51st IUVSTA Workshop on Modern Problems
& Capability of Vacuum Gas Dynamics
9th – 12th July 2007

Monte Carlo Calculations of Pressure Profiles in Particle Accelerator Storage Rings

R. Kersevan*, ESRF, Grenoble, France
kersevan@esrf.fr - Tel.: +33 4 76 88 22 06

ESRF, BP 220, 38043 GRENOBLE, FRANCE

Agenda:

Intro: Particle Accelerators - Where and What For?
Beam Loss Mechanisms
Pressure Profiles
Why MC?
Framework
Examples
Conclusions
References

* On behalf of the Vacuum Group, Technical Services Division, ESRF - 6 Rue Jules Horowitz, Grenoble F-38043 Cedex 09

1. Intro: Particle Accelerators - Where and What For?

Where:

- The total number of particle accelerators, **all categories included**, in operation in the world as of today is practically impossible to know with precision. The are recent estimates which list at about **1,500** the number used in industrial applications, **5,000** in the medical field (radiotherapy and production of radio-isotopes), and **~200** for basic research (particle physics, synchrotron radiation). In addition, about **7,000** units are used as ion implanters or to modify the state of surfaces, and **1,000** more for non-nuclear research. The **grand total** is approximately **15,000** accelerators [1];
- They are located on the 5 continents, although Africa unfortunately barely makes it on the list;
- Total world investment can be estimated at **several billions €/year**;

  Ex.: the ILC (Internation Linear Collider, an international project under study now) would need approximately 14 billion $US to complete in 7 years, if built now with present technology. **Its vacuum system is one of the major contributors to the total budget, and a possible show-stopper for the entire project. Innovative vacuum technology solutions make the top ten list in terms of R&D [2];**

1. Intro: Particle Accelerators - Where and What For?

Where:

• In Europe, the following list shows the names of the accelerators used for basic research purposes in the field of **synchrotron radiation** (25 entries) [3]:

http://www.lightsources.org/"

Europe

- ALBA - Synchrotron Light Facility, Spain
- ANKA - Angstromquelle Karlsruhe, Germany
- BESSY - Berliner Elektronenspeicherrin
- CLIO - Centre Laser Infrarouge d'Orsay
- DAΦNE Light, Italy
- DELSY - Dubna ELectron SYnchrotron, R
- DELTA - Dortmund Electron Test Accele
- Diamond Light Source, UK
- ELETTRA - Synchrotron Light Laboratory
- ELSA - Electron Stretcher Accelerator, G
- ESRF - European Synchrotron Radiation
- FELBE - Free-Electron Lasers at the ELB
- FELIX - Free Electron Laser for Infrared eXperiments, The Netherlands
- HASYLAB - Hamburger Synchrotronstrahlungslabor at DESY, Germany
- ISA - Institute for Storage Ring Facilities, Denmark
- ISI-800 - Institute of Metal Physics, Ukraine
- Kharkov Institute of Physics and Technology, Ukraine
- KSRS - Kurchatov Synchrotron Radiation Source, Russian Federation
- MAX-lab, Sweden
- MLS - Metrology Light Source, Germany
- PSLS - Polish Synchrotron Light Source, Poland (external link)
- SLS - Swiss Light Source, Switzerland
- SOLEIL, France
- SRS - Synchrotron Radiation Source, UK
- TNK - F.V Lukin Institute, Russian Federation

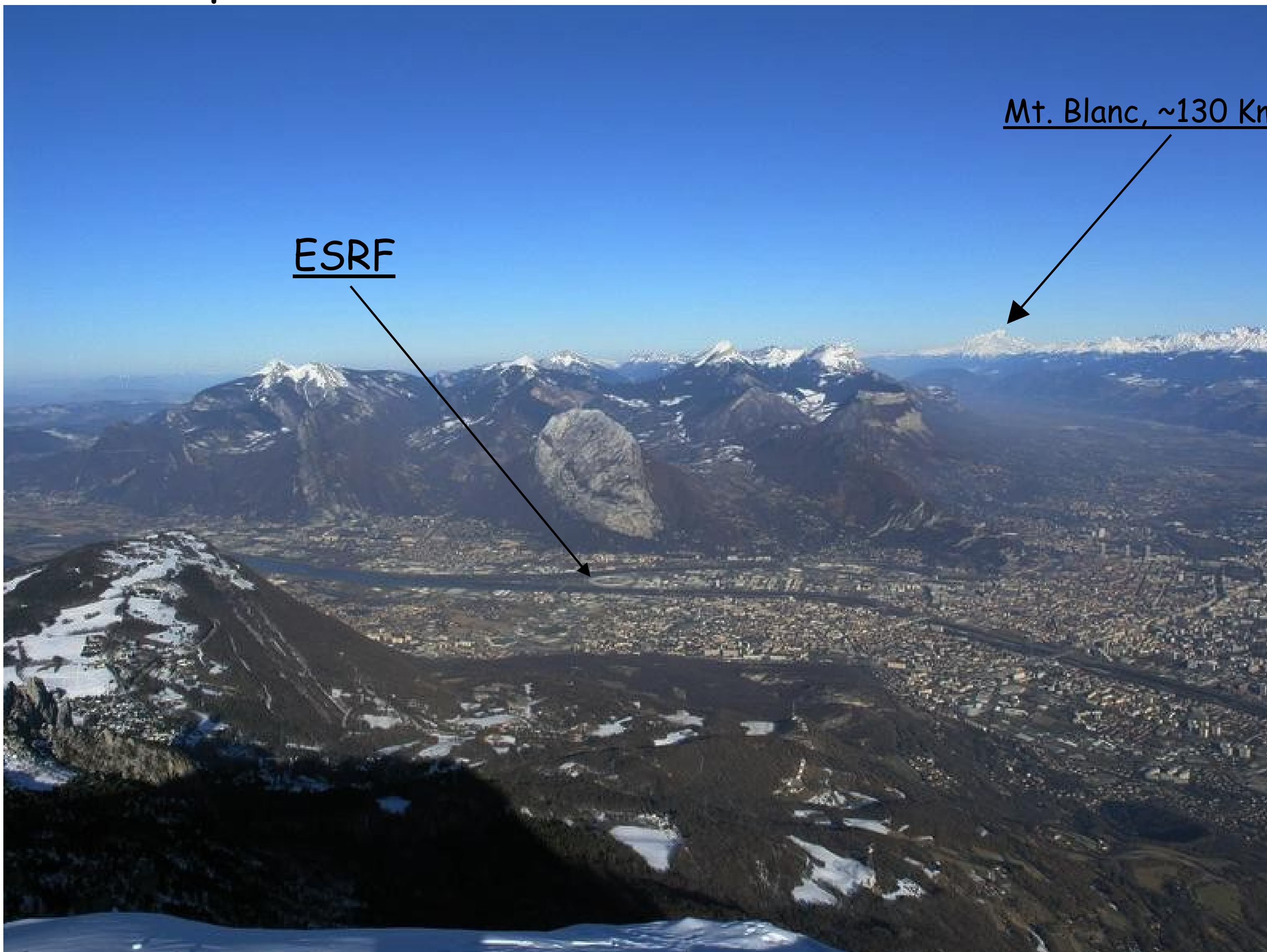
1. Intro: Particle Accelerators - Where and What For?

ESRF

Where: location of the major European particle accelerator laboratories

1. Intro: Particle Accelerators - Where and What For?

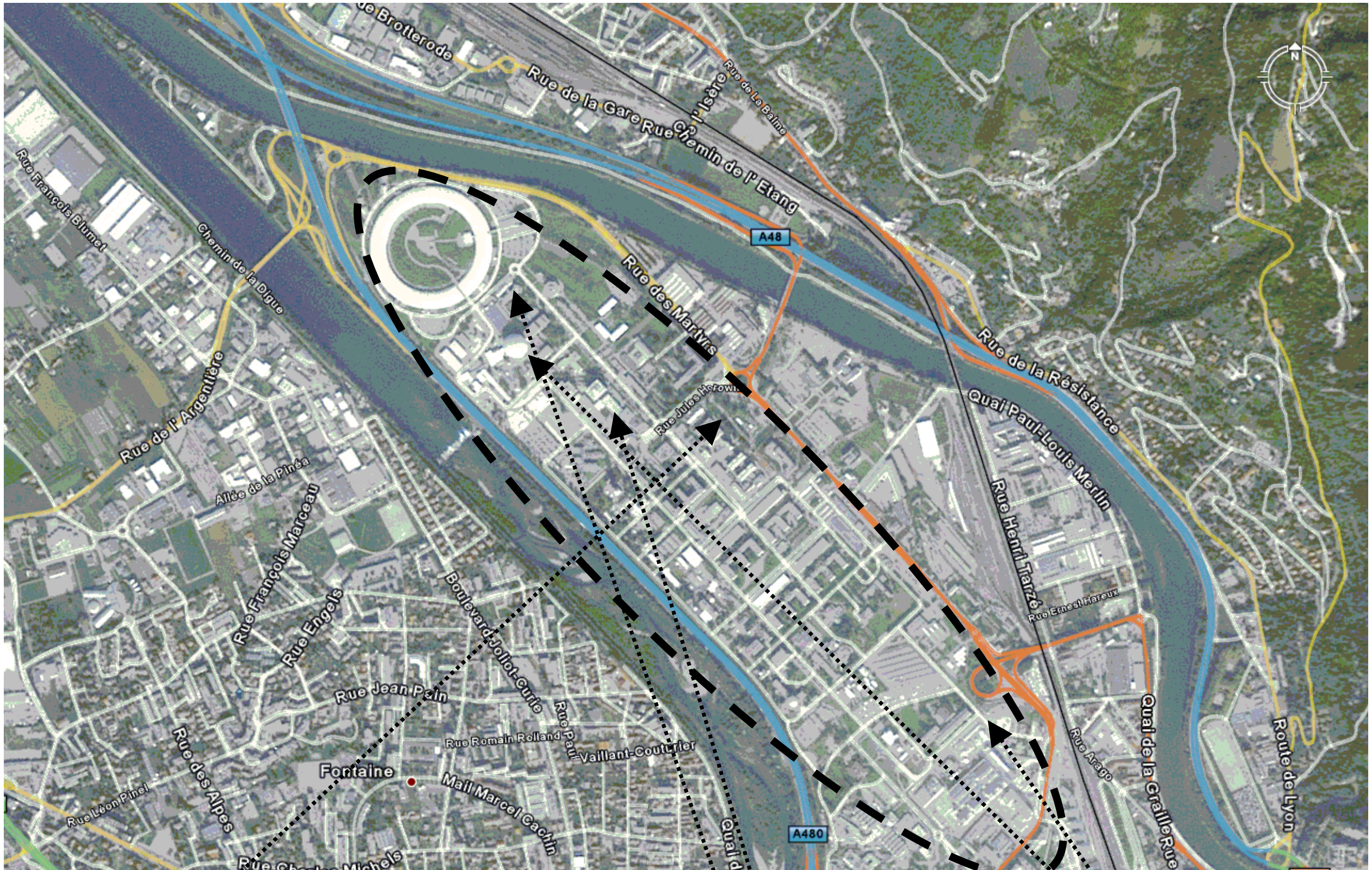
Where: One example: the ESRF in Grenoble as viewed from the Vercors…



1. Intro: Particle Accelerators - Where and What For?

ESRF

Where: One example: the ESRF in Grenoble, and the Polygone Scientifique



@ **Polygone Scientifique "Louis Neel"**, home of **ILL** (neutron research, 50 MW D_2O reactor); **EMBL/IVM** (molecular biololgy); **CNRS** (French Research Council); **ST Microelectronics**, **MINATEC** (nanotecnology), and more, totalling **~3500 people**

European Synchrotron Radiation Facility (ESRF):

- One of only 3 “high-energy” SR light sources (APS-USA, 7 GeV; Spring-8-Japan, 8 GeV);
- Int’l lab, partnership of 19 countries (more coming on board soon);
- In operation since 1993;
- 5 Experimental runs/year (~285 days), ~5500 hours of photon beams delivered to 43 beamlines ;
- Permanent staff: ~480;
- Visiting scientists: ~3500/year;
- **>98% beam availability; ←**

Aerial view of the ESRF site

What For?:

• As already mentioned, particle accelerators are used for **basic** and **applied research**, **industrial**, **medical** and **military** applications;

• **Basic research**:

• Elementary particle: best known example is LHC -under construction at CERN- a multi-billion € machine (27 Km, 22/27 cryogenically cooled down to 1.9K);

• Synchrotron radiation light sources: ex. ESRF, 844 m circumference, 250 M€/y budget;

• ITER will also make use of accelerators, for heating the plasma, although vacuum is not the major issue here;

• **Medical applications**: mainly treatment of tumors (ex. GSI Darmstadt);

• **Military applications**: inertial fusion (study/optimization of thermonuclear devices), directed-energy weapons (aka "Star Wars"), detection of radio-nuclides (ex. US Homeland Security stuff) and more, **mostly classified work**;

• **The common feature is the need for some degree of vacuum: from 10^{-13} mbar for heavy-ion or anti-proton storage rings up to >10^{-5} mbar for low-grade ion-implanters;**

2. Beam Loss Mechanisms

- Depending on the type (collider, storage ring, cyclotron, etc…), the energy of its beam(s), the type of particle(s) being accelerated, and several machine-specific parameters (the "optics" of the machine), each accelerator is subjected to a variety of **beam loss mechanisms**, which affect its performance sometimes in dramatic ways;
- One important class of beam losses is the one related to the **interactions of the beam(s) with the residual gas (RG) inside the vacuum chamber**, along the path of the beam(s);
- These interactions can be due either to **elastic** or **inelastic scattering** off the **nuclei** of the RG molecules or their **electrons**. Examples are **Coulomb scattering**, **Bremsstrahlung** scattering, **charge-exchange**. The result of these interactions can either be a **direct loss** or the generation of **high-energy secondaries** (photons, neutrons);
- These scattering interactions are described by precise analytic formulae, and can be correlated to the beam loss rates measured along/around the accelerator [4];
- **A careful analysis in terms of expected pressure profile <u>-depending explicitly on the gas composition-</u> can be very helpful in order to design and operate efficiently and safely the accelerator itself and <u>the experimental areas around it</u> [5, 6];**

2. Beam Loss Mechanisms

The beam lifetime τ is defined by the current decay rate $1/\tau = -\dot{I}/I$, which is the sum of the Touschek (T) rate and the gas scattering (G) rate

$$\frac{1}{\tau} = \frac{1}{\tau_T} + \frac{1}{\tau_G} = \frac{1}{\tau_T} + c\,n\left(\sigma^N_{elast} + \sigma^N_{inel} + \sigma^e_{elast} + \sigma^e_{inel}\right). \quad (1)$$

The Touschek decay rate can be written as (e.g. [4])

$$\frac{1}{\tau_T} = \frac{N r_e^2 c}{8\pi\sigma_x\sigma_y\sigma_z\,\gamma^2\,(\Delta p/p)^3}\cdot D\left(\frac{(\Delta p/p)^2\sigma_{x'}^2}{\gamma^2}\right), \quad (2)$$

where $D \approx 0.3$ is a slowly varying function that is evaluated numerically. Relativistic effects and beam polarization modify the Touschek rate on the level of 10-20% [5].

The total cross sections for elastic and inelastic scattering on residual gas nuclei (N) and electrons (e) are [4]

$$\sigma^N_{elast} = \frac{2\pi r_e^2 Z^2}{\gamma^2}\frac{\bar{\beta}\beta_a}{a^2} \quad (3)$$

$$\sigma^N_{inel} = \frac{4 r_e^2 Z^2}{137}\frac{4}{3}\left(\ln\frac{183}{Z^{1/3}}\right)\left(\ln\frac{1}{\Delta p/p} - \frac{5}{8}\right) \quad (4)$$

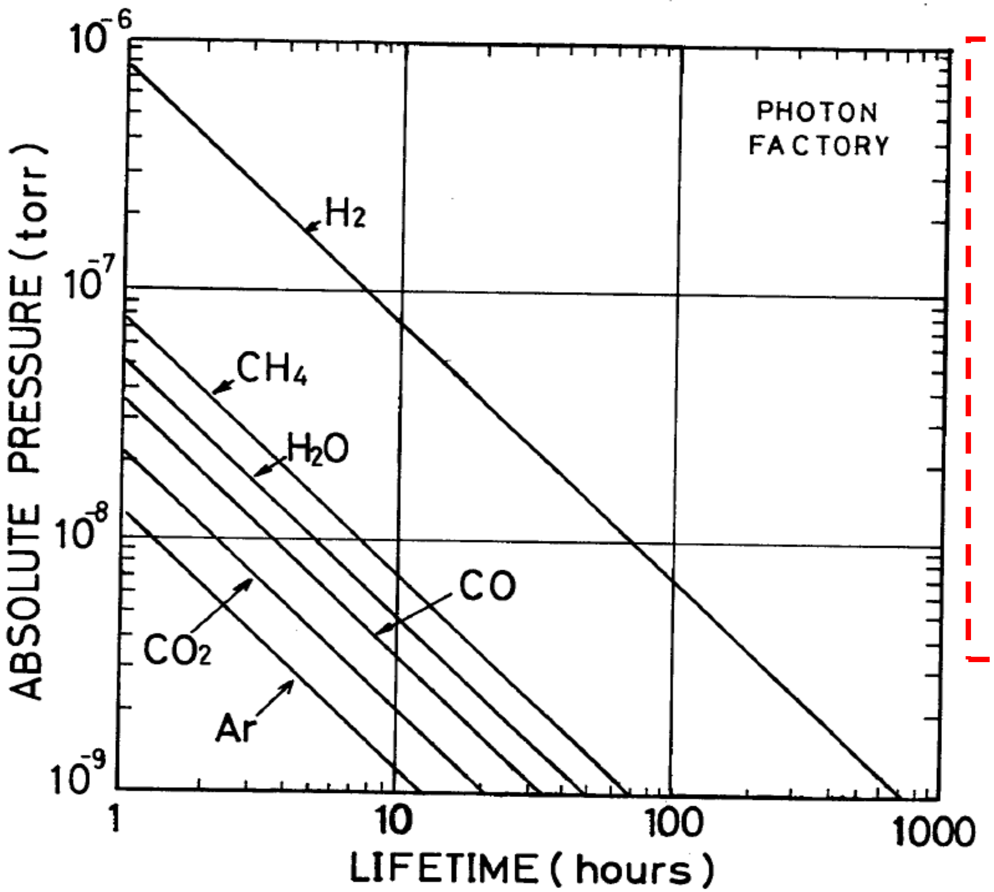
$$\sigma^e_{elast} = \frac{2\pi r_e^2 Z}{\gamma}\frac{1}{\Delta p/p}$$

$$\sigma^e_{inel} = \frac{4 r_e^2 Z}{137}\frac{4}{3}\left(\ln\frac{2.5\gamma}{\Delta p/p} - 1.4\right)\left(\ln\frac{1}{\Delta p/p} - \frac{5}{8}\right),$$

Ref.: S. Khan, "Study of the BESSY II beam lifetime", Proc. PAC-99, NY, p.2831-2833

2. Beam Loss Mechanisms

ESRF

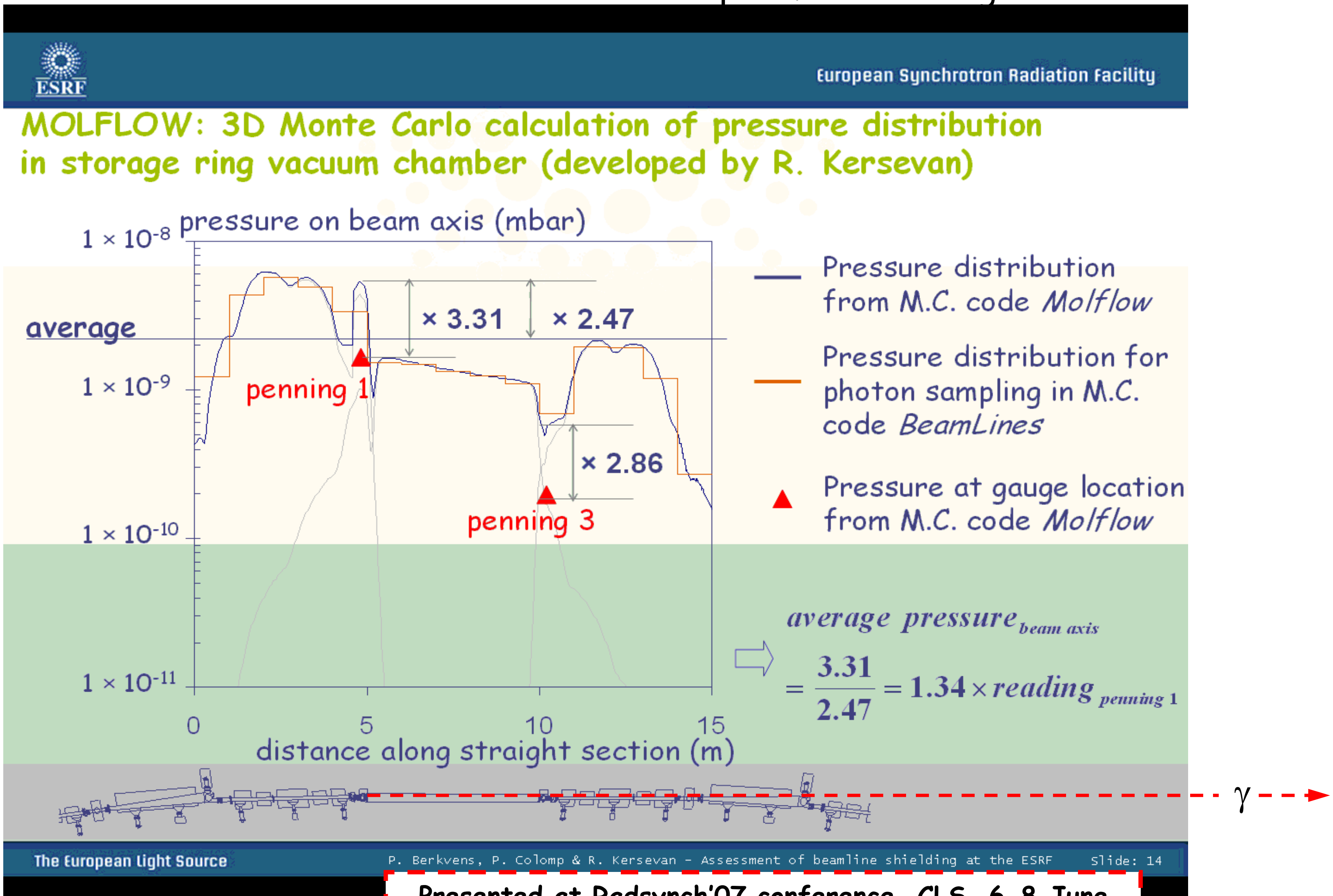


<u>Substance</u>	Molecular <u>Weight</u>	Radiation <u>Length ($g\ cm^{-2}$)</u>
H	1	58
C	12	42.5
O	16	34.2
CH_4	16	45.5
H_2O	18	35.9
CO	28	37.3
Ar	40	19.4
CO_2	44	36.1

Ref.: "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

2. Beam Loss Mechanisms

Bremsstrahlung radiation along experimental straight section:



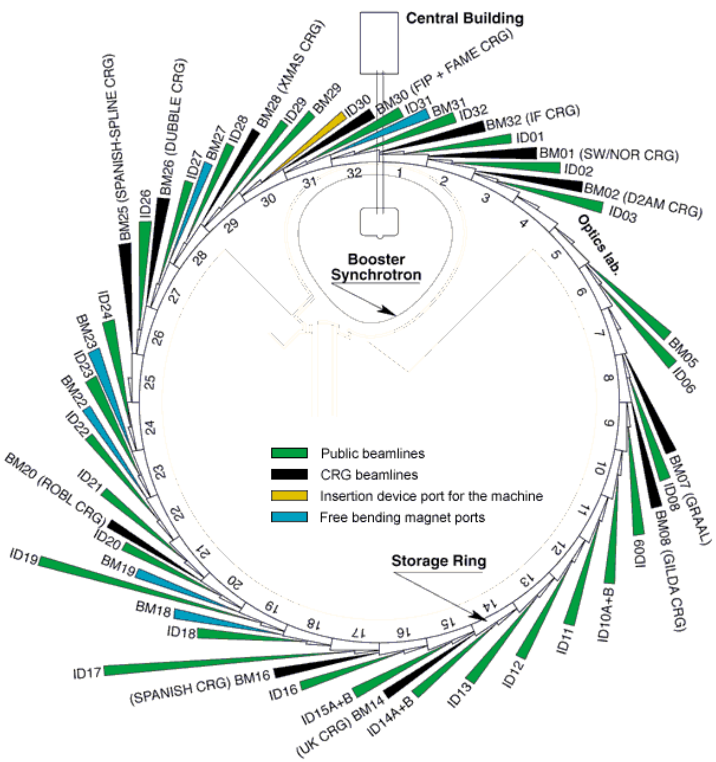
Presented at Radsynch'07 conference, CLS, 6-8 June 2007, Saskatoon, to be published in *Radiation Measurements*

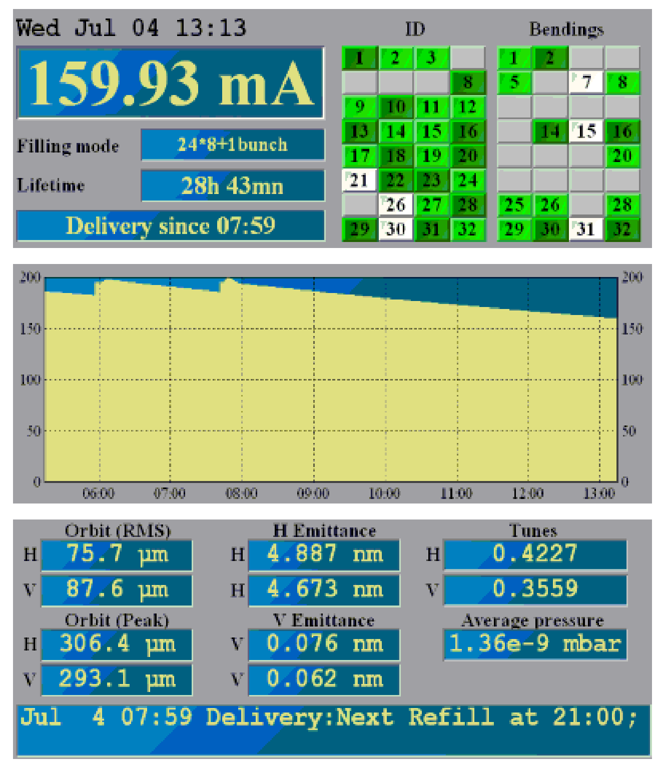
2. Beam Loss Mechanisms

ESRF

Example: the ESRF, a high-energy, 3rd generation light source

Machine Parameters: Quantity	**Nominal Value**	**Units/Comments**
Circumference	844	m
Beam Energy	6	GeV
Beam Current	200	mA (e-)
Lifetime (needed)	**>30**	**hours** (>80 hours achieved)
Average Pressure	**~1.0E-9**	**mbar**
No. of Experimental Beamlines	43	(27 from IDs and 16 from Dipole Magnets)





3. Pressure Profiles

Depending on the type of accelerator, and the specific use being made of it at a particular time, the pressure distribution depends on:

- **Outgassed species**;
- **Pumping speed**, <u>installed</u> and <u>*effective*</u>;
- **Conductance** of the various vacuum chambers making up the complete system;

It is therefore important to know and/or be able to calculate the **outgassing rates** of the different gas species, for all possible **desorption mechanisms** (thermal desorption, beam-induced desorption, etc…);

Generally speaking, all particle accelerators have one feature in common: their vacuum systems are **conductance limited**, mainly due to the need to **minimize the size of the magnets** (cost, field quality,…);

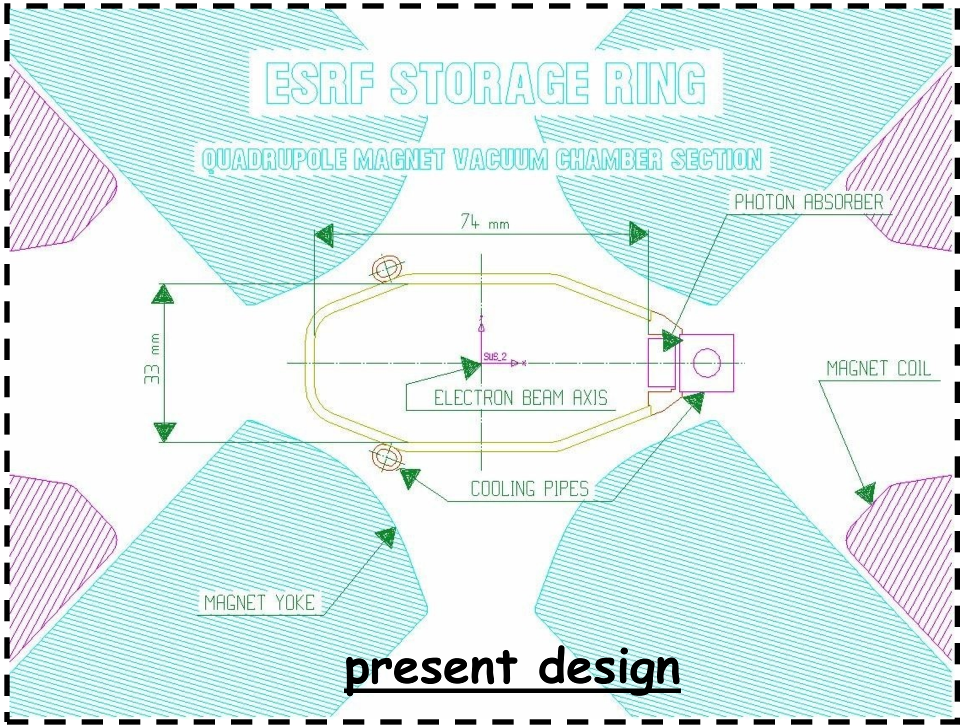
As a consequence, the **effective pumping speed** can be (is!) somewhat smaller than the **installed one**. The location, size and type of vacuum pumps are very important, as is their optimization in order to **maximize the capital investment**.

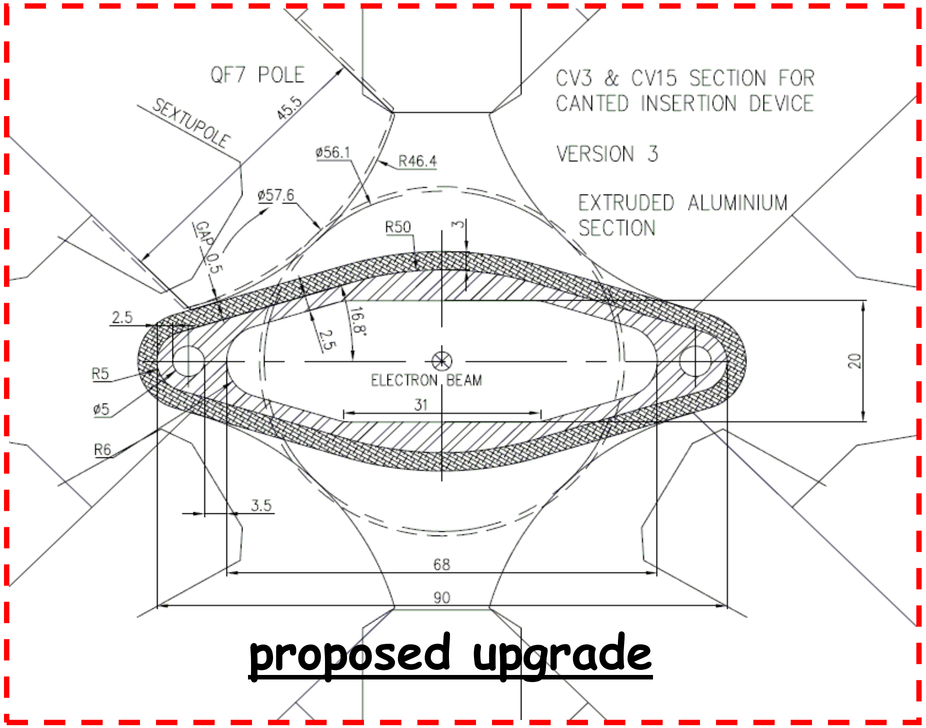
Pumps are expensive to buy, operate and maintain. The ESRF **storage ring** alone has **>800 pumps installed on it, ~1 pump per meter!** At present market prices, just the bare pumps (IPs and NEGs) and their power supplies, **excluding** cabling and manpower for installation, are worth **~3M€**.

Several algorithms and computational schemes have been developed along the years in order to calculate the pressure profile along an accelerator and optimize its vacuum system [7];

3. Pressure Profiles

Generally speaking, all particle accelerators have one feature in common: their vacuum systems are **conductance limited**, mainly due to the need to **minimize the size of the magnets** (material costs, field quality, choice of lattice,…);





Specific conductances: present design ~14 l·m/s, upgrade proposal ~6 l·m/s.

3. Pressure Profiles

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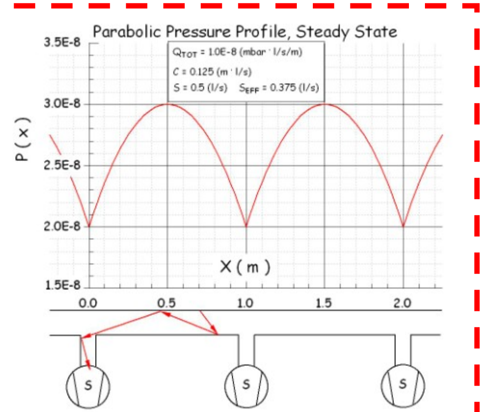
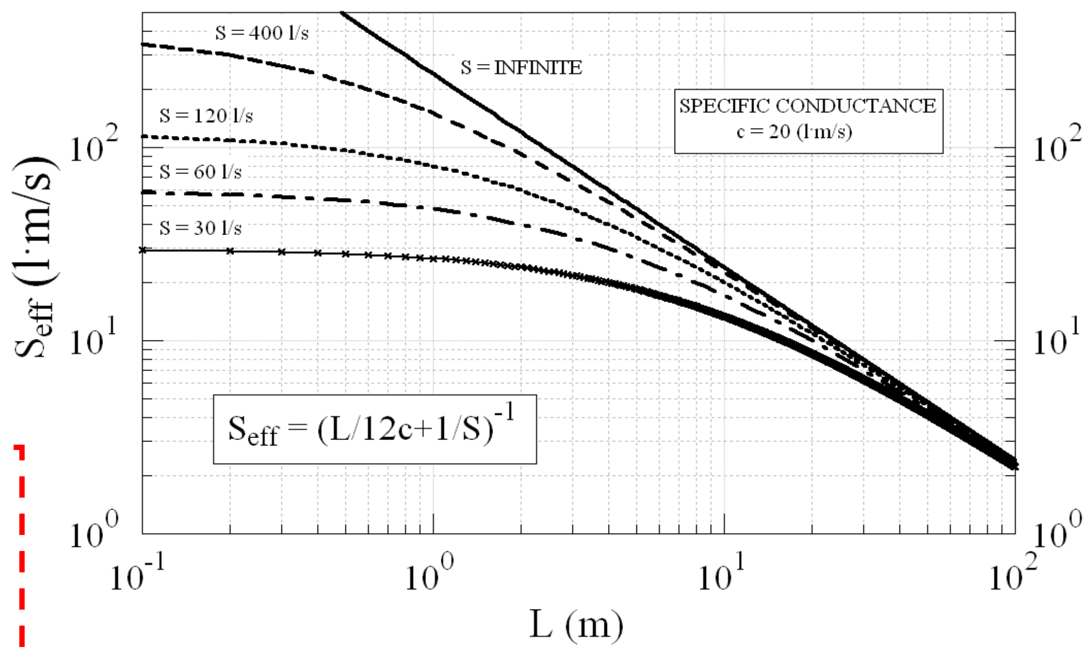


$$\begin{cases} P(x) = \frac{AqL}{2c}\left(Lx - x^2\right) + \frac{AqL}{S} \\ P_{AVG} = \frac{1}{L}\int_0^L P(x)dx = AqL\left(\frac{L}{12c} + \frac{1}{S}\right) = AqL(1/S_{EFF}) \\ P_{MAX} = AqL\left(\frac{1}{8c} + \frac{1}{S}\right); \qquad S_{EFF} = \left(\frac{L}{12c} + \frac{1}{S}\right)^{-1} \end{cases}$$



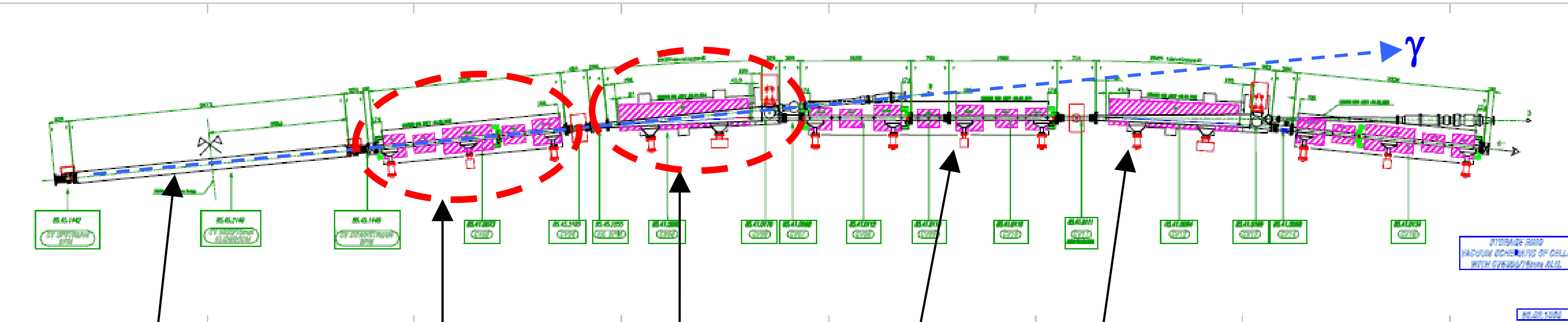
Effective pumping speed vs pump spacing for given installed speeds [7]

(equally spaced pumps installed on uniform cross-section chamber)

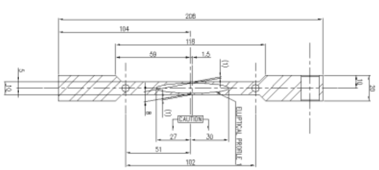
4. Why MC?

Very often, the vacuum system of a particle accelerator is characterized by a **geometry which cannot be treated analytically or via simplified 1- or 2-D FE models** (circles, ellipses, tubes of constant cross-section).

Ex.: one **ESRF standard cell**, 32 cells total, with ID straight section (**Length~26.4 m**):

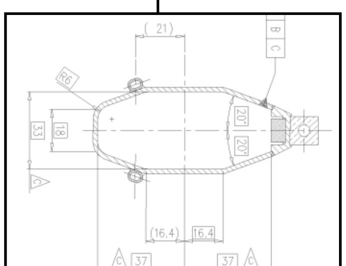


Insertion Device (ID) chamber ~0.9 l*m/s



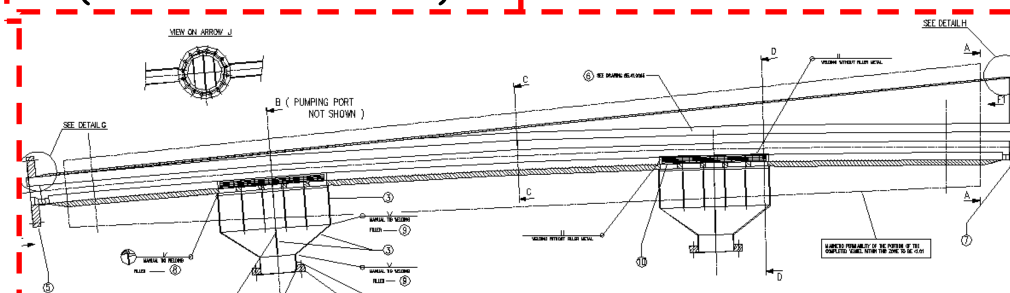
Quad/sext chamber ~14 l*m/s

(2 NEGs + 1 IP)



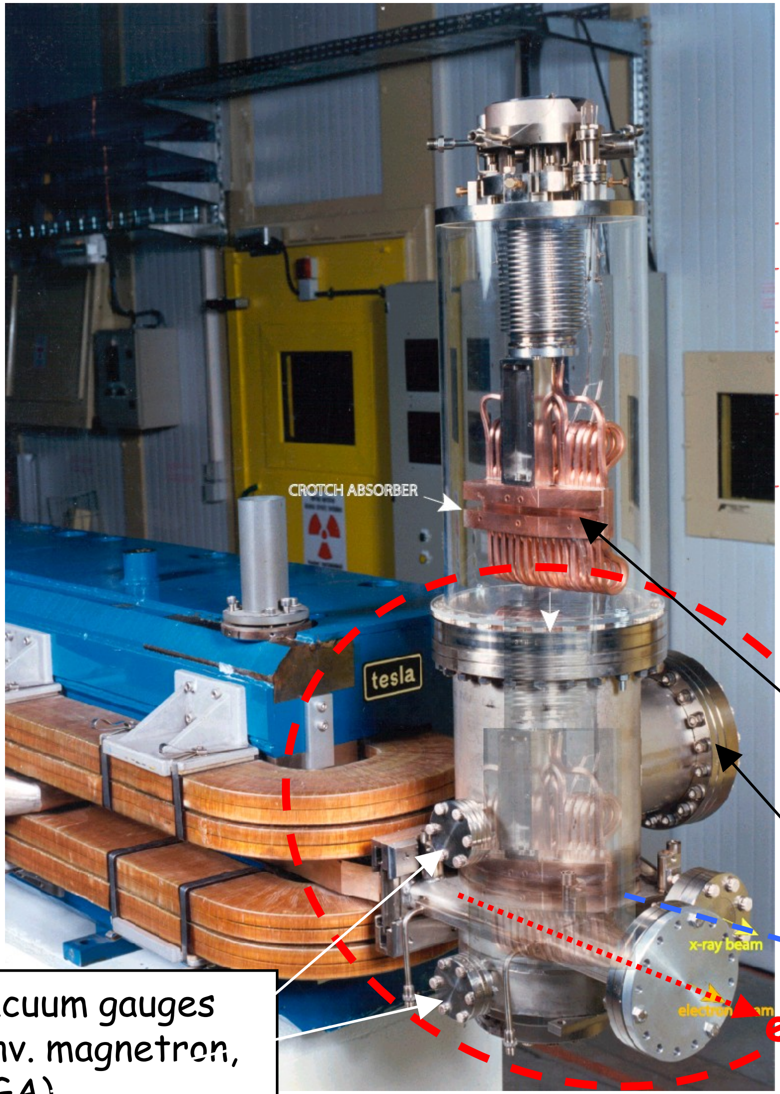
Dipole/Crotch chambers – 2 IPs + 2 NEGs (see also next slide…)

11 ion-pumps (IP) + 11 NEG pumps on standard set-up

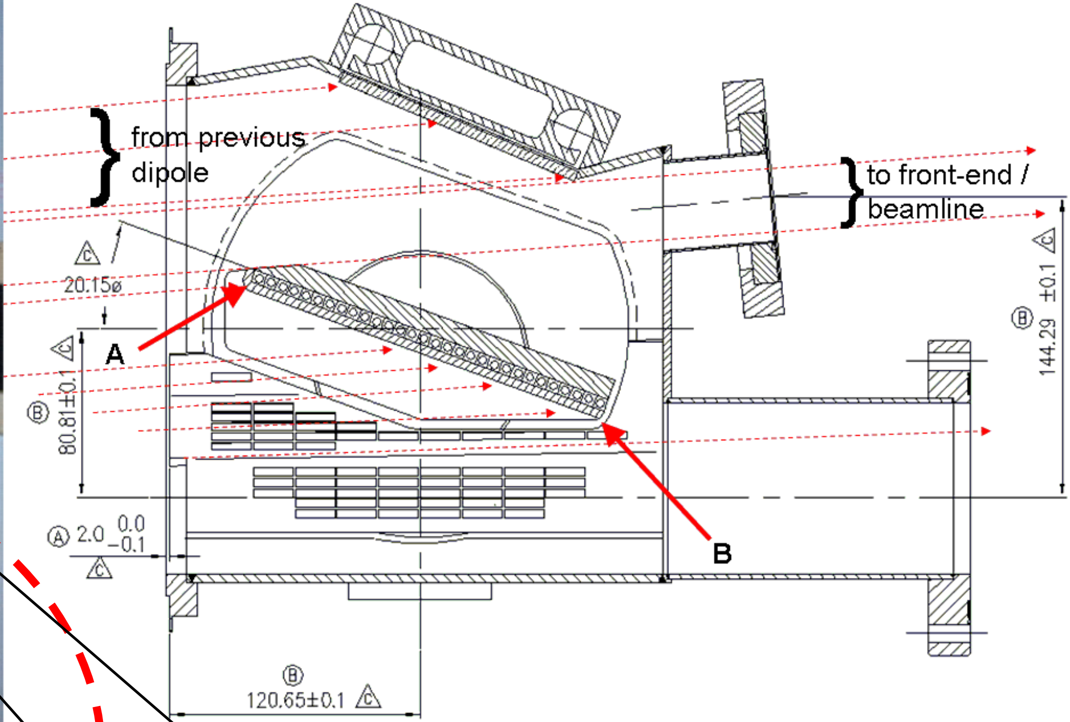


4. Why MC?

Ex.: Details of one ESRF **crotch absorber area**. Real hardware and CAD drawing



crotch 2: P_{tot}=8.2 KW @ 200mA
(has been run already at 300mA)

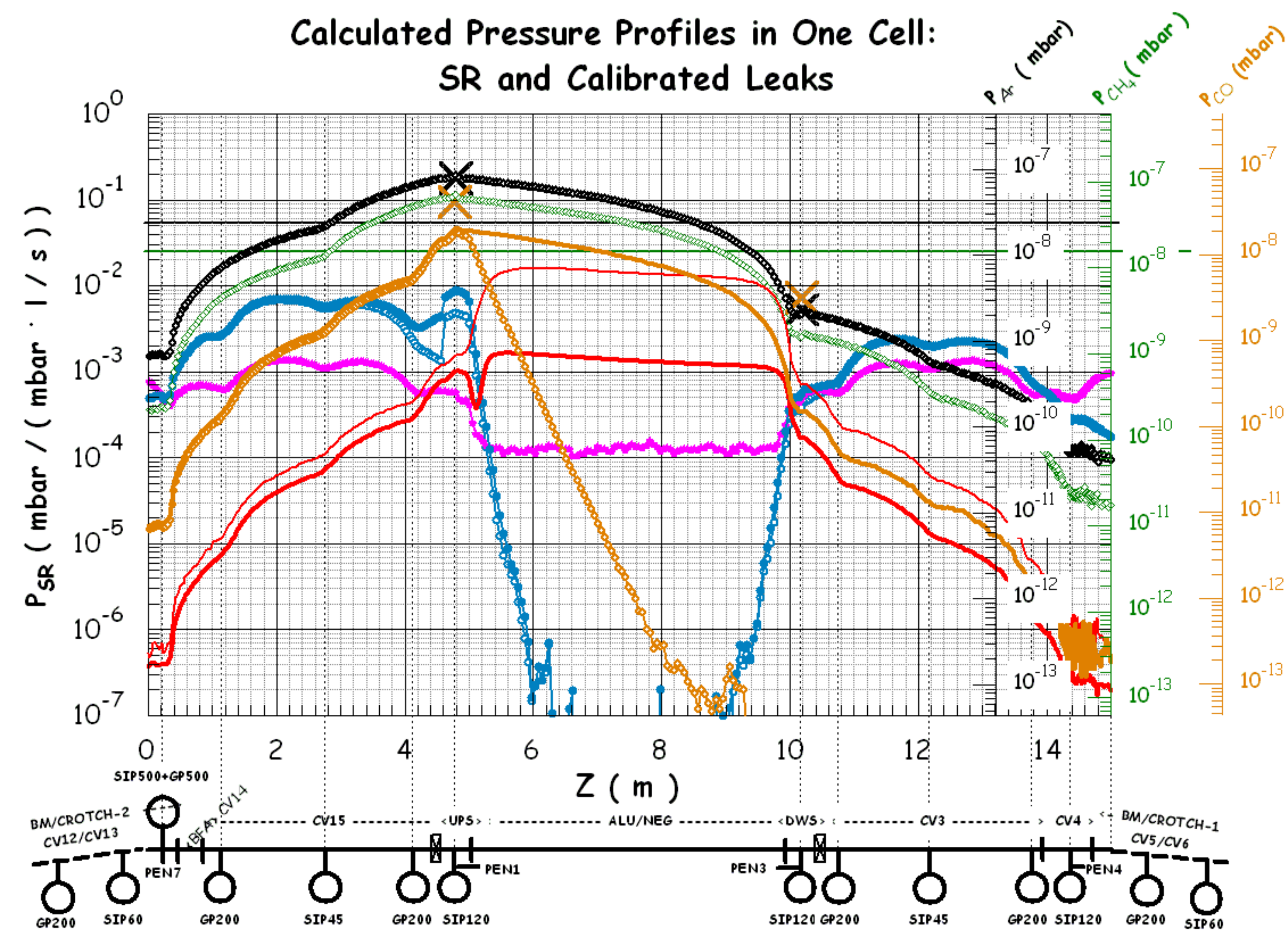


vacuum gauges (inv. magnetron, RGA)

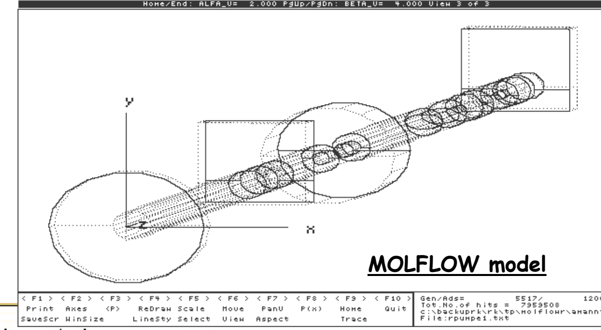
- the GlidCop absorber is positioned vertically inside the crotch chamber;
- 500 l/s ion-pump + GP500 NEG pump on back flange

4. Why MC?

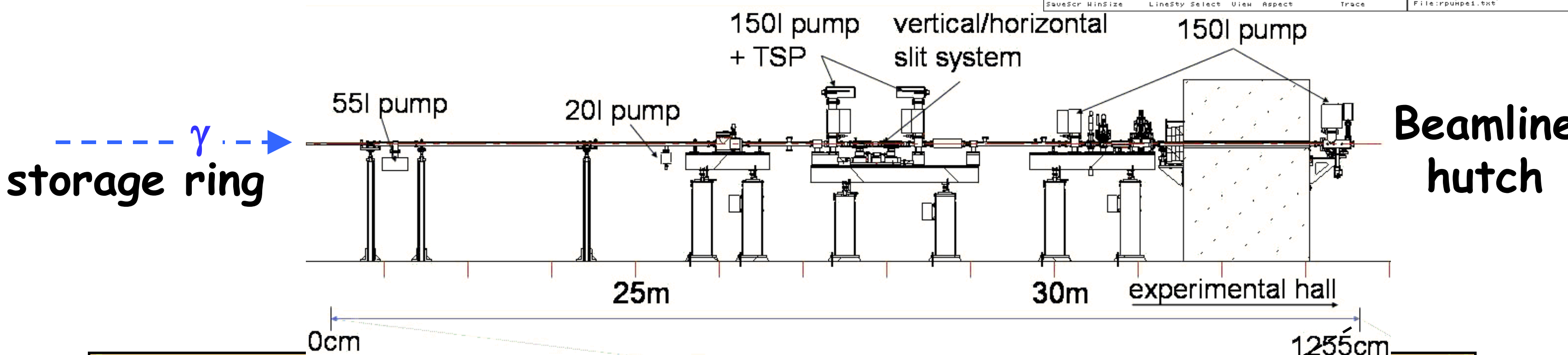
The relationship between the pressure measured at the gauges' location and the e- beam trajectory are important to know. In the following graph, the pressure profile along one full ID straight section (dipole-to-dipole) is shown for various configurations: thermal des.; SR-induced des.; Ar, CO, CH_4 calibrated leaks…

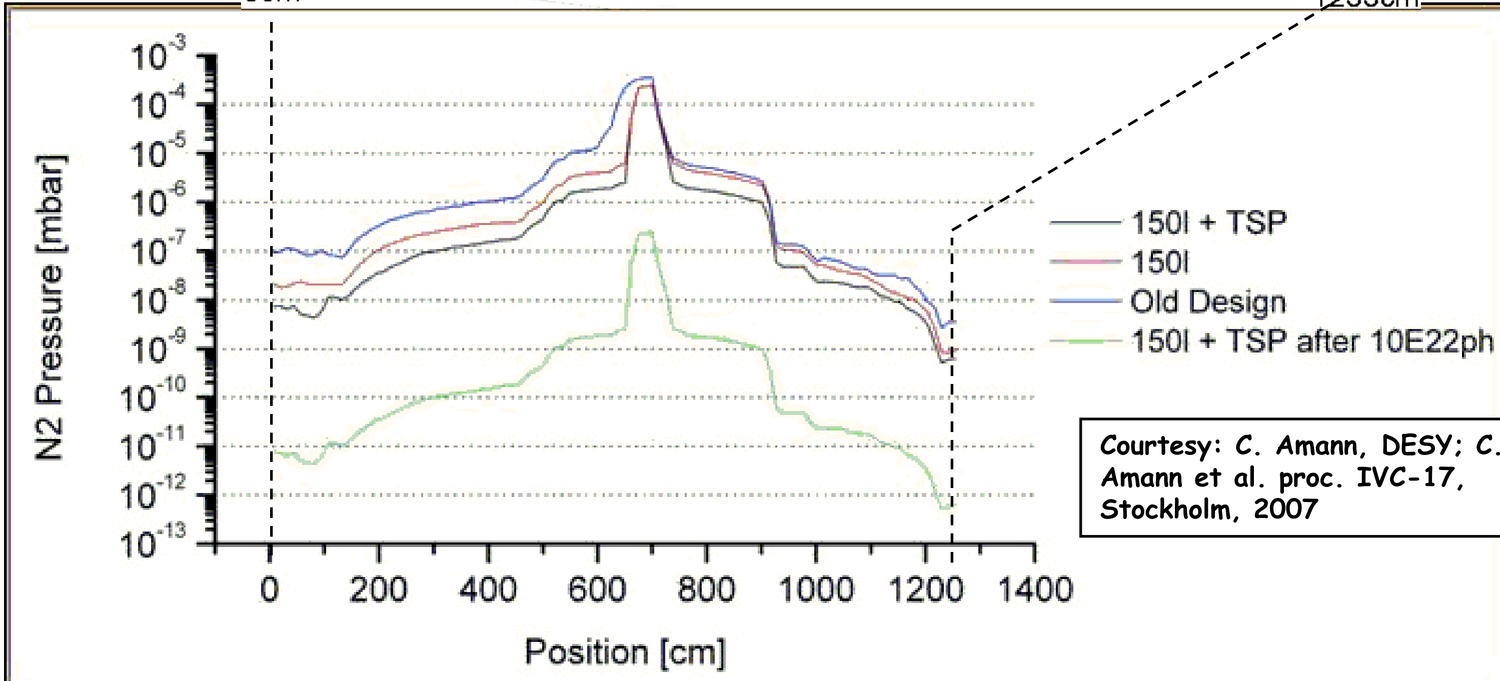


4. Why MC?



Ex.: **PETRA-3 front-ends**: MC simulation of the pressure profiles for different pumping schemes [8]



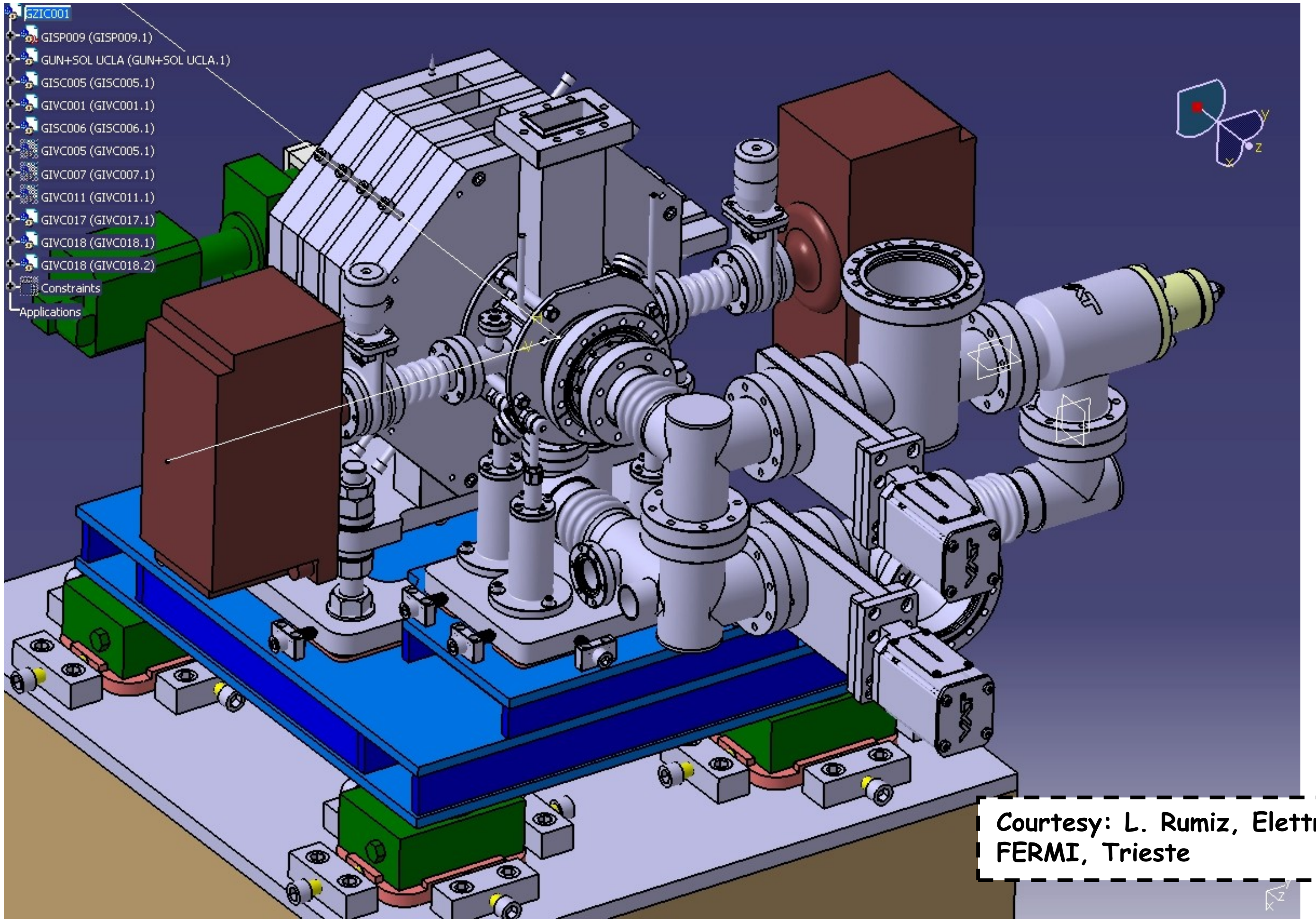


Courtesy: C. Amann, DESY; C. Amann et al. proc. IVC-17, Stockholm, 2007

4. Why MC?

Ex.: FERMI, free-electron laser project at Elettra. Photocathode assembly (CAD dwg):

- Multi-node, variable geometry components, hard to simulate with 1- or 2-D models



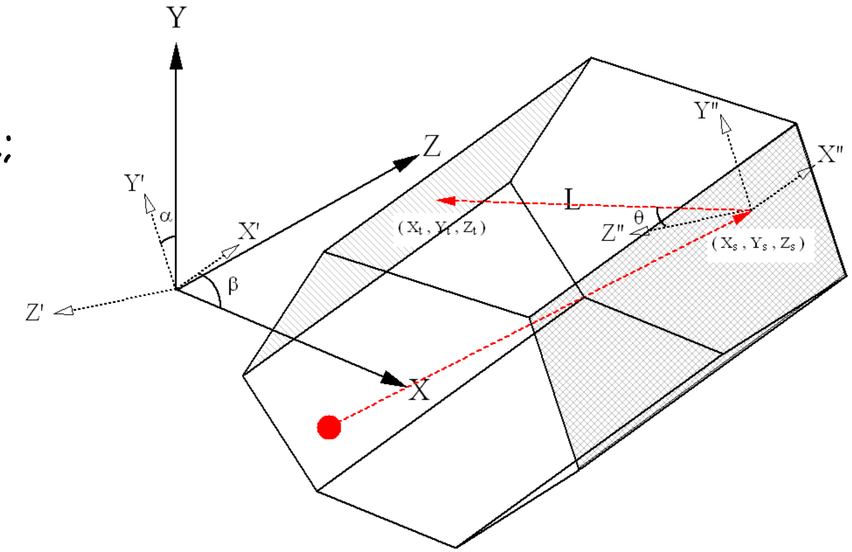
Courtesy: L. Rumiz, Elettra-FERMI, Trieste

5. Framework

The MC code described and used for this talk is **Molflow** [9], which has been under development on and off since quite some time (1991);

Molflow, some features:

- test-particle Monte Carlo simulation software (i.e. **UHV conditions**, **no** intra-molecular interactions): stand-alone editor and MC code;
- 3D model, uses **planar polygonal facets** on a **wireframe model**;



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

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

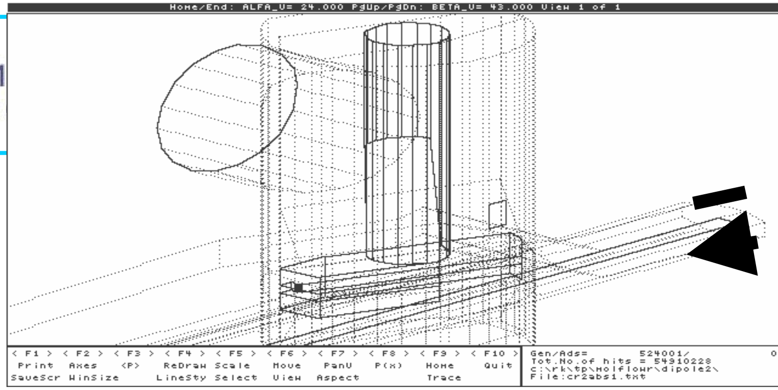
$$\theta = \sin^{-1}(\sqrt{r})$$

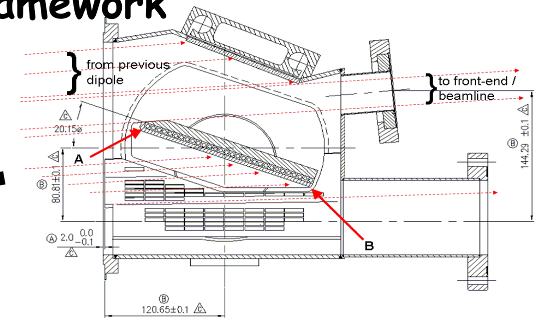
$$\begin{cases} X_t = X_s + L_t(\sin\theta\cos\varphi\cos\beta_s - \sin\theta\sin\varphi\sin\alpha_s\sin\beta_s - \cos\theta\cos\alpha_s\sin\beta_s) \\ Y_t = Y_s + L_t(\sin\theta\sin\varphi\cos\alpha_s - \cos\theta\sin\alpha_s) \\ Z_t = Z_s + L_t(\sin\theta\cos\varphi\sin\beta_s + \sin\theta\sin\varphi\sin\alpha_s\cos\beta_s + \cos\theta\cos\alpha_s\cos\beta_s) \end{cases}$$

$$\begin{cases} L_t = -(A_t X_s + B_t Y_s + C_t Z_s + D_t)/U \\ U = A_t(\sin\theta\cos\varphi\cos\beta_s - \sin\theta\sin\varphi\sin\alpha_s\sin\beta_s - \cos\theta\cos\alpha_s\sin\beta_s) + \\ + B_t(\sin\theta\sin\varphi\cos\alpha_s - \cos\theta\sin\alpha_s) + \\ + C_t(\sin\theta\cos\varphi\sin\beta_s + \sin\theta\sin\varphi\sin\alpha_s\cos\beta_s + \cos\theta\cos\alpha_s\cos\beta_s) \end{cases}$$

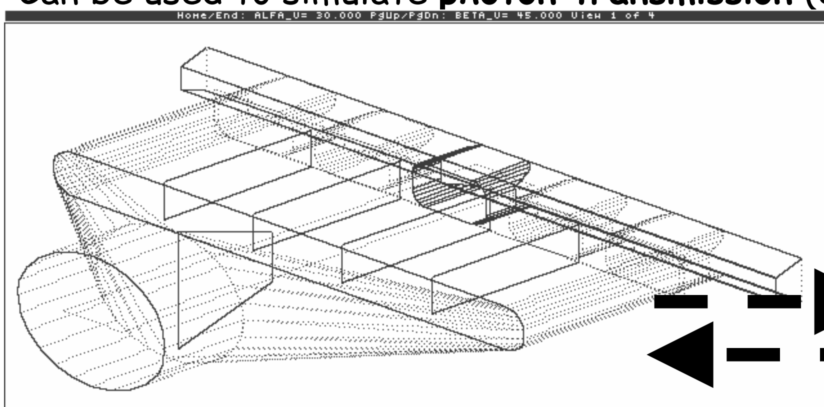
Ref.: R. Kersevan, "Analytical and Numerical Tools for vacuum systems", Proc. CERN Accelerator School, CERN-2007-003, June 2007

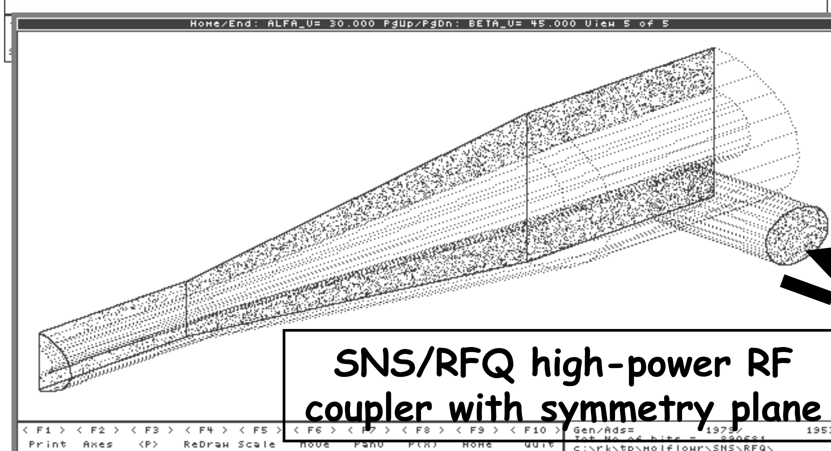
5. Framework



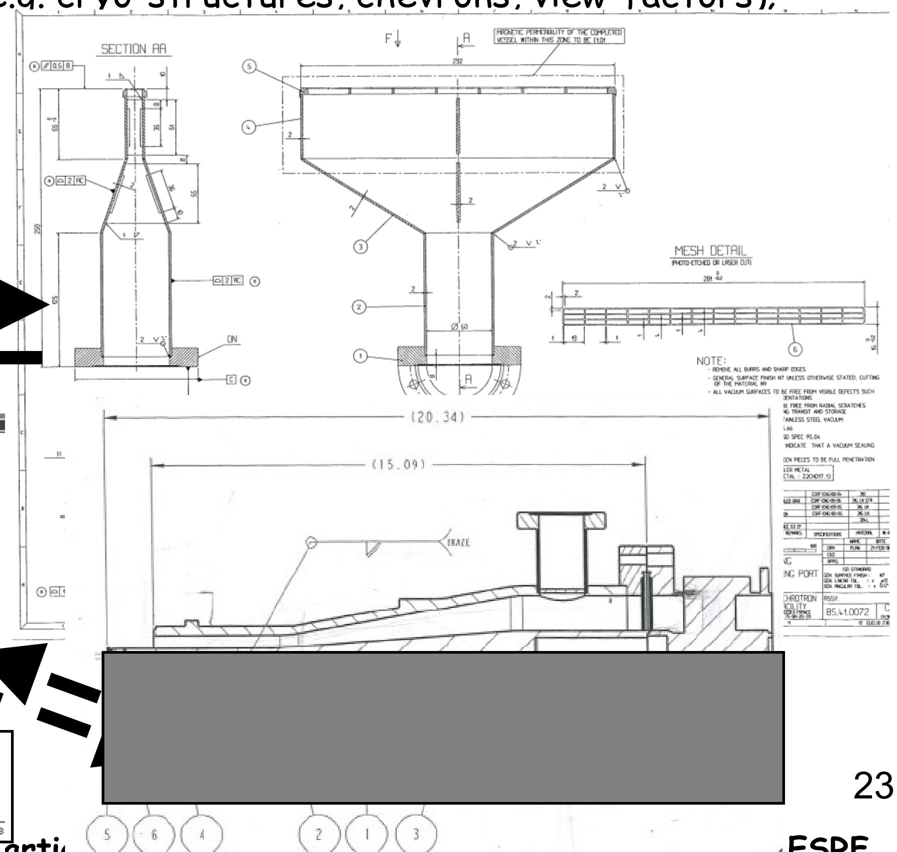


- 3D model, uses **planar polygonal facets** on a **wireframe model**;
- Each facet has **attributes** such as **sticking coefficient**, **transparency**, **desorption**, **desorption function (e.g. $f(\theta)=\cos^n(\theta)$)**, **orientation**;
- Can be used to simulate **photon transmission** (e.g. cryo-structures, chevrons, view-factors);





SNS/RFQ high-power RF coupler with symmetry plane



5. Framework

- Extensively **benchmarked against published results** [9, 10];
- **Time-independent** simulation (time-dependent version has been tested once);
- Random number generator does not implement **yet** Mersenne's algorithm [11] (under dev.);
- Version with graphic output has **limits on complexity** of structures which can be modeled. **New re-compiled version** w/o graphics overcomes this, and allows the simulation of arbitrarily complex structures (hard limit given by the installed memory on PC). Under final test and optimization;

405 Yoshiro Kusumoto: Reflection rules preserving molecular flow symmetry

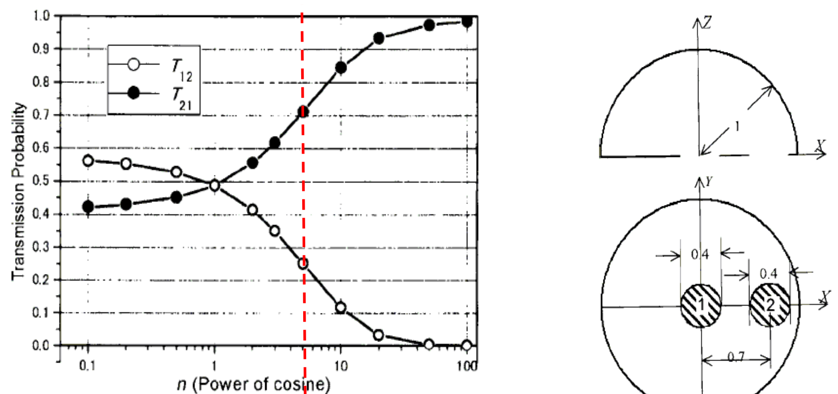
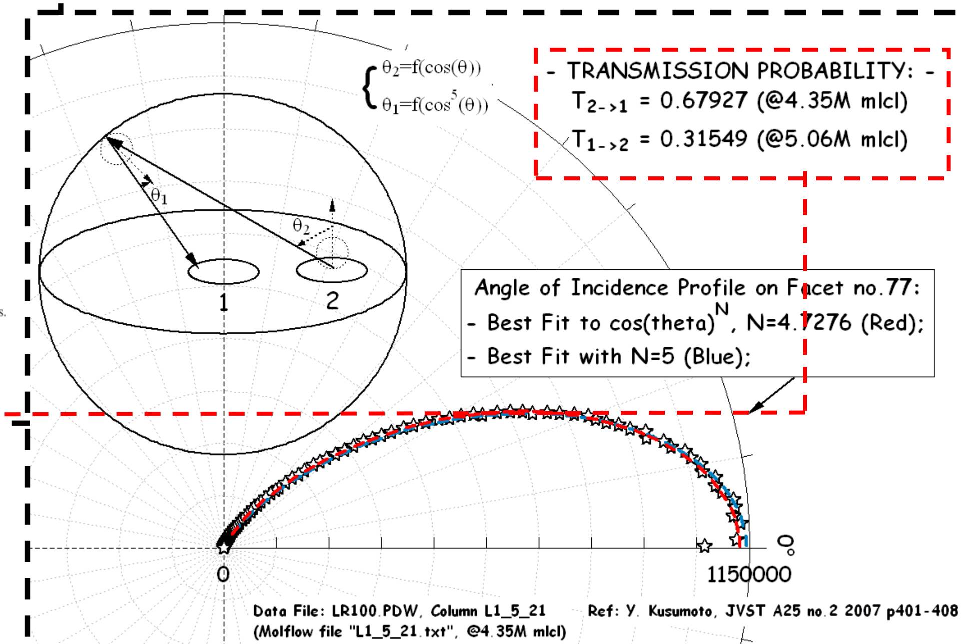


FIG. 5. Transmission probabilities obtained by Monte Carlo calculation using 10^6 test particles are plotted vs power of cosine, n. The equality $T_{12} = T_{21}$ holds if and only if $n=1$.

FIG. 4. Drawing of the hemispherical apparatus.

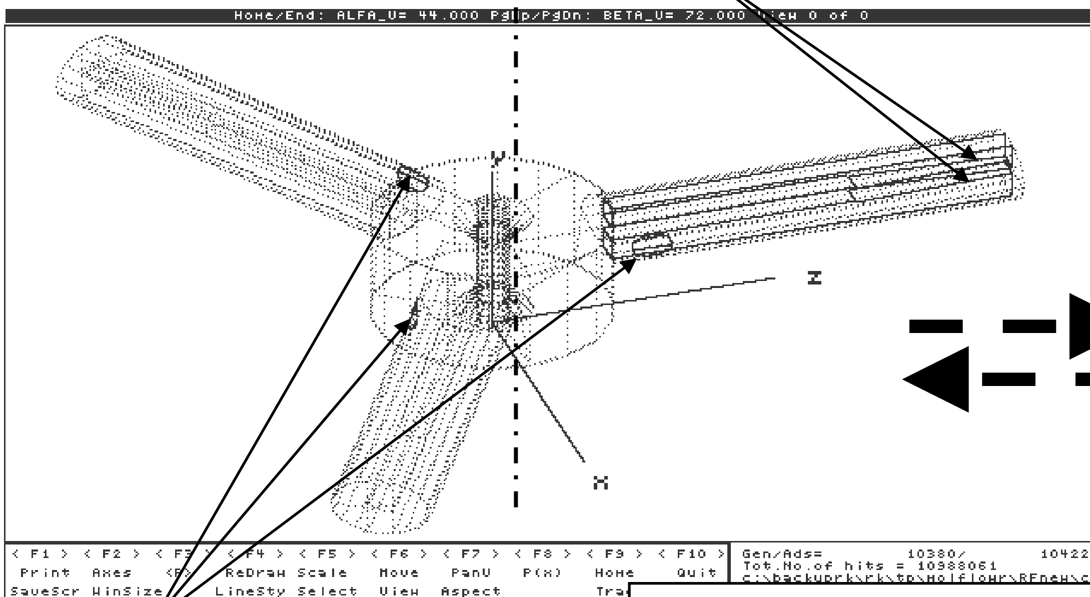
J. Vac. Sci. Technol. A, Vol. 25, No. 2, Mar/Apr 2007



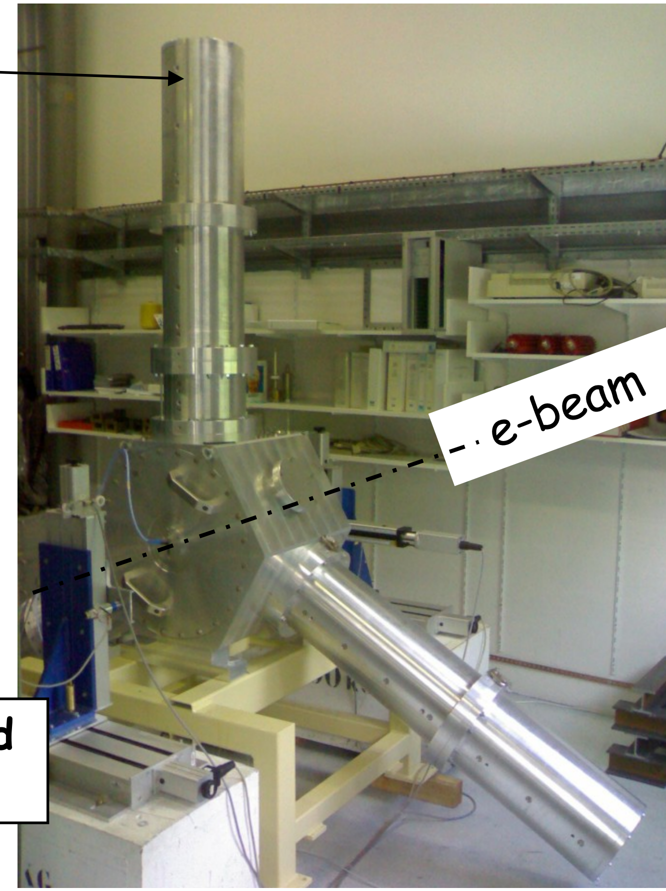
6. Examples

- Optimization of the location and size of the ion-pumps on an RF cavity [12], for the upgrade of the ESRF to 500 mA

outgassing ferrites



ion-pumps

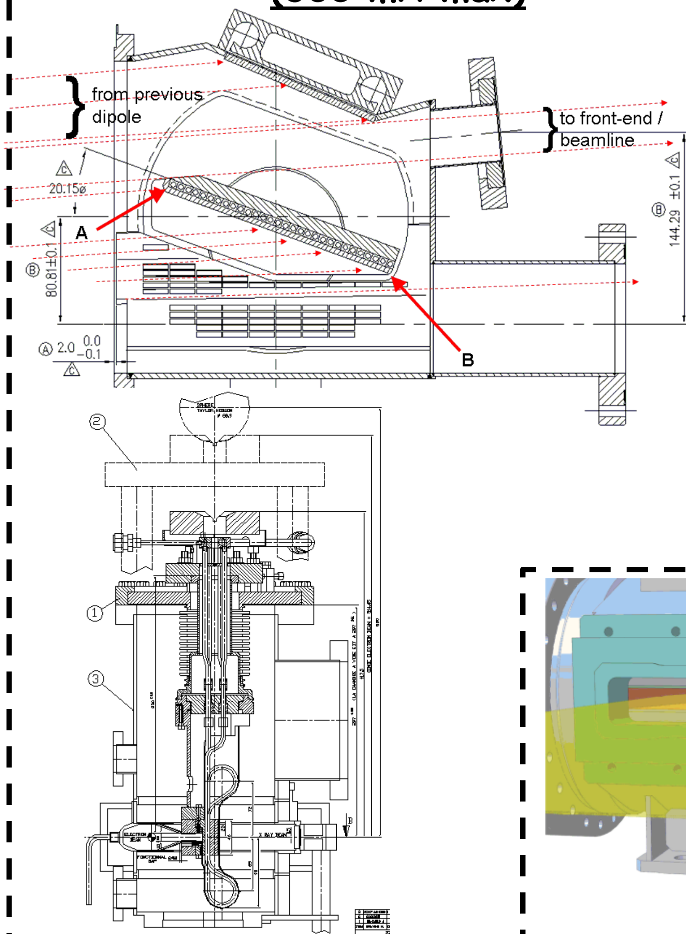


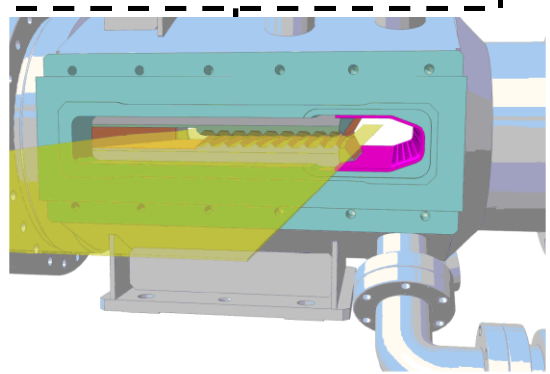
352 MHz HOM-damped
RF cavity Alu model

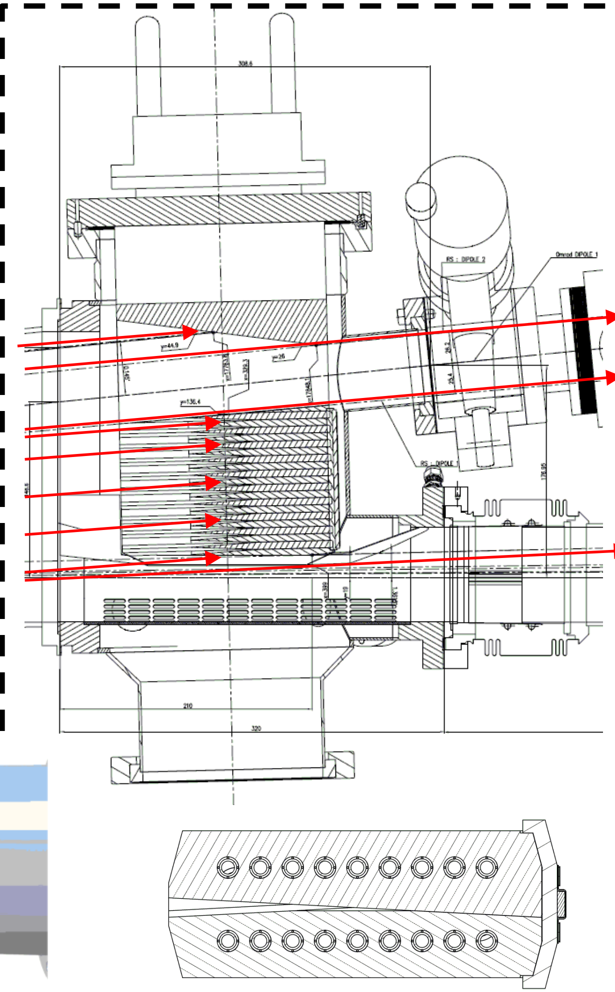
6. Examples

- Optimization of the pumping geometry for the new crotch absorber of the ESRF upgrade [12]:

present version (300 mA max)







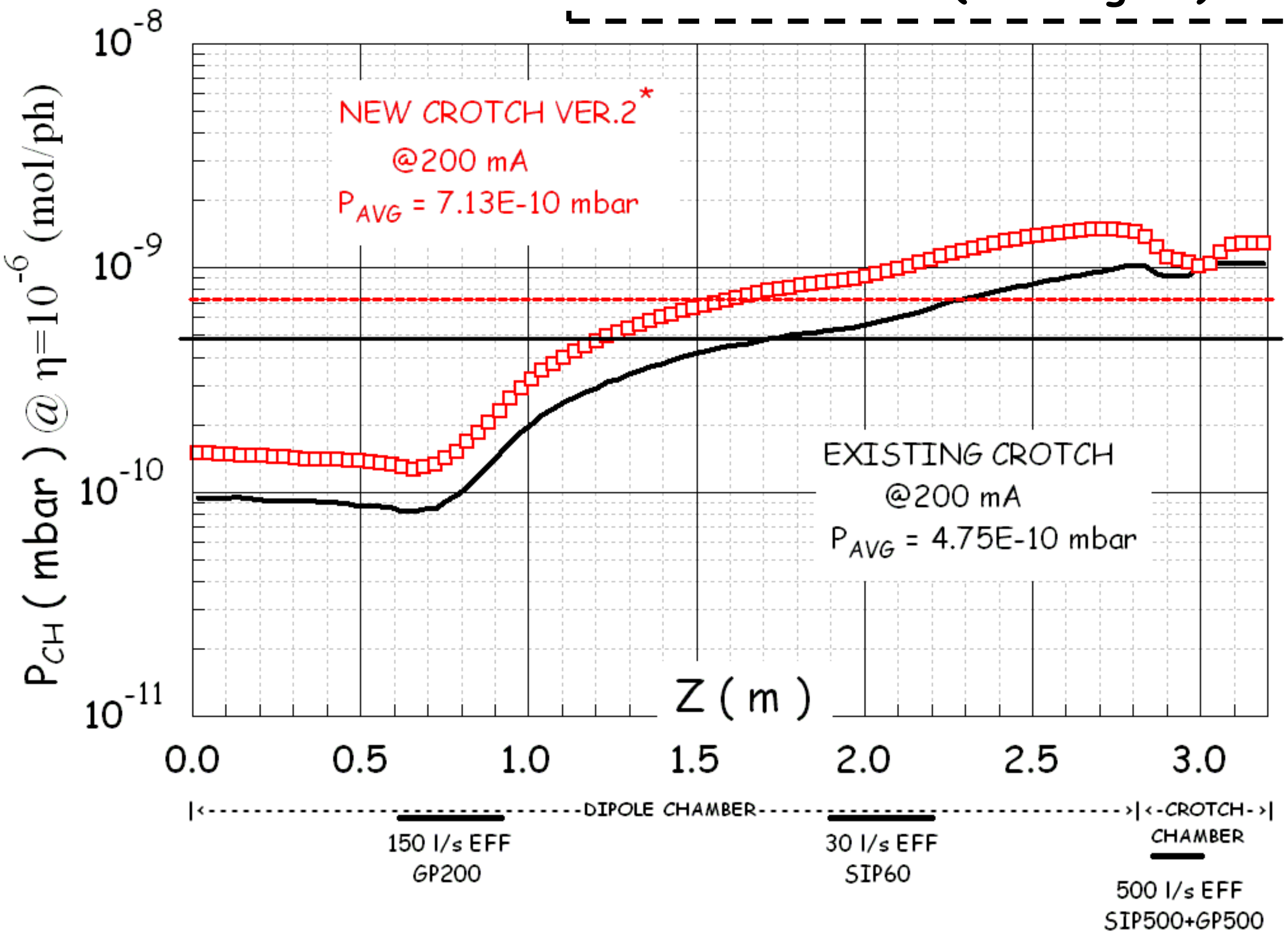
new version (up to 500 mA)

6. Examples

ESRF

- Optimization of the pumping geometry for the new crotch absorber of the ESRF upgrade [12]:

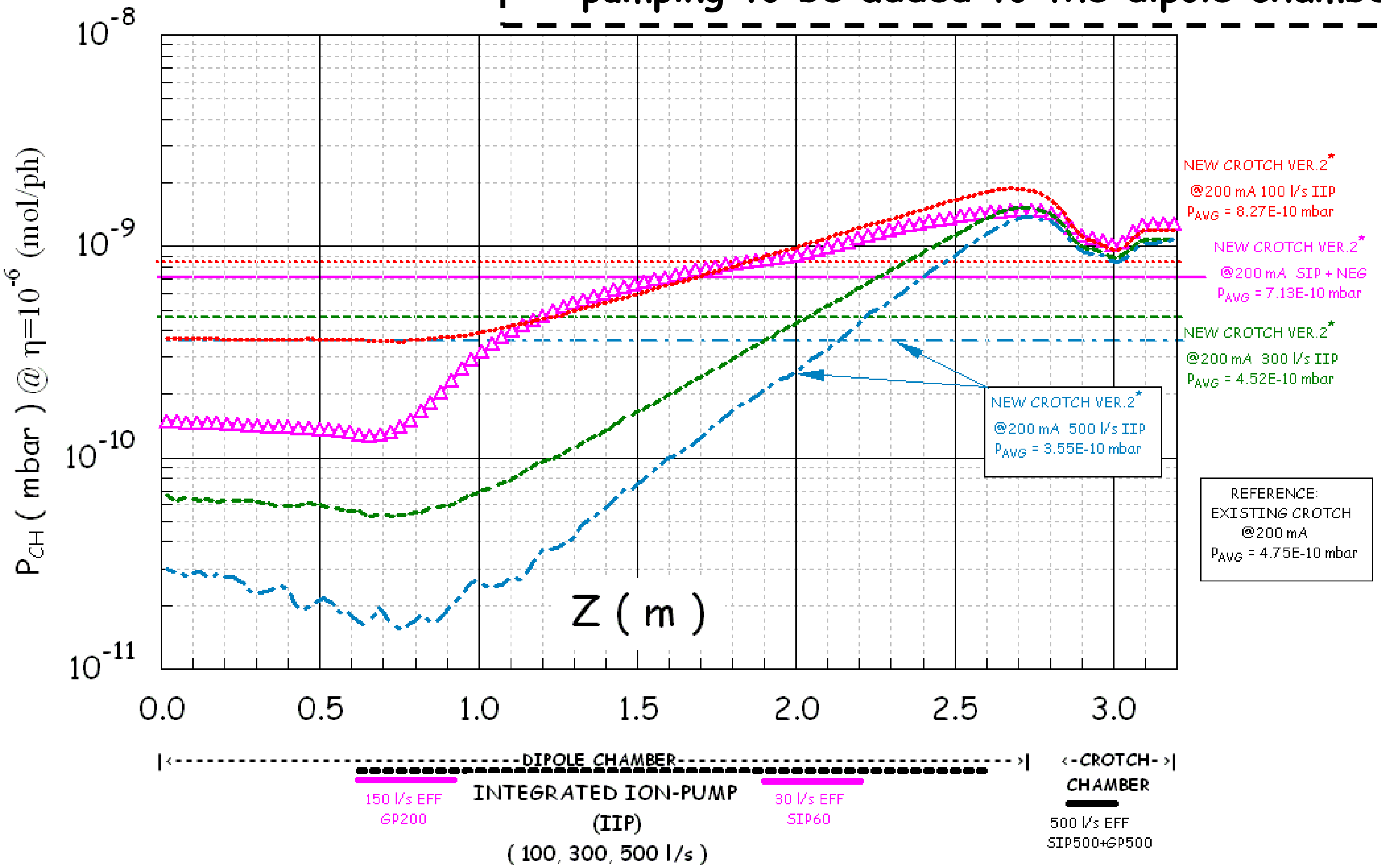
Pumping efficiency of new crotch abs geometry is not as good as that of the present design (50% higher)!



6. Examples

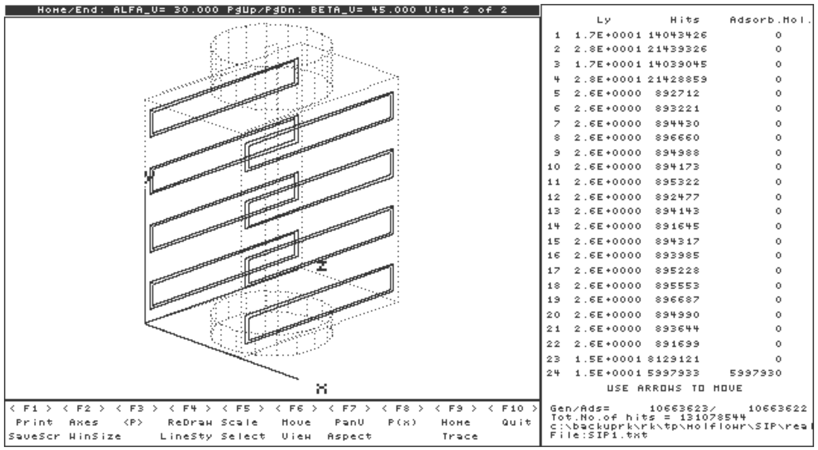
- Optimization of the pumping geometry for the new crotch absorber of the ESRF upgrade [12]:

Change of position of IP/NEG pump and orientation of abs jaws, call for distributed pumping to be added to the dipole chamber

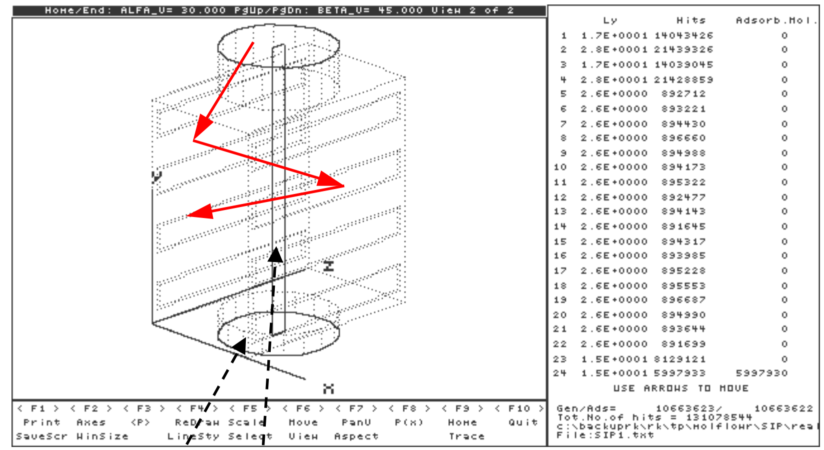


6. Examples

- **Analysis of the pumping efficiency of a 500 l/s StarCell with and w/o a GP500 NEG pump on its back flange [13]. A detailed model is made…**



Pump body with the 8 pumping pockets, where the StarCell triode elements are located

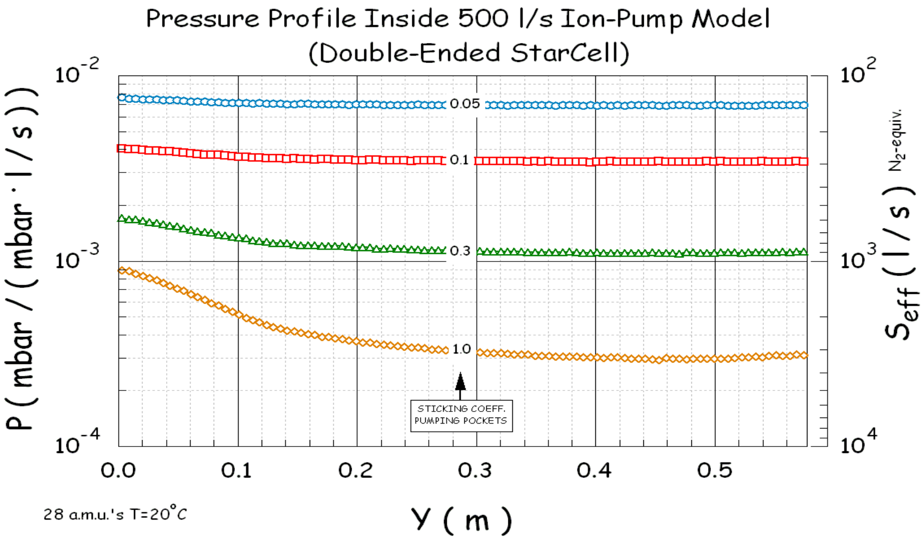


Molecules enter the pump from the upper flange. Pressure is computed along the vertical "<u>pseudo surface</u>" (i.e. transparent).

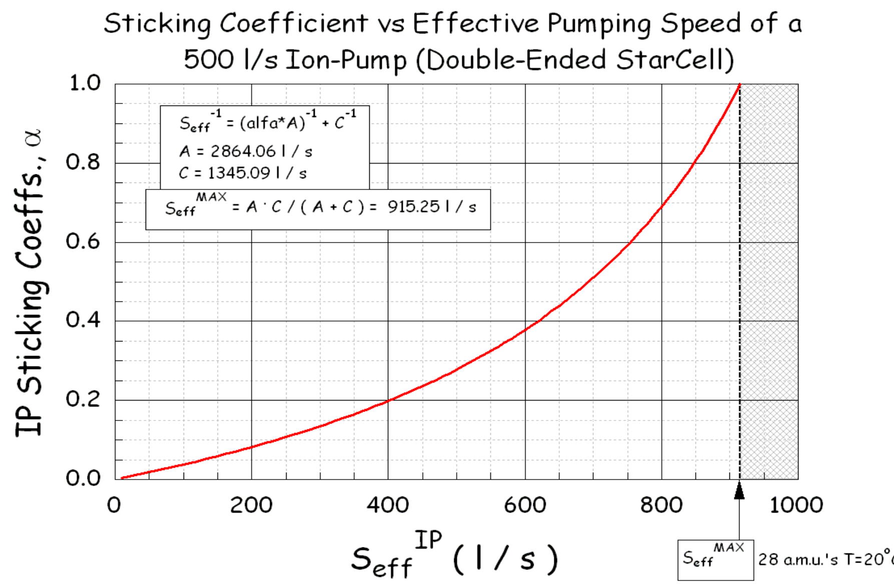
<u>The bottom flange may be used for installing a GP500 NEG pump (not shown here)</u>

6. Examples

- **Analysis of the pumping efficiency of a 500 l/s StarCell with and w/o a GP500 NEG pump on its back flange [13]. A detailed model is made and different configurations are studied: effect of varying the sticking coeff of the pumping pockets; determination of the IP sticking coeff for a measured pumping speed…**



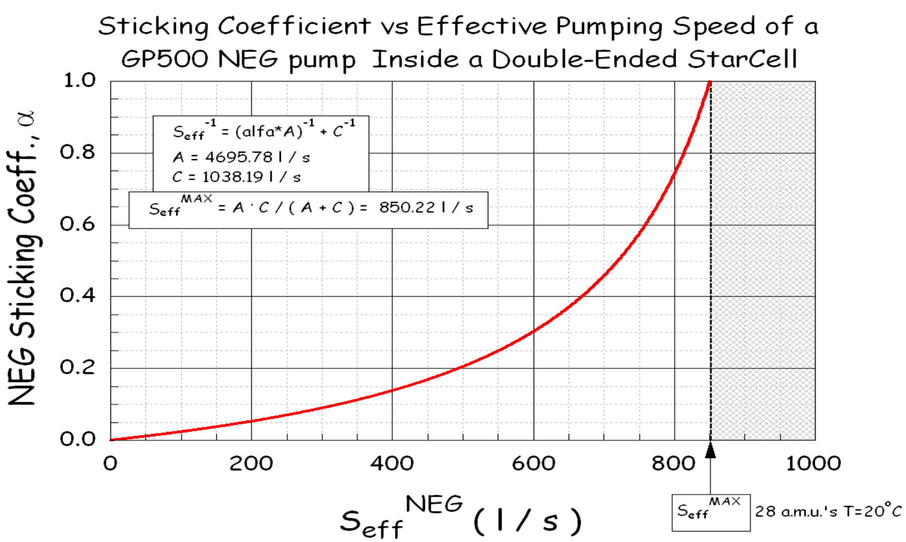
Pressure profile along the pump axis for different values of the effective sticking coefficient



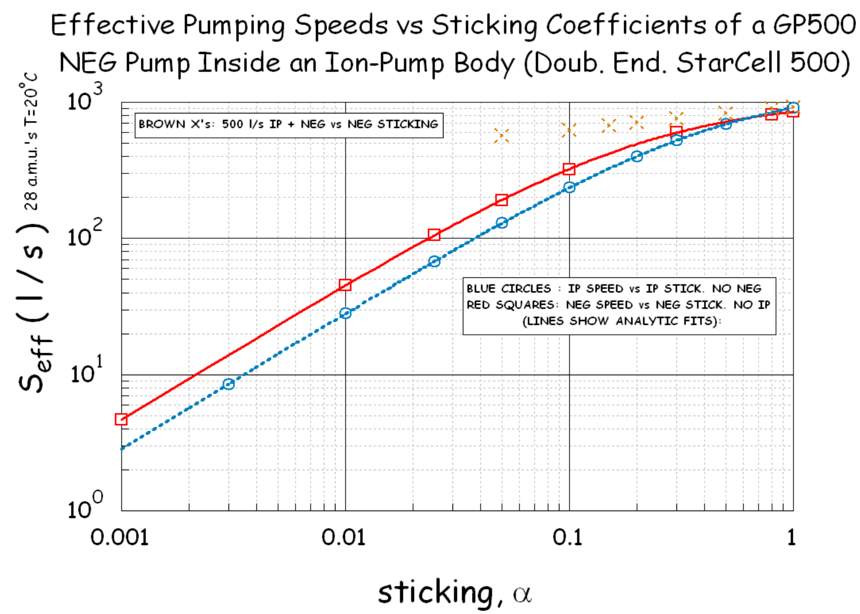
Equivalent sticking coefficient vs pumping speed for a 500 l/s StarCell with no NEG pump in it

6. Examples

- Analysis of the pumping efficiency of a 500 l/s StarCell with and w/o a GP500 NEG pump on its back flange [13]. A detailed model is made and different configurations are studied: determination of the NEG sticking coeff for a measured pumping speed, and more…



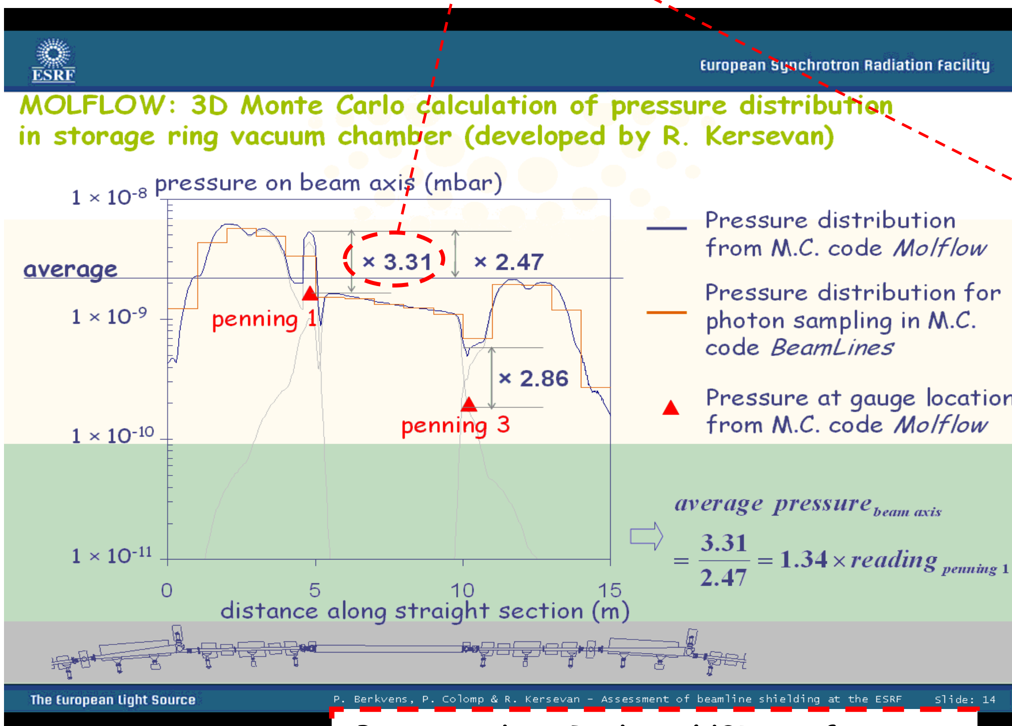
Equivalent sticking coefficient of a GP500 NEG pump vs the pumping speed of the NEG pump inside a 500 l/s StarCell body



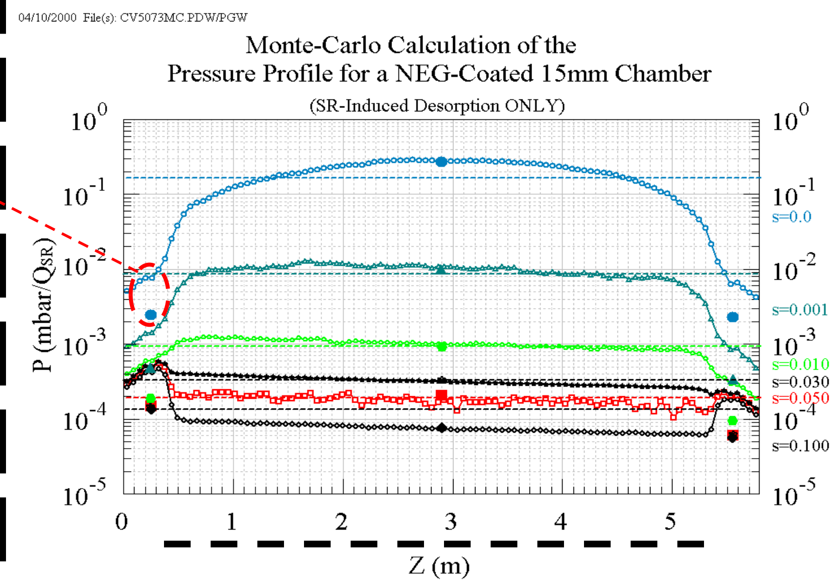
Effective pumping speed of NEG, SIP, and SIP(500) + NEG vs respective sticking coefficients

7. Conclusions

- More often than not, the geometry of a particle accelerator's vacuum system is such that real 3-dimensional mathematical models **should be made**. Failure to do so can lead to rather **large discrepancies** between the calculated values for the pressures and the measured ones;



Presented at Radsynch'07 conference, CLS, 6-8 June 2007, Saskatoon, to be published in *Radiation Measurements*



Pressure measured at extremities of NEG-coated ID chambers (solid dots) on transition chambers, is markedly lower than the pressure inside the chamber at same Z (curves).

(S=NEG-coating sticking coeff.)

7. Conclusions

- More often than not, the geometry of a particle accelerator's vacuum system is such that real 3-dimensional mathematical models **should be made**. Failure to do so can lead to rather **large discrepancies** between the calculated values for the pressures and the measured ones;
- 3D MC calculations can nowadays be used with confidence, as they have been benchmarked against analytic calculations, and rather accurate measurements (calibrated leaks, beam losses);

The speed of the MC is becoming less and less of an issue, thanks to the never ending improvement of the computational speed of modern CPUs (thanks Mr. Moore!) !): faster clocks, multi-core CPUs, parallelization, improved compilers, etc…;

- A **huge improvement** could come from the use of **hardware acceleration**, rather than software, in line with what has happened for graphics applications with the development of faster and faster dedicated graphical CPUs. Instead of drawing polygons on screen, one would have to draw molecular trajectories. How long till the first "molecular flow FPU"?
- In spite of the **lack of a standard reference software**, the vacuum systems of most accelerators conceived during the last 20 years **have been designed** relying, partially or in total, to **test-particle MC simulations**: LEP, ELETTRA, LHC, DIAMOND, ESRF, CESR, NSLS-II, PETRA-III, SESAME, ALBA, just to mention a few.

THANK YOU FOR YOUR ATTENTION

8. References

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