



# Vacuum Technology for Ion Sources

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### Outline

- 1. Aim of this short course
- 2. Gas flow in molecular regime
  - a. Conductance and pumping speed.
  - b. Evaluation of pressure profiles.
  - c. Transient behaviour.
- 3. Electrical analogy

#### 4. Gas pumping:

- a. Momentum transfer pumps (turbomolecular)
- b. Sputter ion pumps
- c. Getter pumps
- d. Comparison of pumps
- 5. Conclusions

#### Appendix

- 1. Basic Notions
- 2. Additional Examples of Electrical Analogy
- 3. Outgassing
- 4. Extra Info about Capture Pumps.



### **Basic Notions (see appendix 1)**

• Ideal gas equation:  

$$P V = N_{moles} \times R T$$
 (thermodynamic)  
 $P V = N_{molecules} \times k_B T$  (statistical mechanics)

 $\varphi = \frac{1}{4}n\langle v \rangle = \frac{1}{4}n \sqrt{\frac{8 k_B T}{\pi m}} \qquad \varphi \text{ rate of impingement}} \\ \text{n gas density} \frac{molecules}{volume}$ Maxwell-Boltzmann model:

m is the molecular mass [Kg]

- $K_n = \frac{l}{D}$ Knudsen number:
- Molecular regime:  $K_n > 1$
- l is the mean free path of gas molecules, D typical distance of the vacuum system

Collisions with the wall of the vacuum system more likely than those between molecules

Gas flow Q in molecular regime:  $Q = C (P_1 - P_2)$ 

C is the gas conductance indipendent of pressure

Gas conductance of a wall slot:  $C = \frac{1}{4}A\langle v \rangle = A C' \rightarrow \propto \frac{1}{\sqrt{M}}$  A is the wall slot area M is the molecular weight [Kg]

Gas conductance of a duct:

Conductance of the duct aperture (A C') x transmission probability  $(\tau)$ 



#### **Gas Flow in Molecular Regime: Conductance**



Analytical expressions for the transmission probability can be found for ducts of circular, rectangular and elliptical cross section (see for example J. M. Lafferty, Foundation of Vacuum Science and Technology, Wiley Interscience).

For more complicated geometry, Test-Particle Monte Carlo methods (TPMC) are used.







# http://cern.ch/test-molflow



#### **Gas Flow in Molecular Regime: Combination of Conductances**





$$Q_{1} = C_{1}(P_{1} - P_{2})$$
  

$$Q_{2} = C_{2}(P_{2} - P_{3})$$
  

$$Q_{TOT} = C_{TOT}(P_{1} - P_{3})$$

In stable conditions, there is no gas accumulation in the whole system:  $Q_1 = Q_2 = Q_3$ 

It can be easily verified that:  $C_{TOT} = \frac{C_1 C_2}{C_{1+} C_2}$  and  $\frac{1}{C_{TOT}} = \frac{1}{C_1} + \frac{1}{C_2}$ :

In general for N vacuum components traversed by the same gas flux, i.e. placed in series :



For components placed in parallel (same pressures at the extremities):



$$Q_{1} = C_{1}(P_{1} - P_{2})$$
$$Q_{2} = C_{2}(P_{1} - P_{2})$$
$$Q_{TOT} = C_{TOT}(P_{1} - P_{2})$$

$$Q_{TOT} = Q_1 + Q_2 \rightarrow C_{TOT} = C_1 + C_2 \rightarrow C_{TOT} = \sum_{i=1}^{N} C_i$$





In vacuum technology a pump is any 'object' that remove gas molecules from the gas phase.

The pumping speed **S** of a pump is defined as the **ratio** between the **pump throughput**  $Q_P$  (flow of gas definitively removed) and the **pressure P at the entrance** of the pump:

$$S = \frac{Q_P}{P}_{\delta O_P} [S] = \frac{[Volume]}{[Time]} = [conductance]$$

In a more general way:  $S = \frac{\delta Q_P}{\delta P}$ 

The gas removal rate can be written as:  $Q_P = \frac{1}{4}A_P n \langle v \rangle \sigma = A_P C' n \sigma$ 



A<sub>P</sub>: is the area of the pump apertureC': is the conductance of the unit surface arean: the gas density

 $\sigma$  : the capture probability, i.e. the probability that a molecule entering the pump is definitively captured (Ho coefficient)





As usual, in term of pressure and PV units:

$$Q_P = A_P C' n \, \sigma(k_B T) = A_P C' \sigma P$$

From the definition of pumping speed:

$$S = A_P C' \sigma$$

S depends on the conductance of the pump aperture  $A_P C'$  and the capture probability  $\sigma$ .  $\sigma$  is <u>in general</u> not a constant; it may depend on many parameters including pressure, kind of gas and quantity of gas already pumped.

The **maximum pumping speed** is obtained for  $\sigma = 1$  and is equal to the conductance of the pump aperture.



Maximum pumping speed [I s<sup>-1</sup>]for different circular pump apertures

ID [mm]	H <sub>2</sub>	N <sub>2</sub>	Ar
36	448	120	100
63	1371	367	307
100	3456	924	773
150	7775	2079	1739



# Gas Flow in Molecular Regime: Effective Pumping Speed



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A gas flow restriction interposed between a pump and a vacuum vessel reduces the 'useful' pumping speed. The effective pumping speed S<sub>eff</sub> seen by the vacuum vessel is easily calculated:



Gas Flow in Molecular Regime: Evaluation of Pressures Profiles





Flux balance at the connexions (node analysis):





$$P_x = P_0 + \frac{Q}{C(x)}$$
$$C(x) = C(L)\frac{L}{x}$$

S

 $\frac{Q}{Q_{off}} = \frac{Q(C+S)}{C \times S}$ 

Ρ

S

Ρ

Q

С



**Gas Flow in Molecular Regime: Time Dependance** 



From the ideal gas equation:  $PV = Nk_BT \rightarrow V\frac{dP}{dt} = k_BT\frac{dN}{dt}$ A gas balance equation can be written as:  $\frac{dN}{dt} = Q_{in} - Q_{out}$ 

$$V\frac{dP}{dt} = k_B T(Q_{in} - Q_{out}); \text{ in PV units: } V\frac{dP}{dt} = (Q_{in} - Q_{out})$$

The pumped gas rate is:  $Q_{out} = SP \rightarrow V \frac{dP}{dt} = Q_{in} - SP$ 

$$P(0) = P_0 \rightarrow P(t) = \left(P_0 - \frac{Q_{in}}{S}\right)e^{-\frac{t}{\tau_p}} + \frac{Q_{in}}{S}$$

$$P(0) = P_0 \rightarrow P(t) = \left(P_0 - \frac{Q_{in}}{S}\right)e^{-\frac{t}{\tau_p}} + \frac{Q_{in}}{S}$$

$$P(0) = 0 \rightarrow P(t) = \frac{Q_{in}}{S}\left(1 - e^{-\frac{t}{\tau_p}}\right)$$

$$\tau_p = \frac{V}{S} \text{ characteristic time of pumping}$$





When Q<sub>in</sub> is a function of time:

$$P(t) = \frac{\int e^{\frac{t}{\tau_p}} \frac{Q_{in}(t)}{V} dt + A}{e^{\frac{t}{\tau_p}}} = \frac{\int Q_{in}(t) dt}{V} - \frac{e^{-\frac{t}{\tau_p}}}{V\tau_p} \int e^{\frac{t}{\tau_p}} \left[ \int Q_{in}(t) dt \right] dt + Ae^{-\frac{t}{\tau_p}}$$

A = integration constant



For a network of vacuum chambers, systems of coupled differential equations for each chamber have to be solved.

However, a simpler method exists. It is based on the analogy between vacuum systems and electrical networks. Very powerful software is available for the time dependent analysis of electrical networks.





Vacuum element	Electrical elements	
Conductance C	Conductance 1/R	••
Gas Flow Q	Current I	
Pressure P	Voltage V	
Volume V	Capacitance C	<b>●   </b>
Pump	Conductance to ground	•
Gas source	Current generator	•
Constant pressure source	Voltage supply	••
Vacuum chamber with conductance and volume		•

- The ground potential is equivalent to zero pressure.
- Long tubes are subdivided in smaller units and considered as single vacuum chambers (conductance + volume) in series.
- Non-linear electric characteristics can be used to simulate pressure and time dependent conductance and pumping speed.
- In this way pressure excursions into viscous regime can be evaluated



## Electric

Simple example: differential pumping

A more complex example: part of the Linac4 H- source (from C. Pasquino et al., CERN, ATS/Note/2012/043 TECH)









**Gas Pumping for Ion Sources** 



In molecular regime:

- gas molecules cannot be removed by suction: the molecules do not transfer energy and momentum amongst them; pumps act on each molecule singularly;
- pumps are classified in two families: ٠
  - momentum transfer pumps; 1.
  - 2. capture pumps.
- Capture pumps remove molecules from the gas phase by fixing them onto an internal wall.
- To do so the sojourn time on the wall has to be much longer than the typical time of the accelerator run. An estimation of sojourn time is given by the Frenkel law J. Frenkel, Z. Physik, 26, 117 (1924):

$$t_s = t_0 e^{\frac{E_a}{k_B T}}$$

where E<sub>a</sub> is the adsorption energy and  $t_0 \approx \frac{h}{k_B T} \approx 10^{-13}$  s.

 $E_a >> k_B T \rightarrow$  Chemical pumps (getter pumps)

$$T \ll \frac{E_a}{k_B} \rightarrow Cryopumps$$





The molecules receive a momentum components pointing toward the pump outlet where the gas is compressed and finally evacuated by pumps working in viscous regime.

In molecular pumps, molecules are headed for the outlet by moving surfaces.

Molecules impinge and adsorb on the moving surface; on desorption the velocity distribution is superimposed by the drift velocity of the wall  $\rightarrow$  a moving wall produces a gas flow



The most important characteristics of molecular pumps are:

1. Pumping speed S

2. Maximum compression ratio 
$$K_0 = \left(\frac{P_{OUT}}{P_{IN}}\right)_{MAX}$$

The parameters affecting S and K<sub>0</sub> can be identified by a simple model.



#### Momentum Transfer Pumps: Turbomolecular Pumps





At any point in time, half of the molecules has just collided with the moving surface and drift in the 'x' direction with velocity 'u'.

The other half comes from the stator where the drift component is lost.

The molecular flow toward an imaginary section (A) is:

$$Q = \frac{1}{2}n \cdot u \cdot bh = \frac{1}{2}\frac{P}{k_B T} \cdot u \cdot bh \text{ in PV units} \rightarrow Q = \frac{1}{2}P \cdot u \cdot bh$$
$$S = \frac{Q}{P} = \frac{1}{2}u \cdot bh$$

The pumping speed of molecular pumps:

- Depends linearly on the speed of the moving wall
- Does not depend on the nature of the gas (in the frame of this model)→ molecular pumps are not selective!





It can be shown that the maximum compression ratio is:

$$K_{0} = \left(\frac{P_{OUT}}{P_{IN}}\right)_{MAX} \propto \exp\left[\frac{u}{\langle v \rangle} \times \frac{L}{h}\right] \propto \exp\left[\left(u\sqrt{m_{i}}\frac{L}{h}\right)\right]$$
L and h  
length and width  
of the nump duct

High compression ratio for molecular pumps can be obtained for:

- Fast moving surfaces: at least of the same order of the average molecular velocity (>100 ms<sup>-1</sup>).
- Narrow and long pumping ducts (lower backstreaming).
- Heavy masses → the maximun compression ratio depends strongly on the molecular mass, the lowest being for H<sub>2</sub> → The ultimate pressure of molecular pumps is dominated by H<sub>2</sub>.





To overcome the problem of the required narrow pump duct, in 1957 Backer introduced the turbomolecular pumps (TMP) based on rapidly rotating blades.



The molecules seen from the blades have a velocity oriented toward the blades' channels when they come from space 1. From space 2, most of the molecules hit the blades and are backscattered  $\rightarrow$  a significant gas flow is set if at least  $\langle v \rangle \approx u$ .

Every series of rotating blades (rotor) is followed by a series of static blades (stator).

The indications given by the simplified model for molecular pumps hold also for the TMP:

S: no strong influence of gas molecular mass + linear dependence on revolution speed

K<sub>0</sub>: exponentially dependent on revolution speed and square root of gas molecular mass



#### Momentum Transfer Pumps: Turbomolecular Pumps (TMP)





TMP pumping speeds are in the range from 10 l/s to 25,000 l/s.

Their ultimate pressure  $(H_2)$  is of the order of  $10^{-10}$ ,  $10^{-11}$  mbar

Courtesy of Pfeiffer Vacuum <u>http://www.pfeiffer-vacuum.com</u> Vacuum Technology KnowHow







Advantages of TMP:

- 1. constant pumping speed in a large range of pressure
- 2. no memory effect (the gas is definitively evacuated) nor gas selectivity
- 3. start working at relatively high pressure (as soon as molecular regime is attained)

Disadvantages of TMP:

- 1. mechanical fragility
- 2. risk of contamination from the backing pump
- 3. need of venting anytime the pump is stopped to block backstreaming of contaminations→need of valve between TMP and vacuum vessel
- 4. intrinsic limitation in ultimate pressure of  $H_2$

Present trend:

- Use of dry pumps as backing pumps (but lower compression ratio than oil pumps)
- 2. Increase compression ratio by adding molecular drag stages below the set of TMP blades (very compact design)
- 3. Remove all lubricated mechanical bearing by magnetic rotor suspension (higher cost).



# Momentum Transfer Pumps: Turbomolecular Pumps (TMP)









Courtesy of Agilent Vacuum

http://www.youtube.com/watch?v=1xZe1H2XHhM&feature=youtube\_gdata\_player





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- <sup>1</sup> In SIP the residual gas is ionized in a Penning cell.
- The ions are accelerated toward a cathode made of reactive metal
- The collisions provoke sputtering of reactive metal atoms that are deposited on the nearby surfaces.
- The pumping action is given by:
  - 1. chemical adsorption onto the reactive metal layer and subsequent burial by additional metallic atoms of gas molecules: all gases except rare gases
  - 2. implantation of gas ions in the cathode and of energetic neutrals bounced back from the cathode in the deposited film: only mechanism of pumping for rare gases



**3.** diffusion into the cathode and the deposited film: only H<sub>2</sub>



# Figure 2.4.12. Example of instabilities in a system with one sputter-ion pump with titanium cathodes, after pumping argon at 5 x $10^{-7}$ Torr for a few hours.

Kimo M. Welch, Capture Pumping Technology, North-Holland, p.106

An excessive quantity of noble gas implanted in the cathode can produce pressure instabilities:

- the continuous erosion extract noble gas atoms from the cathode;
- as a result the pressure increases and the erosion is accelerated;
- a pressure rise is obtained, which terminate when most of the gas is implanted again in the sputtered film or in a deeper zone of the cathode.



#### **Capture Pumps: Sputter Ion Pumps (SIP)**



To increase the pumping efficiency of noble gas, the rate of ions implantation in the cathode has to be reduced while increasing the rate of energetic neutrals impingement on the anode and their burial probability.

Two different approches:

1. Heavier atoms for the cathode

Ta (181 amu) is used instead of Ti (48 amu). The ions, once neutralized, bounce back at higher energy and rate  $\rightarrow$  these pumps are called '**noble diode**'

#### 2. Different geometry of the Penning cell.

- a) Three electrodes are used: **triode pumps**. The cathodes consists of a series of small platelets aligned along the cell axis.
- b) The collisions ion-cathode are at glancing angle → higher sputtering rate of Ti atoms + higher probability of neutralization + higher energy of bouncing + lower probability of implantation in the cathode.





#### **Capture Pumps: Sputter Ion Pumps (SIP)**





An improved triode ion pump is the StarCell (Agilent Vacuum)







Pumping speed for SIP depends on the **pressure at the pump inlet** and the **nature of the gas**.



Fig. 5 Pumping speed vs pressure for a standard diode with  $S_N \approx 100$  l/s (for air after saturation).

Nominal pumping speed for N<sub>2</sub>: Agilent starcell

DN	S [   s <sup>-1</sup> ]
63	50
100	70/125
150	240/500

GAS	DIODE PUMPS	TRIODE PUMPS
AIR	1	1
N <sub>2</sub>	1	1
0 <sub>2</sub>	1	1
H <sub>2</sub>	1.5-2	1.5-2
СО	0.9	0.9
CO <sub>2</sub>	0.9	0.9
H <sub>2</sub> O	0.8	0.8
CH <sub>4</sub>	0.6-1	0.6-1
Ar	0.03	0.25
Не	0.1	0.3

Pumping speed normalized to air



#### **Capture Pumps: Sputter Ion Pumps (SIP)**









#### **Technical Specifications**

	StarCell®	Noble Diode	Diode
Nominal pumping speed for Nitrogen (*) (I/s)	410	440	500
Operating life at 1x10 <sup>-6</sup> mbar (hours)	80,000	50,000	50,000
Maximum starting pressure (mbar)	≤ 1x10 <sup>-2</sup>	≤ 1)	d0 <sup>-3</sup>
Ultimate pressure		Below 10 <sup>-11</sup>	
Inlet flange	8" CFF (NW 150) AISI 304 ESR		
Maximum baking temperature (°C)		350	
Weight, kg (lbs)		120 (264)	
(*) Tested according to ISO/DIS 3556-1-1992			





#### **Capture Pumps: Getter Pumps**



The surface of getter materials reacts with gas molecules by forming **stable chemica compounds**.

This is **possible only if** the surface is clean, **free of contamination and native oxide**.

The clean metallic surface is obtained by:

- 1. Sublimating the reactive metal in situ  $\rightarrow$  Evaporable Getters, Sublimation Pumps
- 2. Dissolving the surface contamination into the bulk of the getter material by heating in situ (activation): Non-Evaporable Getters NEG.

Getter surfaces are characterized by the sticking probability  $\alpha$  :

 $\alpha = \frac{number \ of \ molecules \ captured}{number \ of \ molecules \ impinging}$ 

$$0 \le \alpha \le 1 \ S = \alpha \ A_{getter} C'$$

For  $\alpha=1$ , the pumping speed of the surface is equal to its maximum pumping speed. Getter materials do not pump rare gases and methane at room temperature.



**Capture Pumps: NEG Pumps** 



The dissolution of the oxide layer is possible only in metals having very high oxygen solubility limit, namely the elements of the 4<sup>th</sup> group: Ti, Zr and Hf.







The activation temperature of the 4<sup>th</sup> group elements can be decreased by adding selected elements which increase oxygen diffusivity.

NEG materials are produced industrially by powder technology. Small grains are sintered to form pellets, discs or plates. The grains can also be pressed at room temperature on metallic ribbon.

A typical alloy produced by SAES Getter is **St707**:

Element	Concentration [wt. %]	Main role in the alloy
Zr	70	<ul><li>High O solubility limit.</li><li>Chemical reactivity</li></ul>
V	24.6	<ul><li>Increases O diffusivity,</li><li>Chemical reactivity</li></ul>
Fe	5.4	- Reduces pyrophoricity

Full pumping speed is obtained after heating at 400°C for 45' or 300°C for 24h



#### **Capture Pumps: NEG Pumps**



St 171<sup>®</sup> and St 172 - Sintered Porous Getters





The maximum  $H_2$  sorption capacity is limited by  $H_2$  embrittlement of the NEG elements. In general a safe limit is 20 Torr I/g is given by the supplier.

The stored H<sub>2</sub> can be desorbed by heating and pumping with an auxiliary pump (for example a TMP).

June 5th, 2012

Paolo Chiggiato - TMP). Technology for ion sources



#### **Capture Pumps: NEG Pumps**

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The high porosity of NEG materials allows pumping of relatively high quantities of gas without reactivation: for CO about 100 times higher than those for sublimation pumps per unit of geometrical surface of active metal.





#### **Typical Pump Characteristics**

Alloy Type		St 172®
Alloy Composition		ZrVFe
Getter Mass(g)		225
Getter Surface (cm <sup>2</sup> )		1900
Pumping Speed (I/s)	H <sub>2</sub>	2000
	СО	1000
Sorption	H <sub>2</sub>	4500
Capacity (Torr I)	CO Room Temperature	5
	CO Total	2000
Note: Dumping speed data refer to the initial values of the pump		

Note: Pumping speed data refer to the initial values of the pump without the pump body. CO capacity based on speed below 50 l/s.



# **Comparison of Pumps**



	Advantages	Disadvantages
ТМР	<ul> <li>No memory effects</li> <li>Constant pumping speed for pressures lower than 10<sup>-3</sup> mbar</li> <li>Pumping speed independent of total gas load</li> <li>Starts working at high pressures (molecular regime)</li> </ul>	<ul> <li>Mechanical fragility</li> <li>Risk of contamination from the backing pump</li> <li>Need of venting anytime the pump is stopped</li> <li>Need of valve on the main flange</li> <li>Intrinsic limitation in ultimate pressure of H<sub>2</sub></li> <li>Possible vibrations</li> <li>Maintenance</li> </ul>
SIP	<ul> <li>Clean pumping</li> <li>No maintenance</li> <li>No vibrations</li> <li>Installation in any orientation</li> <li>Relatively long lifetime</li> <li>Relatively low cost</li> <li>Limited but high H<sub>2</sub> capacity</li> <li>The pump current gives a pressure reading</li> </ul>	<ul> <li>Low capture probability</li> <li>Gas Selectivity and limited capacity</li> <li>Memory effects (in particular for rare gases)</li> <li>Ignition in 10<sup>-5</sup> mbar range</li> <li>Bulky</li> <li>Difficult starting for old pumps</li> <li>Production of charged particles in particular at start-up</li> <li>Field emission problems for old pumps</li> <li>Fringing magnetic field</li> <li>Safety issue: high voltage</li> </ul>



# **Comparison of Pumps**



	Advantages	Disadvantages
NEG pumps	<ul> <li>Clean vacuum</li> <li>High pumping speed for reactive gases</li> <li>With SIP, extremely low vacuum can be achieve</li> <li>High gas capacity for porous NEG</li> <li>Low cost</li> <li>Electrical power needed only for activation; it works in case of power cut</li> <li>No maintenance</li> <li>No vibration</li> </ul>	<ul> <li>Selective pumping (no pumping of rare gases and methane)</li> <li>H<sub>2</sub> enbrittlement if regeneration is not applied</li> <li>Formation of dust particles is not excluded</li> <li>Safety issue: pyrophoric, it burns when heated in air at high temperature</li> </ul>





#### **Final Remarks**

- For vacuum technology, an ion source is a special place in particle accelerators. Gas is injected at high rate for the beam production. The main task of vacuum experts is to remove this gas as close as possible to the source.
- The gas removal efficiency is limited by space constraints and the available pumping mechanism.
- The requirement for high vacuum in presence of high gas load define the choice and combination of pumps.
- I have chosen to focus this course on pumps because in ion sources, as in no other places in modern accelerators, they work near their limits.
- Pressure measurement is not an issue in ion sources: commercial Penning-Pirani heads are generally used.




# Appendix



# Appendix 1 Basic Notions : Gas Pressure



Definition of pressure: *|Force component in normal direction| Surface area* 

Unit of measurement:  $\frac{[Force]}{[Surface]} \rightarrow \frac{N}{m^2} = Pa \rightarrow 10^5 Pa = 1 \ bar \rightarrow 1 \ atm = 1.013 \ bar$ 

In vacuum technology : *mbar or Pa* 

Still used in vacuum technology:

1 Torr = pressure exerted by a column of 1 mm of Hg; 1 atm = 760 Torr

#### Conversion Table

	Ра	bar	atm	Torr
1 Pa	1	10 <sup>-5</sup>	9.87 10 <sup>-6</sup>	7.5 10 <sup>-3</sup>
1 bar	10 <sup>2</sup>	1	0.987	750.06
1 atm	1.013 10 <sup>5</sup>	1.013	1	760
1 Torr	133.32	1.33 10 <sup>-3</sup>	1.32 10 <sup>-3</sup>	1



Operation of ion sources

## Appendix 1 Basic Notions : Gas Pressure



#### **Degree of Vacuum**

	Pressure boundaries [mbar]	Pressure boundaries [Pa]
Low Vacuum LV	1000-1	10 <sup>5</sup> -10 <sup>2</sup>
Medium Vacuum MV	1-10 <sup>-3</sup>	10 <sup>2</sup> -10 <sup>-1</sup>
High Vacuum HV	10-3-10-9	10-1-10-7
Ultra High vacuum UHV	10 <sup>-9</sup> -10 <sup>-12</sup>	10-7-10-10
Extreme Vacuum XHV	<10 <sup>-12</sup>	<10 <sup>-10</sup>

Pressures and gas quantities are correlated by the gas equation of state. In vacuum the ideal gas law is always fulfilled :

P V = n R T (thermodynamic)

 $P \ V = N \ k_B \mathsf{T}$  (statistical mechanics)

**P** pressure, **V** volume, **T** temperature, quantity of gas in moles (**n**) and number of molecules (**N**)

**R** gas constant, **k**<sub>B</sub> Boltzmann constant



# Appendix 1 Basic Notions : Gas Quantity



 $\frac{molecules}{cm^3}$ 

$$P V = N k_B T \rightarrow P = \left(\frac{N}{V}\right) k_B T$$
  $k_B = 1.38 \ 10^{-23} \ \frac{Pa m^3}{K} = 1.04 \ 10^{22} \ \frac{Torr \ l}{K}$ 

	Pressure [Pa]	Gas Density 293 K	Gas Density 4.3K
Atmosphere	1.013 10 <sup>5</sup>	2.5 10 <sup>19</sup>	1.7 10 <sup>21</sup>
Plasma chambers	1	2.5 10 <sup>14</sup>	1.7 10 <sup>16</sup>
LINAC pressure upper limit	<b>10</b> <sup>-5</sup>	2.5 10 <sup>9</sup>	1.7 10 <sup>11</sup>
Lowest pressure ever measured at room T	10 <sup>-12</sup>	250	1.7 10 <sup>4</sup>

#### Gas quantities can be expressed in:

- Number of molecules: N
- Moles:  $\frac{N}{N_A} \left( N_A = 6.022 \ 10^{23} \left[ \frac{molecules}{mole} \right] \right)$
- PV quantities if the temperature is known and constant :  $PV = N(k_BT)$

Example: 1 Pa m<sup>3</sup> at 293K contains  $N = \frac{1 \left[ Pa.m^3 \right]}{1.38.10^{-23} \left[ \frac{J}{K} \right] 293 \left[ K \right]} = 2.47 \ 10^{20}$  molecules

1 Torr I = 3.3 10<sup>19</sup> molecules; 1 mbar I =2.47 10<sup>19</sup> molecules



## Appendix 1 Basic Notions : Molecular Mean Speed



Maxwell-Boltzmann Molecular Speed Distribution for Noble Gases



In the kinetic theory of gas the mean speed of a molecule is the mathematical average of the speed distribution:

$$\langle v \rangle = \sqrt{\frac{8 k_B T}{\pi m}} = \sqrt{\frac{8 R T}{\pi M}}$$

m is the molecular mass [Kg] M is the molecular weight [Kg]

Courtesy of Wikipedia: http://en.wikipedia.org/wiki /Maxwell%E2%80%93Boltzmann\_distribution

Gas	$\langle v \rangle$ at 293 K $\left[\frac{m}{s}\right]$	$\langle v \rangle$ at 4.3 K $\left[\frac{m}{s}\right]$
H <sub>2</sub>	1761	213
Не	1244	151
CH4	622	75
N <sub>2</sub>	470	57
Ar	394	48



## Appendix 1 Basic Notions : Impingement Rate with a Surface



Gas	Pressure [mbar]	Impingement rate 293 K [cm <sup>-2</sup> s <sup>-1</sup> ]
	10 <sup>-3</sup>	1.1 10 <sup>18</sup>
H2	10 <sup>-8</sup>	1.1 10 <sup>14</sup>
	10 <sup>-14</sup>	1.1 10 <sup>8</sup>
NO	10 <sup>-3</sup>	2.9 10 <sup>17</sup>
IN Z	10 <sup>-8</sup>	2.9 10 <sup>13</sup>
<b>A r</b>	10 <sup>-3</sup>	2.4 10 <sup>17</sup>
AI	10 <sup>-8</sup>	<b>2.4</b> 10 <sup>13</sup>

$$\varphi = \frac{1}{4}n\langle v \rangle = \frac{1}{4}n\sqrt{\frac{8\,k_BT}{\pi\,m}}$$

$$\varphi[cm^{-2}s^{-1}] = 2.635 \ 10^{22} \frac{P \ [mbar]}{\sqrt{M[g]T[K]}}$$



Appendix 1 **Basic Notions : Mean Free Path** 



The molecular collision rate  $\omega$  in a gas is:

$$\omega = \sqrt{2} n \langle v \rangle \sigma_c$$

where  $\sigma_c$  is the collision cross section.

For a single gas, in case of elastic collision of solid spheres:

$$\sigma_c = \pi \delta^2 \rightarrow \omega = \sqrt{2} \pi n \langle v \rangle \delta^2$$

and  $\delta$  is the molecular diameter.

The mean free path l, i.e. the average distance travelled by a molecule between collisions, is given by:

$$l = \frac{\langle v \rangle}{\omega} = \frac{1}{\sqrt{2} \pi n \, \delta^2} = \frac{k_B T}{\sqrt{2} \pi P \, \delta^2}$$

 $l_{H_2}[m] = 4.3 \ 10^{-5} \frac{T[K]}{P[Pa]}$ 

Gas	$\sigma_c [nm^2]$
H <sub>2</sub>	0.27
Не	0.21
N <sub>2</sub>	0.43
0 <sub>2</sub>	0.40
CO <sub>2</sub>	0.52

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Appendix 1 Basic Notions : Knudsen Number



$$K_n = \frac{l}{D}$$

*l* is the mean free path and **D** is a characteristic dimension of a vacuum system (p.ex. the diameter of a beam pipe).

K <sub>n</sub> range	Regime	Description
K <sub>n</sub> >0.5	Free molecular flow	The gas dynamic is dominated by molecular collisions with the walls of the system
K <sub>n</sub> <0.01	Continuous (viscous) flow	The gas dynamic is dominated by intermolecular collisions
0.5 <k<sub>n&lt;0.01</k<sub>	Transitional flow	Transition between molecular and viscous flow



Appendix 1 Basic Notions : Knudsen Number





Technology for Ion Sources



#### Appendix 1 Basic Notions : Knudsen Number









In molecular regime the net flux of molecules from one point (1) to another (2) is proportional to the pressure drop:

$$Q = C \left( P_1 - P_2 \right)$$

C is called the gas conductance from the two points. It does not depend on pressure.

The simplest example is the gas flow through a small wall slot of area A and infinitesimal thickness



Gas flow 1 -> 2 : 
$$\varphi_{1 \rightarrow 2} = \frac{1}{4} A n_1 \langle v \rangle$$
  
Gas flow 2 -> 1 :  $\varphi_{2 \rightarrow 1} = \frac{1}{4} A n_2 \langle v \rangle$ 

Net flow: 
$$\frac{1}{4}A(n_1 - n_2)\langle v \rangle = \frac{1}{4}A\frac{\langle v \rangle}{k_B T}(P_1 - P_2)$$

In PV units  $(PV = Nk_BT) \rightarrow Q = \frac{1}{4}A\langle v \rangle (P_1 - P_2) \rightarrow C = \frac{1}{4}A\langle v \rangle$ 





Conductance of a wall aperture in PV units, per unit area:  $C' = \frac{1}{4} \langle v \rangle$ 

T= 293 K	Gas	$\langle v \rangle$ at 293 K $\left[\frac{m}{s}\right]$	$C'at 293 K\left[\frac{m^3}{s m^2}\right]$	$C' \text{ at } 293  K\left[\frac{l}{s  cm^2}\right]$
	H <sub>2</sub>	1761	440.25	44
	Не	1244	311	31.1
	CH₄	622	155.5	15.5
	H <sub>2</sub> O	587	146.7	14.7
	N <sub>2</sub>	470	11.75	11.75
	Ar	394	98.5	9.85

Example:  $H_2 P_1 = 5 \ 10^{-4} mbar$ ,  $P_2 = 7 \ 10^{-5} mbar$ ,  $A = 0.8 \ cm^2$ 

$$\begin{array}{c|c} \mathsf{P}_1 & \mathsf{P}_2 \\ \mathsf{A} & \\ \end{array} \rightarrow Q = 44 \times 0.8 \times (5 \ 10^{-4} - 7 \ 10^{-5}) = 1.5 \times 10^{-2} \frac{mbar \ l}{s} \\ \rightarrow Q = 1.5 \times 10^{-2} \frac{mbar \ l}{s} \times 2.47 \ 10^{19} \frac{molecules}{mbar \ l} = 3.74 \ 10^{17} \frac{molecules}{s} \end{array}$$





For more complicated gas flow restrictions, the transmission probability  $\tau$  is introduced.



Gas flow 1 -> 2 : 
$$\varphi_{1\to 2} = \frac{1}{4} A_1 n_1 \langle v \rangle \tau_{1\to 2}$$

Gas flow 2 -> 1 :
$$\varphi_{2\to 1} = \frac{1}{4} A_2 n_2 \langle v \rangle \tau_{2\to 1}$$

In absence of net flow:  $\varphi_{1 \rightarrow 2} = \varphi_{2 \rightarrow 1}$ and  $P_1 = P_2 \rightarrow A_1 \tau_{1 \rightarrow 2} = A_2 \tau_{2 \rightarrow 1}$ 

$$Q = \frac{1}{4} A_1 n_1 \langle v \rangle \ \tau_{1 \to 2} - \frac{1}{4} A_2 \ n_2 \langle v \rangle \ \tau_{2 \to 1} = \frac{1}{4} A_1 \langle v \rangle \ \tau_{1 \to 2} \ \frac{(P_1 - P_2)}{k_B T}$$

In PV units:

$$Q = \frac{1}{4} A_1 \langle v \rangle \tau_{1 \to 2} (P_1 - P_2) = C (P_1 - P_2)$$
  
$$C = C' A_1 \tau_{1 \to 2}$$

# $C = [conductance of the aperture] \times [molecular transmission probability]$





The molecular transmission probabilities:

- depend only on the geometry of the vacuum system;
- can be calculated only for simple geometry;
- nowadays are accurately obtained by Monte Carlo methods.

Example:

• Tubes of uniform circular cross section (*L* length, R radius); Santeler formula (max error 0.7%):

$$\tau = \tau_{1 \to 2} = \tau_{2 \to 1} = \frac{1}{1 + \frac{3L}{8R} \left( 1 + \frac{1}{3\left(1 + \frac{L}{7R}\right)} \right)}$$
  
For long tubes  $\left(\frac{L}{R} \gg 1\right)$ :  $\tau \approx \frac{1}{1 + \frac{3L}{8R}} \approx \frac{8}{3} \frac{R}{L}$ 

For N<sub>2</sub> and 
$$\frac{L}{R} \gg 1 \rightarrow C = C'A \tau \approx 11.75 \times \frac{\pi D^2}{4} \times \frac{4D}{3L} = 12.3 \frac{D^3}{L} \left[\frac{l}{s}\right] ([D] and [l] = cm)$$











Other expressions can be found for ducts of rectangular and elliptical cross section (see J. M. Lafferty, Foundation of Vacuum Science and Technology, Wiley Interscience).

For more complicated geometry, Test-Particle Monte Carlo methods (TPMC) are used.

The TPMC:

- generates "random" molecules according to the cosine distribution at the entrance of the tube;
- then follows their traces until they reach the exit of the tube
- the molecules are re-emitted from the wall again randomly
- each collision with the walls is followed by a random emission
- many simulated molecules are needed in order to reduce the statistical scattering

The software used at CERN is Molflow+, written and maintained by **Roberto Kersevan** and Marton Szakacs (CERN, TE-VSC)



#### Appendix 2: Additional Examples of Electrical Analogy



#### The full simulation of the MedAustron facility.





#### Appendix 2: Additional Examples of Electrical Analogy



Evaluation of pressure profile during pump-down in the SPS ring J. A. Ferreira Somoza, CERN, TE-VSC internal note, 05-2012



Equivalent electrical network for sector 560.



#### Appendix 2: Additional Examples of Electrical Analogy



Current dependent resistances simulate conductance variations in the whole pressure range, even in viscous regime.



Comparison between calculated pumpdown curves for original (green) and halved (orange) longest SPS vacuum sector.







**Solvents**: their molecules interact and transport contaminants away by diffusion (dilution) -> quite selective! ( $C_2Cl_4$ , wide spectrum; HFC, more restricted action)

**Detergents in water**: allows organics and water to combine by forming micelle (surfactant: **surf**ace **act**ing **a**ge**nt**). Based on molecule with hydrophilic heads and lipophilic tail: less selective than solvents

June 5th, 2012





Materials of which a vacuum system is made of are spontaneous source of gas.

## Two main categories of materials:

**Metals** After state-of-art surface cleaning

 <u>If not heated in situ</u>: mainly H<sub>2</sub>O for the first months in vacuum, then also H<sub>2</sub>.

 $q_{H_2O} \approx \frac{3 \times 10^{-9}}{t[h]} \left[ \frac{mbar \, l}{s \, cm^2} \right]$ 

The source of  $H_2O$  is recharged after each venting to air.

 If heated in situ (baked-out): mainly H<sub>2</sub>. The outgassing rate can be assumed as constant; it depends on the accumulated effect of the previous thermal treatments

# **Organics (Polymers)**

- High solubility of gas in the bulk, in particular H<sub>2</sub>O.
- In general, the outgassing process is dominated by H<sub>2</sub>O release.
- In the initial phase of pumping:

$$q_{H_2O} \propto \frac{1}{\sqrt{t}}$$

- Heavier gas molecules can be outgassed (remnant of polymerisation, fraction of polymeric chains)
- The permeation of light molecules is not negligible, in particular He



Technology for Ion Sources









#### Outgassing rate of water vapour for unbaked metals



H.F. Dylla, D. M. Manos, P.H. LaMarche Jr. Journal of Vacuum Science and Tech. A, 11(1993)2623





Outgassing rate of water vapour for polymers







Pressure profiles with distributed outgassing can be calculated analytically (for simple geometry), by electrical analogy or by Monte Carlo simulation.







Cryopumps rely on three different pumping mechanisms:

- **1. Cryocondensation**: is based on the mutual attraction of **similar** molecules at low temperature:
  - a. the key property is the saturated vapour pressure, i.e. the pressure of the gas phase in equilibrium with the condensate at a given temperature. The attainable pressure is limited by the saturated vapour pressure.
  - b. Only Ne,  $H_2$  and He have saturated vapour pressures higher than 10<sup>-11</sup> Torr at 20 K.



c. The vapour pressure of H<sub>2</sub> at 4.3 K is in the 10<sup>-7</sup>
 Torr range, at 1.9 lower than 10<sup>-12</sup> Torr.





#### Appendix 4: Extra Info about Capture Pumps/Cryopumps



- 2. Cryosorption: is based on the attraction between molecules and substrate. The van der Waals forces are much stronger than those between similar molecules:
  - a) Gas molecules are pumped at pressure much lower than the saturated vapour pressure providing the adsorbed quantity is lower than one monolayer.
  - a) Porous materials are used to increase the specific surface area; for charcoal about 1000 m<sup>2</sup> per gram are normally achieved.
  - b) The important consequence is that significant quantities of H<sub>2</sub> can be pumped at 20 K and He at 4.3 K.
  - c) Submonolayer quantities of all gases may be effectively cryosorbed at their own boiling temperature; for example at 77 K all gases except He, H<sub>2</sub> and Ne.
- **3. Cryotrapping** : low boiling point gas molecules are trapped in the layer of an easily condensable gas. The trapped gas has a saturation vapor pressure by several orders of magnitude lower than in the pure condensate. Examples: Ar trapped in CO<sub>2</sub> at 77 K; H<sub>2</sub> trapped in N<sub>2</sub> at 20 K.





Modern cryopumps take advantages of the first two mechanisms.

- The cryocondensation takes place on a cold surfaces, in general at 80 K for H<sub>2</sub>O and 10 or 20 K for the other gases.
- 2. The cryosorption of  $H_2$ , Ne and He is localised on a hidden surface where a porous material is fixed. This surface is kept away from the reach of the other molecules.





#### Courtesy of Oerlikon Leybold Vacuum www.oerlikon.com/leyboldvacuum



#### 800 BL UHV (CF)

High vacuum flange	DN	160 CF	
Fore vacuum flange	DN	40 CF	
Flange for other purpose	es DN	16 CF (1x), 40 CF (1x)	
Safety valve with DN 40 connection for gas exha	KF flange ust line	burst disk mounted on DN 16 CF	
Pumping speed H <sub>2</sub> O Ar / N <sub>2</sub> H <sub>2</sub> / He	x s <sup>-1</sup>   x s <sup>-1</sup>   x s <sup>-1</sup>	2600 640 / 800 1000 / 300	- <b>*</b>
Capacity Ar / N <sub>2</sub> H <sub>2</sub> at 10 <sup>-6</sup> mbar He	bar x I (Torr x I) bar x I (Torr x I) bar x I (Torr x I)	300 (225 000) / 300 (225 000) 4.3 (3225) 0.5 (375)	
Built-in cold head	COOLPOWER	7/25	
Max. throughput Ar / N <sub>2</sub> mbar x H <sub>2</sub> mbar x	l x s⁻¹ (Torr x l x s⁻¹) l x s⁻¹ (Torr x l x s⁻¹)	4 (3) / 4 (3) 2 (1.5)	45° 13, 13,5
Crossover value	mbar x I (Torr x I)	150 (112)	
Cool down time to 20 K	min	50	-4
Overall height	mm (in.)	538 (21.18)	
Weight	kg (lbs)	12 (26.5)	
Silicon diode for tempera at second stage of the co	ture measurements old head	built-in to a DN 16 CF with 4 way	Dimensiona



Top turned by 90°

COOLVAC 800 BL UHV (160 CF)

Cryopumps require periodic regeneration to evacuate the gas adsorbed or condensed.

To remove all captured gas, the pump is warmed at room temperature. The desorbed gas is removed by mechanical pumps (in general, for accelerators, mobile TMP). During regeneration, the rest of the system must be separated by a valve.



# Appendix 4: Extra Info about Capture Pumps/Cryopumps

# Characteristics of Cryopumps

# 1. Starting Pressure

- Cryopumps should be started when the mean free path of molecules is higher than the pump vessel diameter: P<10<sup>-3</sup> mbar. Otherwise the thermal load is too high.
- In addition a thick condensate layer must be avoided.
- They need auxiliary pumps.

# 2. Pumping speed

- High effective pumping speed for all gases. Pumping speed from 800 l/s up to 60000 l/s are commercially available .
- Pumping speed for water vapour close to the theoretical maximum.

## 3. Maximum Gas Intake (Capacity)

- At the maximum gas intake, the initial pumping speed of the gas is reduced by a factor of 2.
- Condensed gases: the limitation is given by the thermal conductivity of the gas layer.
- Adsorbed gases: the capacity depends on the quantity and properties of the sorption agent; it is pressure dependent and generally several orders of magnitude lower compared to that of condensable gases.





Cryopumps require periodic regeneration to evacuate the gas adsorbed or condensed.

To remove all captured gas, the pump is warmed at room temperature. The desorbed gas is removed by mechanical pumps (in general, for accelerators, mobile TMP).

During regeneration, the rest of the system must be separated by a valve.

In the majority of application, the performance deterioration is given by the gas adsorbed on the second stage (10-20 K). A partial regeneration may be carried out for a shorter time while water vapour is kept on the first stage at temperatures lower than 140 K.





# Appendix 4: Extra Info about Capture Pumps/Cryopumps



	Advantages	Disadvantages
Cryopumps	<ul> <li>Very large pumping speed for all gases</li> <li>Clean vacuum</li> <li>High pumping capacity</li> <li>Limited selectivity</li> </ul>	<ul> <li>Cost and maintenance</li> <li>Relatively large volume needed (including refrigerator)</li> <li>Gas release in case of power cut</li> <li>Reduced pumping efficiency for H<sub>2</sub> for high quantity of gas adsorbed: regeneration needed</li> <li>Need of valve on the main flange</li> </ul>





For particle accelerators Ti is the sublimated metal.

Ti alloy rods are heated up to 1500°C attaining a Ti vapour pressure of about 10<sup>-3</sup> mbar.



*Courtesy of Kurt J. Lesker Company http://www.lesker.com/newweb/Vacuum\_Pumps* 

The sticking probabilities depend on the nature of the gas and the quantity of gas already pumped.

$$\max - \begin{bmatrix} H_2 : \ 10^{-2} \le \alpha \le 10^{-1} \\ CO : 5 \times 10^{-1} \le \alpha \le 1 \end{bmatrix}$$

The sticking probability is negligible:

- For CO, one monolayer adsorbed
- For of O<sub>2</sub> several monolayer
- For N<sub>2</sub> fraction of monolayer



Hydrogen diffuses in the Ti film→much higher



Paolo Chiggiato - CERN - Vacuum Technology for Ion Sources





A K Gupta and J H Leek, Vacuum, 25(1975)362





	Advantages	Disadvantages
Sublimation Pumps	<ul> <li>Clean vacuum</li> <li>High pumping speed for reactive gases</li> <li>With SIP, extremely low vacuum can be achieve</li> <li>Low cost</li> <li>Electrical power only for sublimation; it works in case of power cut</li> <li>Limited maintenance (filament change)</li> <li>No vibration</li> </ul>	<ul> <li>Very limited capacity</li> <li>Need frequent sublimations at high pressure</li> <li>Ti film peel-off for high sublimation rates</li> <li>Selective pumping (no pumping of rare gases and methane)</li> <li>Risk of leakage current in high voltage insulators</li> <li>Ideal for low pressure applications</li> </ul>





#### Hydrogen pumping by SIP

- H<sub>2</sub> is mainly pumped by diffusion into the cathode.
- To be adsorbed, H<sub>2</sub> must be dissociated. Only 2.5% of the ions created in a low-pressure H<sub>2</sub> Penning discharge are H+ ions.
- The dissociation is possible only on atomically clean Ti.
- H<sub>2</sub> + ions have poor sputtering yield: 0.01 at 7 KeV on Ti.
- When H<sub>2</sub> is the main gas, it takes a long time to clean the cathode surface by sputtering.
- As a consequence, at the beginning of the operation the pumping speed for H<sub>2</sub> is lower than the nominal and increases gradually with time.
- The simultaneous pumping of another gas has strong effects on H<sub>2</sub> pumping speed.
  - Higher sputtering yield→faster cleaning→ higher pumping speed
  - Contaminating of the Ti surface  $\rightarrow$  lower pumping speed
  - Desorption of implanted H ions  $\rightarrow$  lower pumping speed
- When the concentration of H<sub>2</sub> is higher than the solubility limit in Ti, hydride precipitates are formed → Ti expansion and hydrogen embrittlement → short circuits and cathode brittleness (for 500 l/s pumps: typical value are 10000 Torr l of H<sub>2</sub>)





#### **High Pressure Operation**

- High pressure (>10<sup>-5</sup> mbar) operation can generate thermal run-away. It is frequently noticeable during the pumping of H<sub>2</sub> or after the absorption of high quantity of H<sub>2</sub> (for example due to pumping of H<sub>2</sub>O).
- The Penning discharge heats the cathode and provokes gas desorption, which enhance the discharge. This positive feedback mechanism can melt locally the cathode.
- The total electrical power given to the pump has to be limited at high pressure.

#### Pressure measurement by ion pumps

- The discharge current of the penning cells can be used for pressure measurement.
- In the low pressure range, the current measurement is limited by field emission (leakage current): pressure reading limitation in the 10<sup>-9</sup> mbar range.
- By reducing the applied voltage in the lower pressure range, the pressure measurement is possible down to 10<sup>-10</sup> mbar.




## Appendix 4: Extra Info about Capture Pumps/NEG



Courtesy of SAES Getters, www.saesgetters.com



Figure 3 - Hydrogen equilibrium pressure for the St 707 alloy





The time  $t_R$  needed to regenerate a NEG pump is given by:

$$t_{R} = \frac{M_{NEG}}{S_{aux}} \left( \frac{1}{q_{f}} - \frac{1}{q_{i}} \right) \cdot 10^{-\left(A + \frac{B}{T}\right)}$$

Where:

 $q_f$  and  $q_i$  are the final and initial concentrations in Torr I/g  $S_{aux}$  is the pumping speed of the TMP  $M_{NEG}$  the mass of the NEG in g A and B typical values of the NEG material For St707: A=4.8, B= -6116



The pressure during the regeneration heating is given by:  $Log(P) = A + 2Log(q) + \frac{B}{T}$ q is the actual hydrogen concentration