over)estimate of the value of C may "propagate" through the array of elements which make up the model

ANALYTICAL METHODS:

- As far as analytic calculations are concerned, again the same argument holds: the resolution of the Clausing (integro-differential) equation for arbitrary 3D geometries cannot be tackled easily, if at all. In general, it can be said that only when the accelerator´s chamber resembles a long straight tube with circular cross section, the use of the analytic formula is fully justified.

One example will be given now, which will make clear what all this means...





- The transmission probab
generating molecules at
value is then multiplied
(@20C): $C_{Tr} = 11.7$

- Calculated data for the
which the specific condu

$$P(x) = \frac{Q}{2c}\left(Lx - x^2\right) + \frac{Q}{S}$$

- As can be seen, there is not a univocal value of the specific conductance: it depends from where, in the cross-section, it is calculated. The spread between the smallest value (Knudsen) and the highest (transmission probability) is more than 26%. The spread between the chamber and the ante-chamber values is almost 10%;

- As a general statement, it can be said that the correct determination of the value of the conductances of all the elements used in the calculation is of paramount importance.

3 It´s all about the conductance… and the gas load!

GAS LOADS #1:

- In order to calculate correctly the pressure profiles, it is clear that the determination of the gas loads Q must be made correctly. Failing to do so could lead, for instance, to pumps being placed in the wrong position;

- To this aim, at the ESRF, just to make an example, the whole machine has been carefully studied and documented ("Blue Book") in terms of points where the intense synchrotron radiation generated by the 200 mA, 6 GeV beam is hitting the vacuum chamber and absorbers:

ESRF

SYNCHROTRON RADIATION
POWER DISTRIBUTION
IN THE ESRF STORAGE RING
VACUUM CHAMBERS

* FAN DRAWINGS

* POWER DISTRIBUTION ON THE ABSORBERS

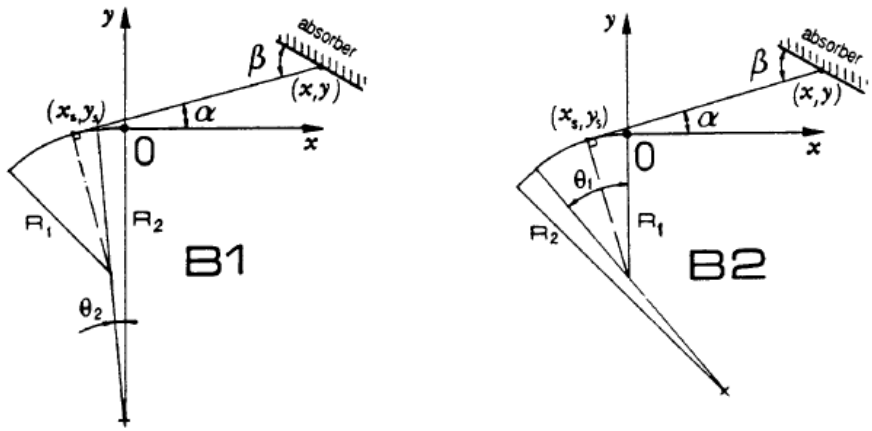
Update March 2004

B. OGIER - B. PLAN - L. ZHANG

Geometrical calculation

There are two types of dipole bending magnets per cell in the ESRF storage ring :

1) with downstream soft end B1
2) with upstream soft end B2

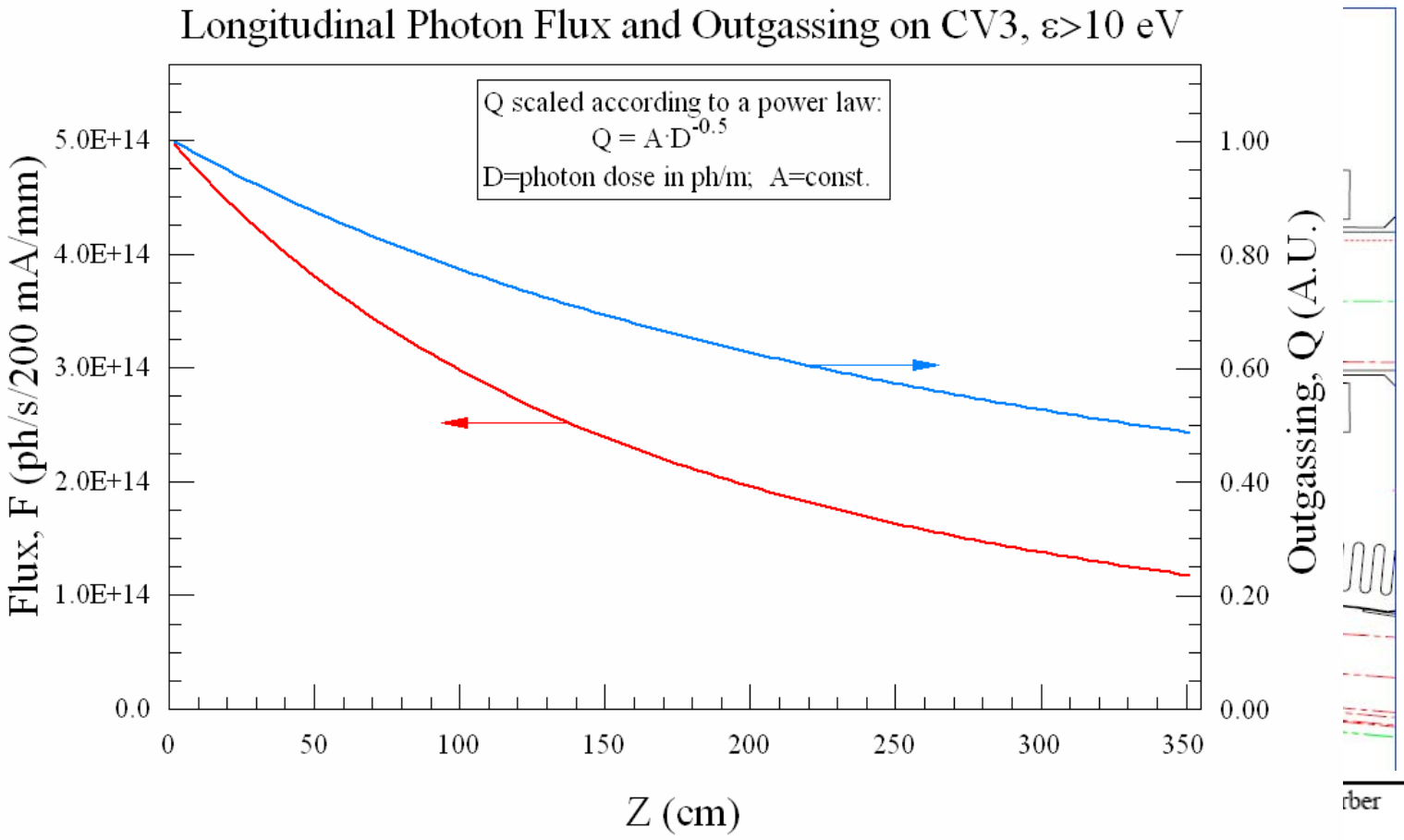


case 1 : dipole magnet B1 case 2 : dipole magnet B2

3 It´s all about the conductance… and the gas load!

GAS LOADS #2:

- **The ESRF Blue Book: the XY coordinates of the source point, the angles of emission and absorption, the e- beam size at the source, the linear (Pl) and surface (Pa) power densities, and the total power intercepted by each chamber/absorber, are shown:**



It is important to choose the right outgassing profile!

4 Conclusions #1

The following table shows a comparison of the different types of calculations we have seen so far:

MODEL	PROs	CONs
Analytic	FAST, ANY SUPPORT (paper sheet to supercomputer)	Usually 1D (cylindrical approx.); No molecular beaming effects; If really accurate →slow (integro-diff eq.); May need pre-calculation of conductances;
FEM/View-Factor	Accurate; multi-purpose. Fast; Integrated environment: mechanical/thermal/vacuum calculations on same model; Gets molecular beaming effects OK;	Can be expensive (license); Needs training; Time consuming modeling;
Montecarlo	Accurate; Fast; Gets molecular beaming effects OK;	Slow; Reference program doesn´t exist yet;
CPoGF	Fast; Intuitive;	Practically limited to 1D problems; Needs pre-calculation of conductances;
Kirchhoff Law Equiv.	Fast; Pedagogically useful;	Prone to keep the user away from the real vacuum issues;
Symbolic Processors	Elegant; Large choice of programs;	Can be expensive (license); Large choice of programs;

4 Conclusions #2

- As we have seen, nowadays pressure distributions inside the vacuum chamber of particle accelerators can be calculated in many different ways, using both commercially available programs and "freeware" codes. Many of the latter are shared on the internet;
- Analytic calculations are leaving the place to advanced and sophisticated numerical simulations, which take advantage of the never ending increase in computing power of today's personal computers;
- There is no general agreement on which the code of choice be: engineers will prefer FEM calculations, while physicists will probably go for modifications of machine-lattice codes, or Montecarlo simulations;
- Vastly different mathematical approaches may be behind each program: care must be put into checking that the physics of the process be correctly described by the algorithm chosen;
- Ideally, more than one calculation should be carried out, and in case of large discrepancies a careful determination of which solution is correct should be reached;
- New codes should always be carefully benchmarked against existing, published results and analytic calculations of simple geometries (e.g. straight round tubes and Clausing's result);
- Together with codes for the calculation of pressures, also codes which evaluate the correct desorption profile should be used. A wrong estimate of the gas load (dynamic and static) will lead to the wrong pressure profiles being obtained.

Tomorrow's particle accelerators will need tomorrow's vacuum calculation codes: take your chance at developing the code everybody wants to use!

5 References

Many references have already been indicated on the previous slides. The following non-exhaustive list is worth consideration:

On analytic calculations:

- "The pressure profile in a long outgassing vacuum tube ", K.M.Welch, Vacuum 23 (8) p271, 1973
- "The calculation of the pressure distribution in the vacuum systems of particle detectors for the colliding beams", Y.Z.Kalinin et al., Vacuum 46 (7) p717, 1995
- "Dynamic vacuum in the beam tube of the SSCL collider – cold beam tube and liner options", W.C.Turner, Proc. PAC-93, Washington D.C., p.3833

On numerical calculations:

- "Monte Carlo calculation of molecular flow rates through a cylindrical elbow and pipes of other shapes", D.H.Davis, J.Appl.phys. 31, p1169, 1960
- "Monte Carlo simulations of molecular flow: some applications in accelerator vacuum technology using a versatile personal computer program", A.Pace et al., Vacuum 41 (7-9) p1910, 1990
- "Matrix calculation of pressures in high-vacuum systems", H.Hirano et al., JVST A6(5) p2865, 1988
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- "An analysis of a complex network of vacuum components and its application", G.Horikoshi et al., Vacuum 41 (7-9) p2132, 1990
- "Vacuum system design using symbolic numeric processors ", W.D.Cornelius, IEEE paper 199
- "PEP-II vacuum system pressure profile modeling using EXCEL", C.Perkins et al., Proc. EPAC-94 conference, London, 1994