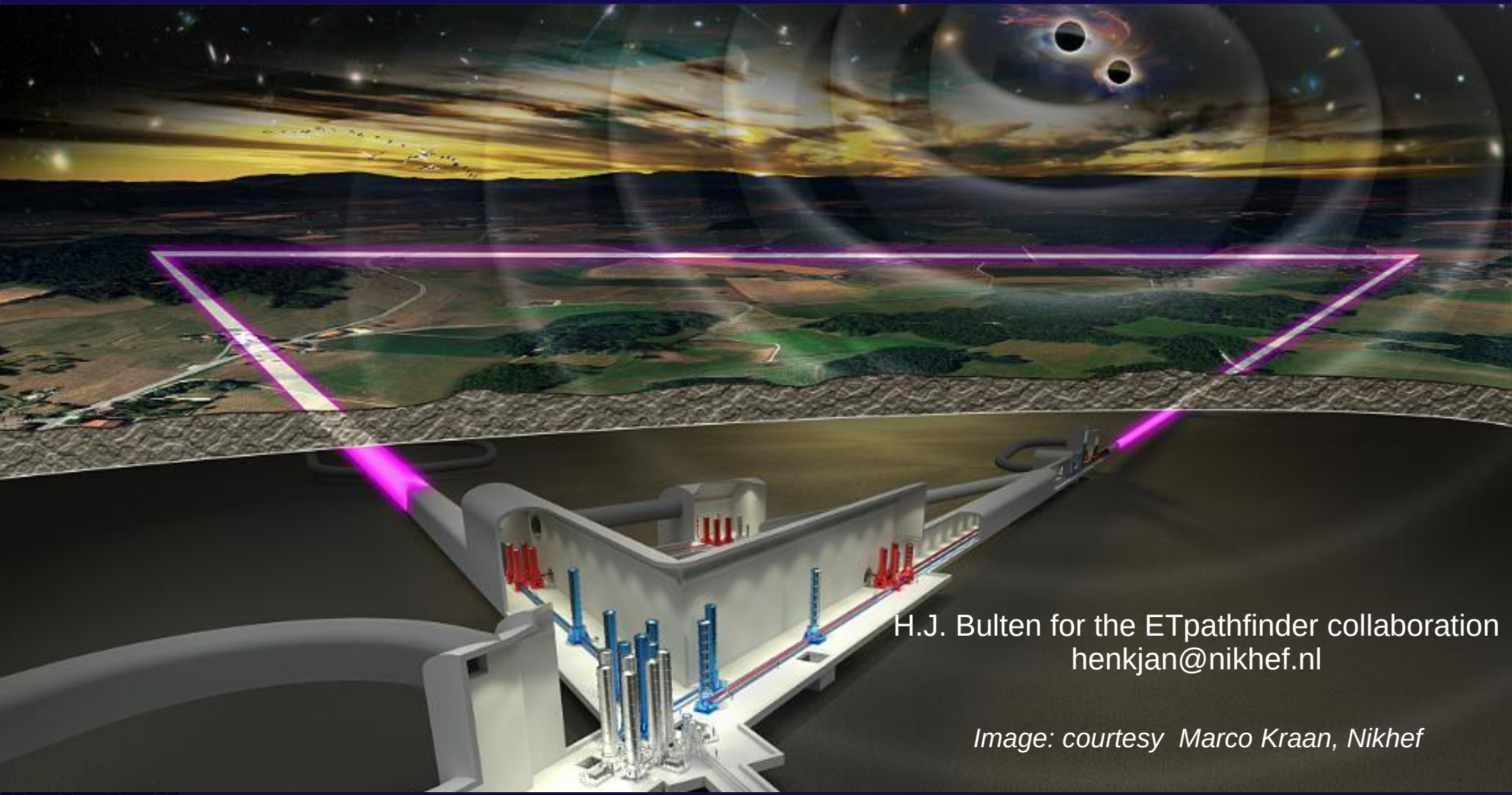
Vacuum & Cryogenic simulations for gravitational-wave interferometry



H.J. Bulten for the ETpathfinder collaboration
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Image: courtesy Marco Kraan, Nikhef

3rd generation GW interferometry – cryogenics and vacuum

Improve sensitivity:

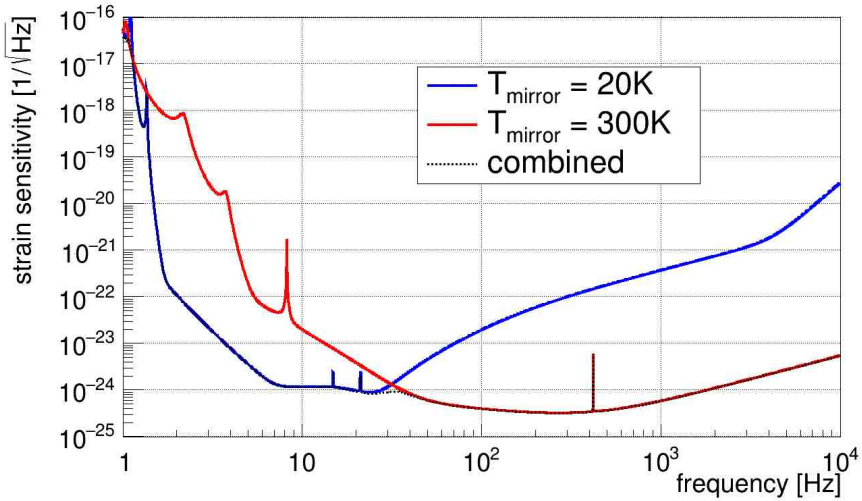
- Use heavy mirrors (reduces the radiation pressure fluctuations, helps at low frequency)
- More stored laser power (reduces shot noise but increases radiation pressure noise)
- Go underground: reduces the gravitational attraction of seismic activity on the mirror
- Cool the mirrors: reduces the thermal noise that makes vibrations in the mirror suspensions, the mirror bulk movement, and the mirror coatings.
- Better vacuum – reduces residual gas noise

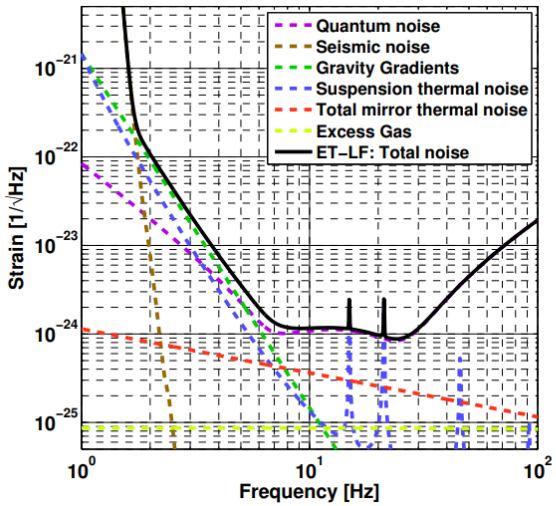
Cryogenic challenges

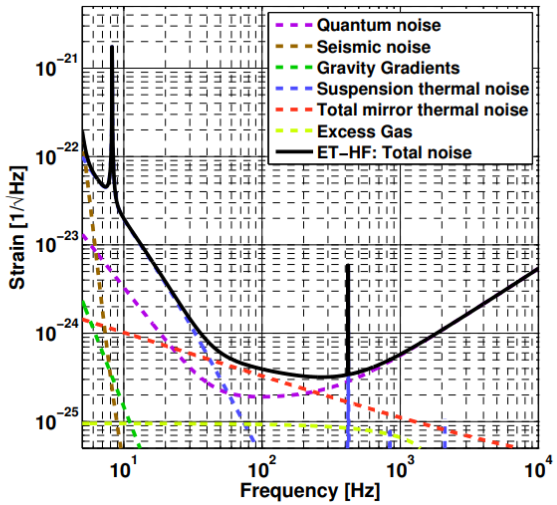
- Vibration-free cooling
- Initial cool-down cryogenic mass (GJ of heat)
- Design shields that:
  - Absorb thermal radiation from environment
  - Emit little thermal radiation towards mirror
  - Help protect mirror against ice build-up
  - Can be pumped down

Vacuum noise contributions

- Optical path length changes in FP-cavities
- Brownian motion, mirror
- Ice build-up on cryogenic optics



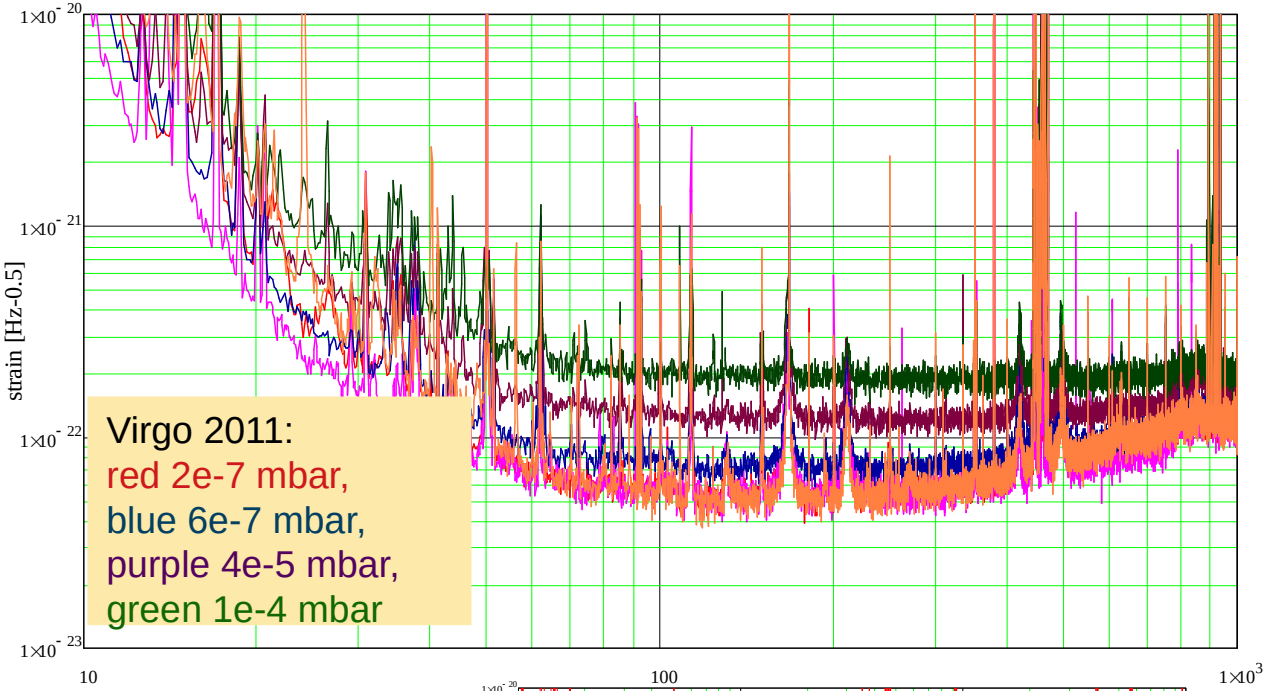




Noise from residual gas: 1 - optical path length changes

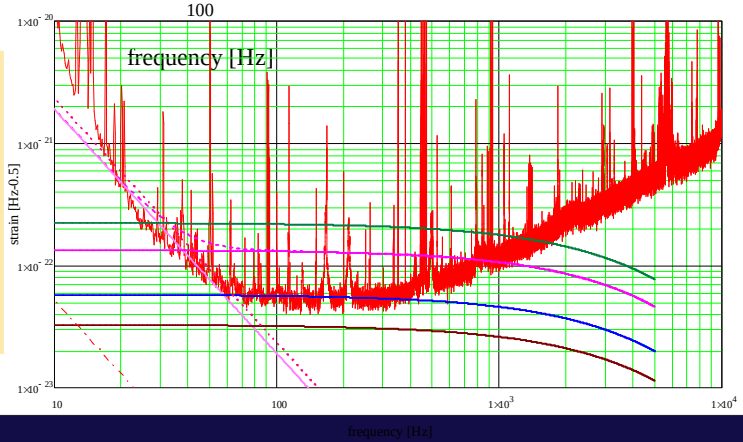
- Residual gas in the arm can cause optical path length changes. These changes depend on the beam profile, the residence time of a molecule in the beam, and the polarizability, and scale with the square root of the gas pressure.
- The effects are calculated from model simulations, but also measured by both LIGO and Virgo.7 At the end of the Virgo science run in 2011 the beam was in steps partially vented with N2 gas and the loss in sensitivity was measured.
- For ET, the aim is to have residual gas noise contribute max 10 percent to the design sensitivity. Tfor current design, this leads to maximal total pressures along the arm as stated in the table below:

Gas species	ET-LF [mbar]	ET-HF [mbar]
hydrogen	1.1e-9	1.0e-10
water	1.2e-10	1.1e-11
Nitrogen	6.2e-11	6e-12
CO2	2e-11	2e-12



LIGO : S. Whitcomb and M. Zucker, "Measurement of Optical Path Fluctuations due to Residual Gas in the LIGO 40 Meter Interferometer," 7th Marcel Grossman Meeting on General Relativity, July 1994, Stanford University, pp. 1434–1436, 1994.

Virgo: Pasqualeti, Cella, et al, TDS Vir-0667A-11



Noise from residual gas: 2 - Brownian motion

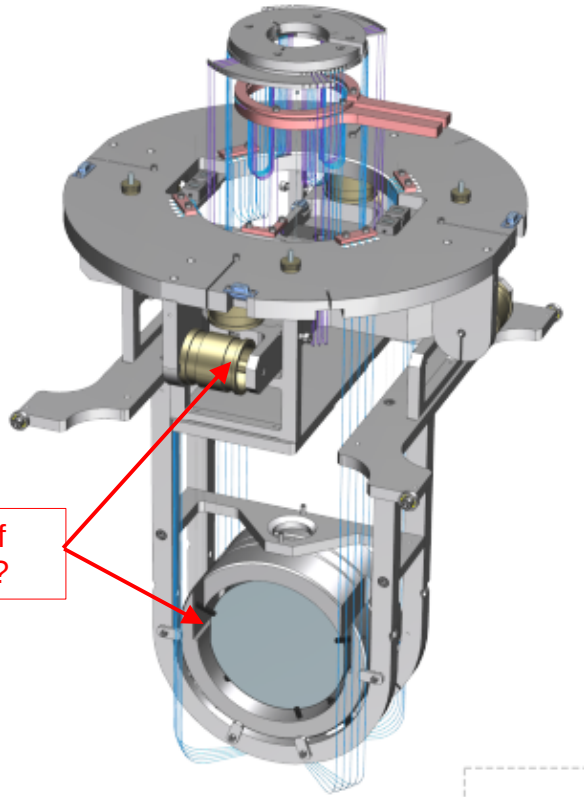
- Residual gas: Brownian motion, mirror
  - Scales with pressure, surface area, mirror mass as sqrt(p A)/m – gas kinetics.
  - Calculation for a cylindrical mirror: based on Energy fluctuation dissipation theorem: Cavalleri et al., Phys. Lett. A374, 4465 (2010)

$$S_f = \sqrt{p\sqrt{\frac{8}{\pi}mk_bT}\left[\pi R^2\left(1+\frac{h}{2R}+\frac{\pi}{4}\right)\right]}\ [\mathrm{N}/\sqrt{\mathrm{Hz}}]$$

Spectral noise — Side of cylinder — scattering

  - For ET, using the cryogenic interferometer (T~ 15K, m=2): $S \approx 3\times10^{-13}\sqrt{p}[N/\sqrt{Hz}] \approx 4\times10^{-17}\sqrt{p}/f^2[m/\sqrt{Hz}]$
    Aim: 10 times lower than sensitivity curve
    Pressure in mirror tower for cryogenic mirror: $S<10^{-21}$ at 7Hz thus $p < 10^{-6}$ Pa in mirror tower.

The mirror towers contain many wires/coils/feedthroughs: vacuum poorer than in arms. Brownian motion seems OK but gas trapped between the mirror and the reaction mass may increase the noise: modeling required.



ETpathfinder mirror with reaction mass, safety frame, cooling, and suspension filter above it. Gas may be trapped between mirror and reaction mass or between the coils that rotate the filter, leading to significant enhancement of the Brownian motion noise

Residual gas noise: freezing

Mirrors are cryogenic: anything except He may freeze on them. Mirrors are shielded by sets of radiation shields, but the optical aperture to the beam is huge.

Particle incidence rate:

$$J = \frac{\rho <v>}{4} = \frac{N}{4V}\sqrt{8 k_b \frac{T}{\pi m}} \qquad 3.6\times10^{22}\, H_2O\,@\,1\,Pa$$

a monolayer can freeze on the mirror in 1 minute at a pressure of 10^{-5} Pa
A monolayer might already spoil the resolution. The partial pressures at the mirror, when cooled, should therefore be far below 10^{-9} Pa

Designing and building the vacuum system for ET poses a major challenge. Apart from stringent vacuum techniques we also need state-of-the art modeling: we want to know

- Outgassing rates as a function of time, temperature, and surface history
- Monolayer coverage, concentration profiles of dissolved materials over years
- Outgassing rates after different baking cycles/or after cooling
- Particle tracking: how do the particles migrate? Do they freeze on the shields or the mirror/suspension? If pumped, when are pumps saturated? NEG strip performance over years? Brownian noise from particles between mirror and actuators?

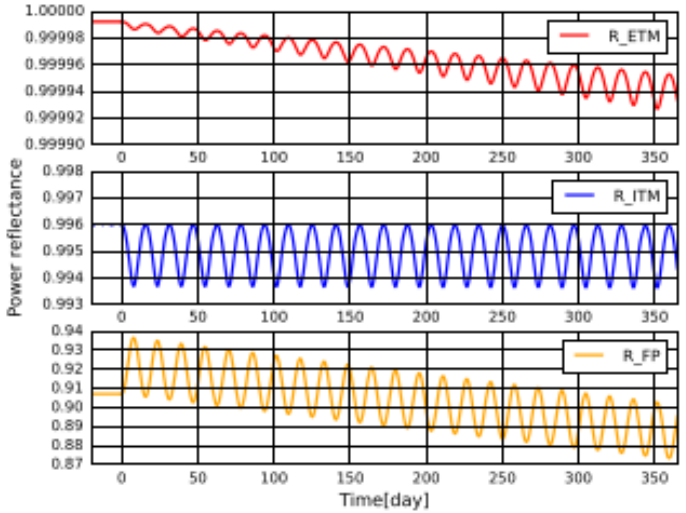


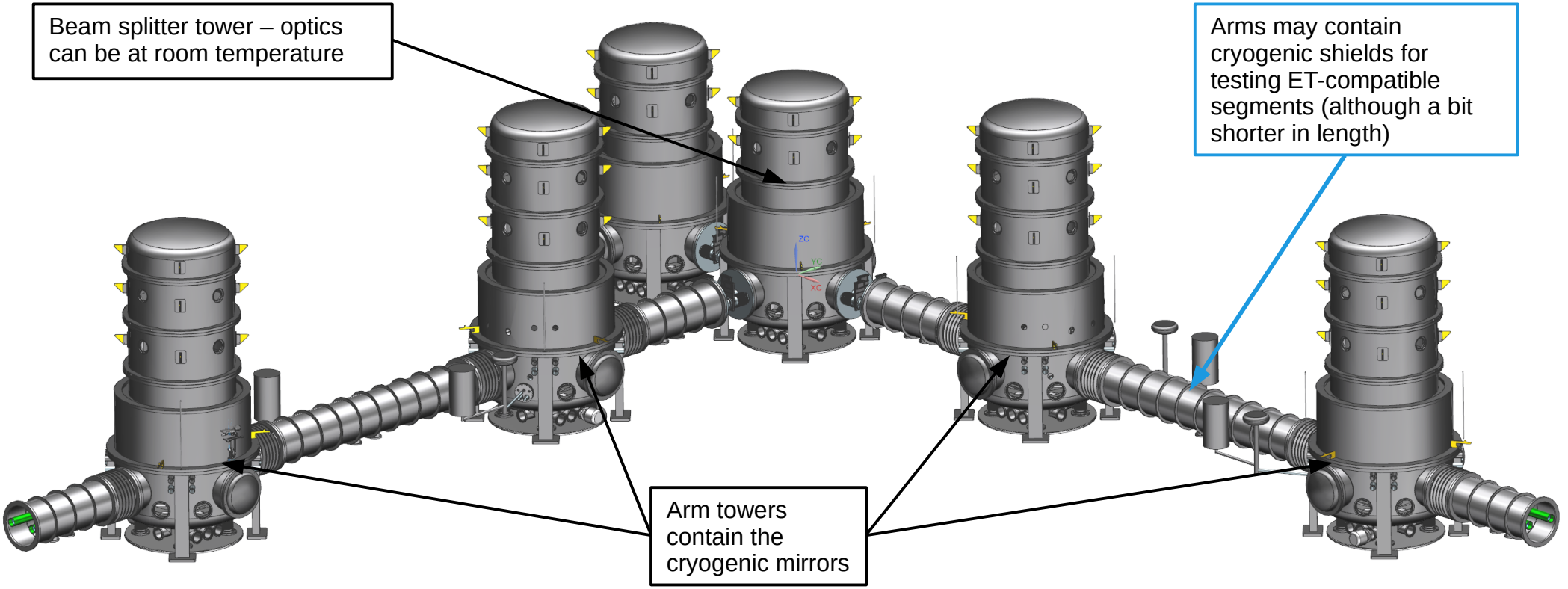
FIG. 9. Reflectance oscillations of the ITM (top), ETM (middle), and the arm FP cavity (bottom) of KAGRA due to the molecular adlayer by using the parameters in Table II. In this calculation, the formations of a molecular adlayer for the ETM and ITM start at the same time. Because the original reflectance of the ETM is higher than that of the ITM, the amplitude of reflectance oscillation of the ITM is larger than that of the ETM. The reflectance of the ETM decreases over time due to the optical absorption inside the adlayer. On the other hand, the reflectance of the ITM does not decrease. This is because the ITM reflectance is lower than the ETM reflectance, and the absorption of the adlayer is not large enough to significantly reduce the ITM reflectance. The reflectance of the arm cavities increases when the reflectance of the ITM decreases because the reflectance of the ETM is higher than that of the ITM.

Kagra data, from Hasegawa et. Al, PRD 99, 022003 (2019).)

ETpathfinder – a research facility for future GW interferometers

Research facility to test and develop cryogenic techniques for future GW detectors

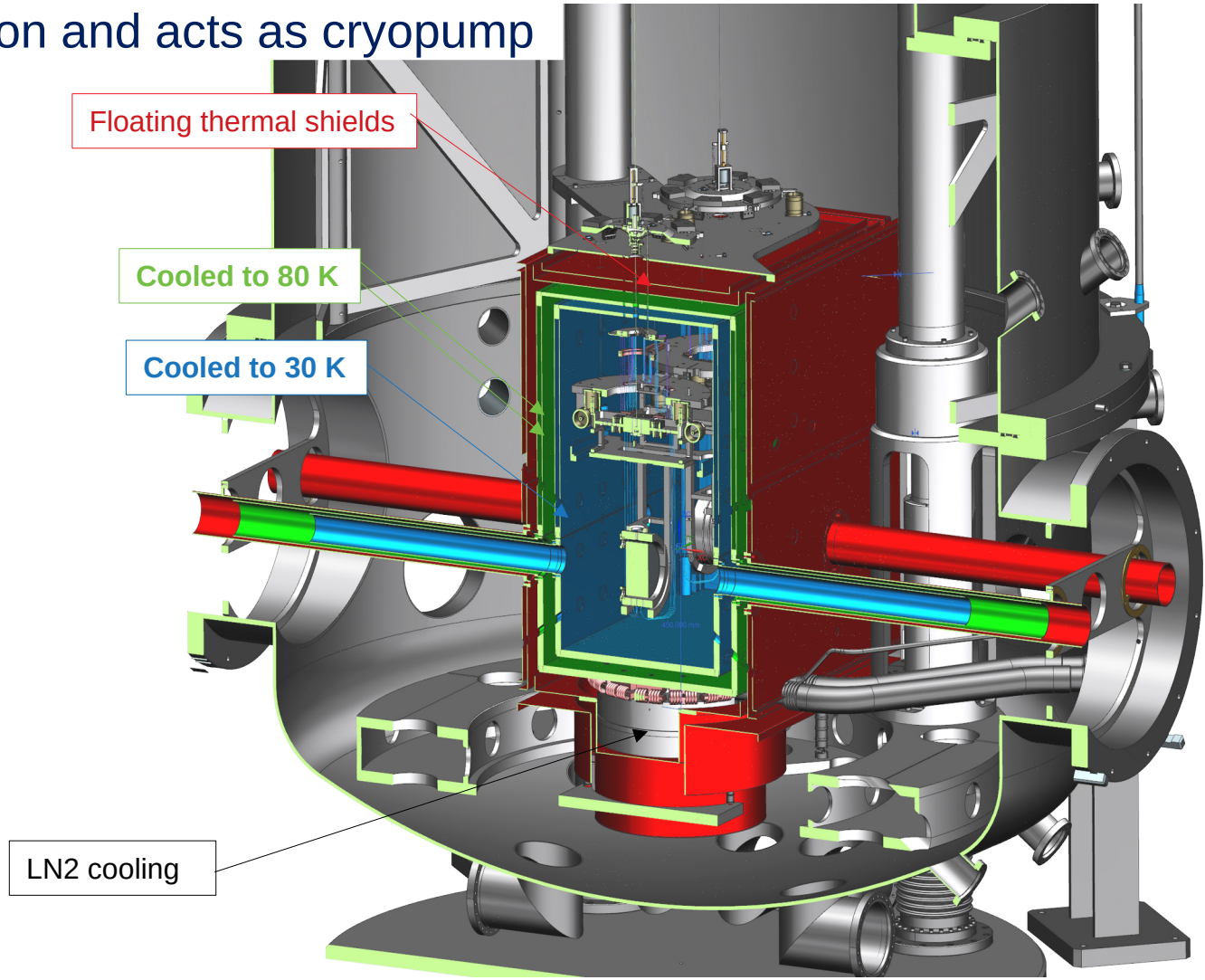
- Being constructed right now in Maastricht, the Netherlands
- 2 arms ~ 10m long: each arm can host 2 Fabry-Perot cavities for small optics (150mm diameter, 3.5 kg Si mirrors) or 1 FP cavity with large optics (ET-size, up to 250 kg mirrors)
- Aim is to to develop and test cryogenic techniques and interferometer operations at room temperature, at 123K, at 10-20 K; mirror ASD < 10^{-18} m/sqrt(Hz) above 10 Hz (sufficient to be limited by thermal noise)



ET pathfinder, thermal shields

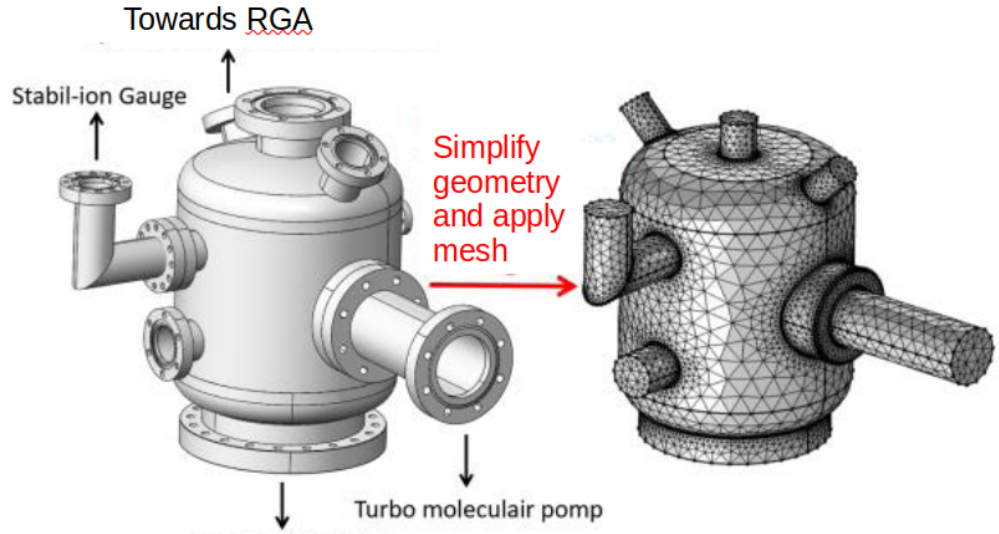
Allows to reduce thermal radiation and acts as cryopump

- UHV – we cannot use MLI foils
- Double-walled shields with holes for vacuum conductance
- Thermal radiation scales with $\sigma_{SB}\ T^4$ – the mirror should not see more than 0.01% of thermal radiation from the ambient room-temperature environment
  - Tubes along the laserbeams
  - Three sets of shields with holes
  - Modeling needed for: temperature gradients and cool-down curves - emissivity – how much radiation bounces through the pumpholes and enters the inner shield? Emissivity shields?
  - Outgassing of vacuuum walls, cables, optics – where does the gas go? Where does it freeze
  - Design a cool-down strategy and design the shields to obtain minimal freezing of water when cryogenically operated
- We developed an extensive simulation packet for just that: Vacrysim.

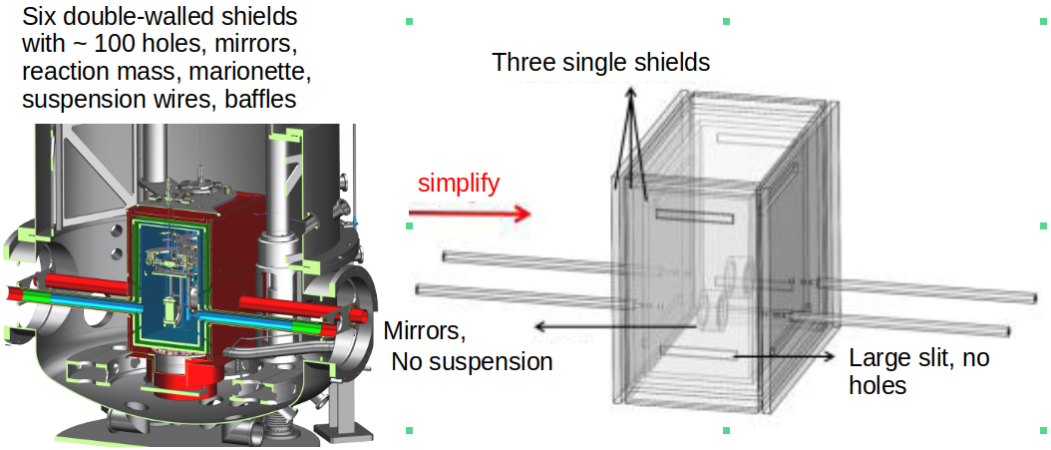


Modeling – Vacrysim versus FEM (Comsol and Molflow)

- Standard approach: finite-element modeling
  - Render the structure in small elements with connecting surfaces
  - Calculate currents through surfaces and update central values in elements
  - Solve for all elements, all surfaces – static equilibrium is reached when the sum of the currents through the surfaces of all elements equals zero
- Size of elements: should represent shape of object: e.g. elements < wire diameters, wall thicknesses, holes.
- To solve for one full cryogenic tower: millions of elements needed.
  - 1 time step : billions of flops.
  - Stiff equations: e.g. the current through a jellyfish wire in 1 microsecond changes the temperature of that wire by 10 percent at low temperatures! When not in equilibrium, microsecond steps are needed. For a cool-down calculation of 1 tower for 1 month: unpractical (hundreds of Petaflops)
- Vacrysim: many orders of magnitude faster than FEM
  - Simpler elements: track to pre-defined surfaces
    - Cylinders, disks, rectangular blocks, cones, spheres, all with circular holes supported. Need only hundreds - thousands of elements to simulate one tower exactly.
  - Decouple time evolution from tracking results. Use sixth-order adaptive Runge-Kutta (for far less elements) to speed up time evolution by many orders of magnitude.

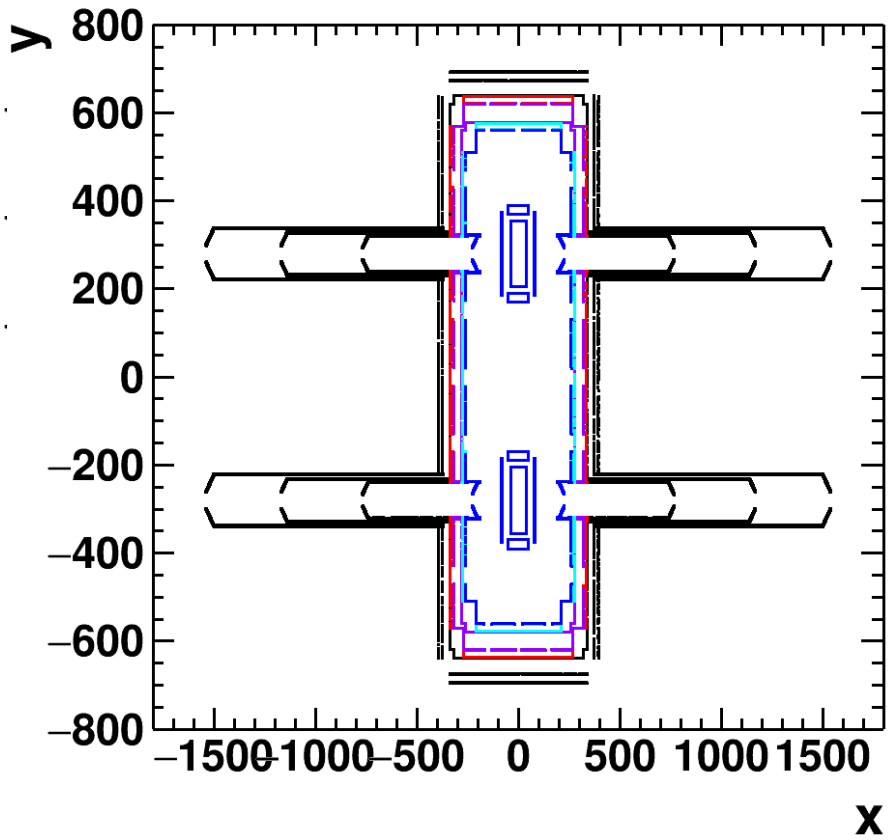


Reduction of object: Vera Erends, Nevac, Oct 2020



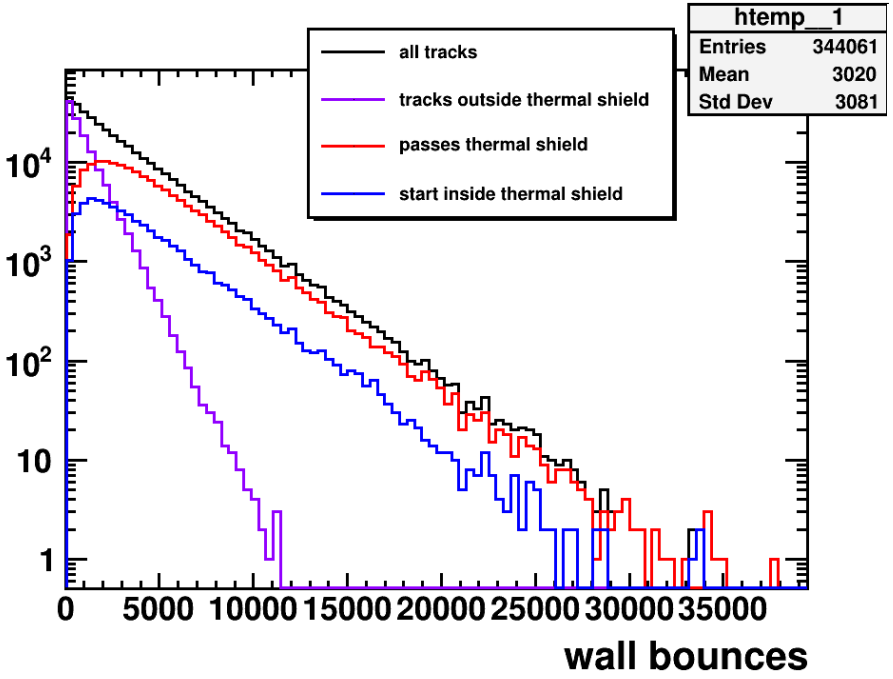
Modeling – ETpathfinder setup

- Raytracing code: we generate particles/radiation at the surface and follow them until absorbed (EM radiation) or pumped out (molecules)
- Weigh the tracks with surface area (and emissivity for radiation).
- Store the track results: how many times which surface is hit, starts and stops of tracks.
- Then off-line, you can do the time-dependent modeling:
  - Outgassing per surface: depends on temperature, monolayer coverage, material type, history
  - Molecular flow: start with incidence rate (follows from pressure and temperature). Account for adsorption and desorption per surface: depending on dissolved concentrations/monolayer coverage/surface temperature. Track also concentration profile for dissolved species.
  - Calculate which percentage of the molecules is transferred from surface X to Y, which percentage is pumped out, and adsorped/desorped
  - Solve coupled equations – group surfaces facing the same volume together for better speed (same incidence rate for these surfaces after each time step.
  - Coupled equations: stiffness problematic (e.g. desorption/adsorption terms change monolayer coverage in microseconds but net outgassing of hydrogen changes over decades) – for water, initially nanosecond steps are needed.

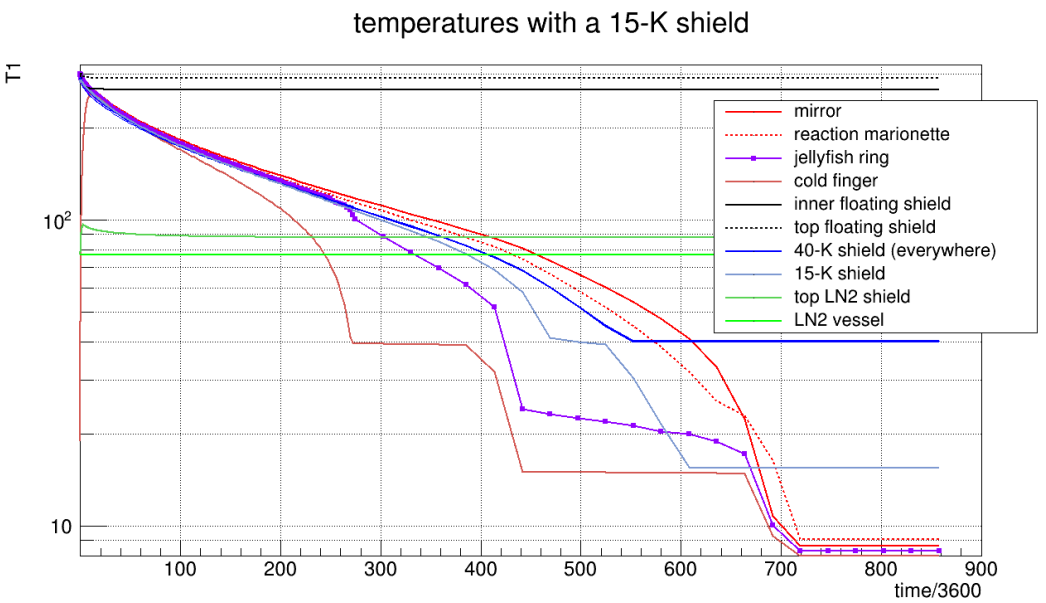


Cross section of the shields, mirror and reaction mass at beam height. Volume around the mirror dark-blue, between the walls of inner shield light blue, LN2 shield purple/red, passive shields and baffles black.An almost exact replica of the shields is reconstructed using 172 basic shapes.

Modeling – ETpathfinder setup



Example of raytrace results: one ETpathfinder tower with shields, mirror, marionette, baffles and reaction mass has been modeled. The number of hits per track before reaching the turbopump is plotted for different start positions – 10 billion tracks calculated in ~ 4 hours (using 12 threads on an iCore7)



Cool-down of the mirrors in about 1 month – using liquid Nitrogen cooling for the LN2 shield, 30W cooling power for the 40K shield until T=40K, then 3W sorption cooling power, 1.5W cooling power at a 15-K screen (not shown in drawings, and 0.1 W cooling power at cold finger.

About 400 elements are needed to describe the system, the heat transfer between each pair of elements is solved in each time step. (5 days CPU on an iCore7)

Time-dependence outgassing

- Adsorption/Desorption: Metal surfaces: water – dominant after venting
  - Relatively strong binding for monolayer – 0.7-1 eV
  - Sojourn times from milliseconds to hours
  - Strongly temperature-dependent
  - Typically thousands of wall bounces before water reaches a pump – 1/t behavior due to balance of adsorption and desorption

- Permeation/dissolved gas:
  - polymers (Teflon, PTFE, Kapton, Viton-A) : different gases can dissolve in these. Outgassing rate depends on diffusion speed and temperature, permeation on solubility. Build-up of concentration profile, depends on squared. Initial decay 1/sqrt(t), ultimate exponential.
  - Hydrogen in stainless steel – a few ppm dissolved during production. Outgassing rate depends on diffusion speed and on recombination cross section at the surface.
  - Initially diffusion-limited (1/sqrt(t) decay), ultimately recombination-limited – more or less linear

- Sublimation: desorption constant, exponentially depending on T; ice build-up depending on pressure.

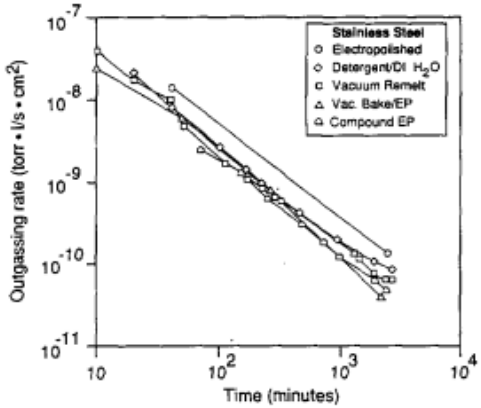
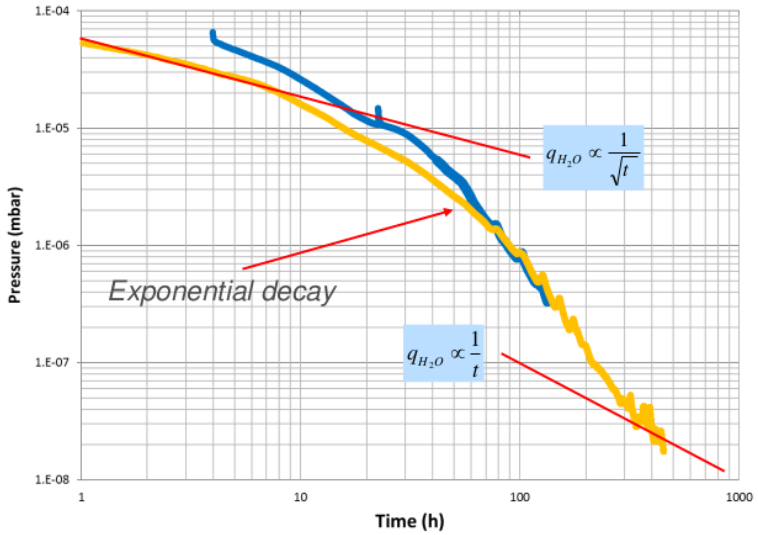


FIG. 3. Outgassing results for the stainless steel surface treatments.

Left: Water outgassing: Dylla, Manos. Lamarche, J. Vac. Sci. Techn 11, 2623 (1993)

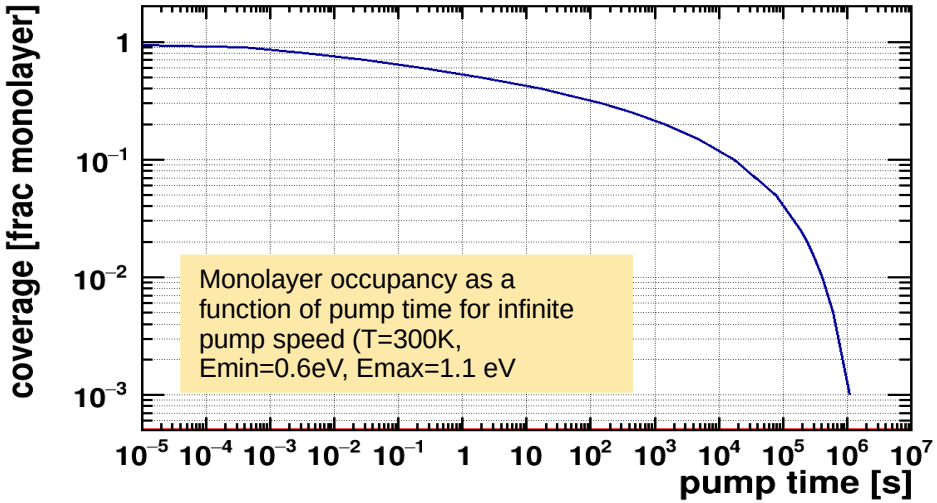
Bottom: 0.2mm thick Kapton wire: from Chiggiato, Cern Accelerator School Lund, June 2017



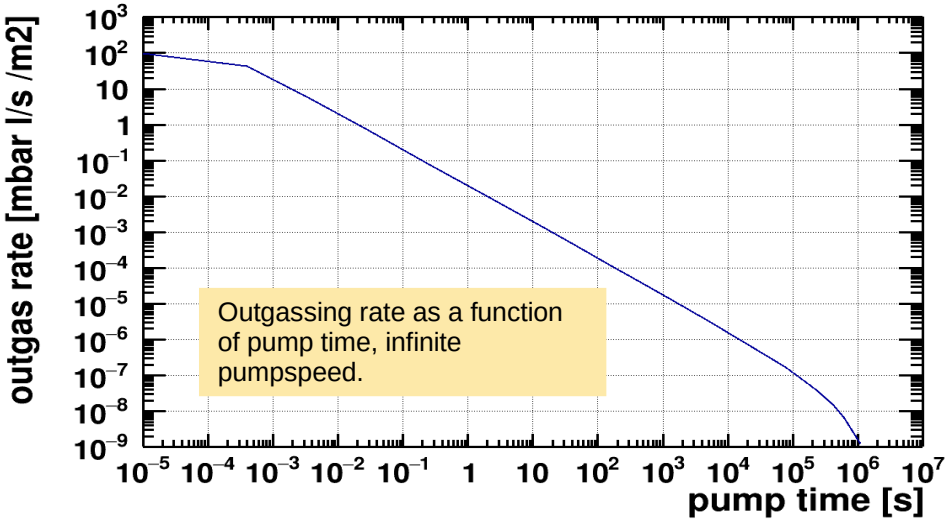
Courtesy of Jose Antonio Ferreira Somoza

Water Outgassing, model calculation

- We assume a Temkin-like isotherm; average binding energies of the monolayer varies from 0.7 eV (fully occupied , eta=1) to 1.05 eV (fully depleted, all sites are available):



$$E_{bind} = E_{min} + (1-\eta)(E_{max} - E_{min})$$



- The outgassing rate can be calculated analytically:

$$\eta'(t) = -\eta(t)/t_{soj}(\eta);\quad t_{soj} = e^{a+b(1-\eta)}$$
$$a = \log(10^{-13}) + E_{min}/kT;\quad b = (E_{max} - E_{min})/kT$$
$$k_1 - e^{-a}t = e^{b}\,Ei(-b\,\eta(t));\quad t = e^{b+a}(Ei(-b) - Ei(-b\,\eta(t)))$$
$$with\quad Ei = \int_{-x}^{\infty} \frac{e^{-t}}{t}\,dt$$

- However, also adsorption takes place. For water we use the coupled equations:

$$\eta'(t) = -\eta(t)/t_{soj}(\eta) + \frac{J_{impingement}}{n_{mono}}\,stick(1-\eta);\quad t_{soj} = e^{a+b(1-\eta)}$$
$$J'_{impingement} = \sum_{surfaces} \frac{-A_{surf}}{A_{tot}} n_{mono}\,\eta' \left\langle \frac{n_{bounces}}{t_{av}} \right\rangle + \sum_{volumes} (J - J_{vol}) \frac{A_{cond,i}}{\sum_{volumes} A_{cond,i}} \frac{1}{t_{av}}$$

- n_mono is the number of molecules per unit area for a full monolayer

The occupancy of the monolayer is a balance between adsorption and desorption.

The impingement rate depends on the desorption (introduction of new water molecules), adsorption (pumping of water by the surface) and the flow towards neighboring volumes (pressure differential).

To solve the coupled equations for all surfaces, temperatures, times, pressures, the coupled differential equations are integrated numerically in time. This is tedious because of the stiff conditions (sojourn times of days versus flow towards other volume regions in milliseconds).

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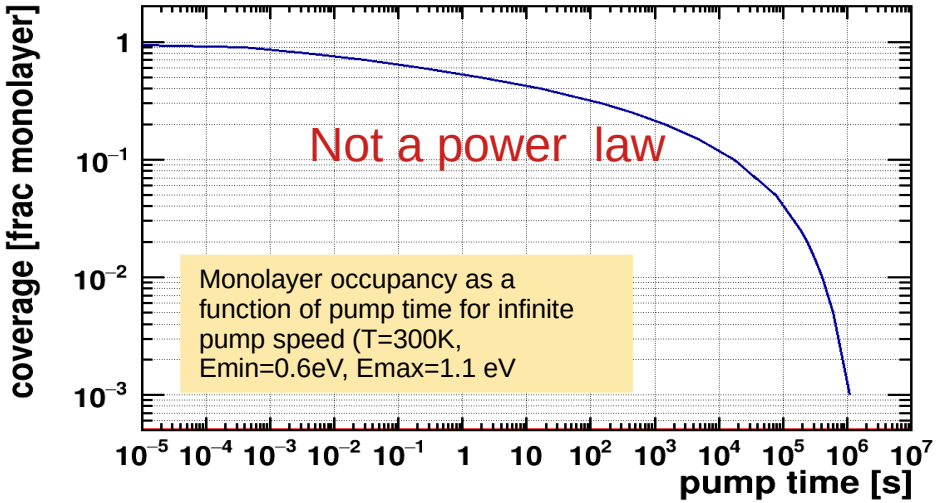

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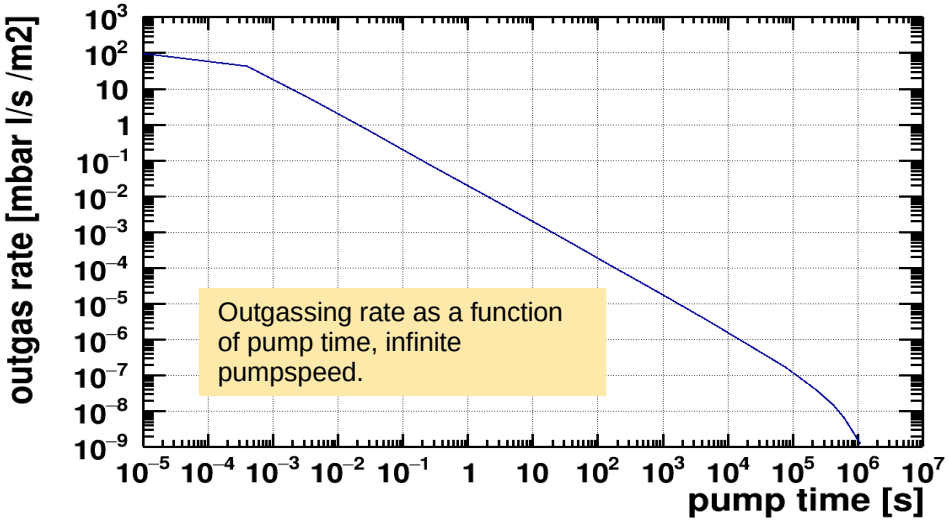

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Hydrogen outgassing from steel, different trapping mechanisms

Different mechanisms to trap hydrogen, can be numerically modeled. From F. Berg, Tata steel, and the ETT-WP2 project. See also e.g. Robert F. Berg; Journal of Vacuum Science & Technology A 1 May 2014; 32 (3): 031604.

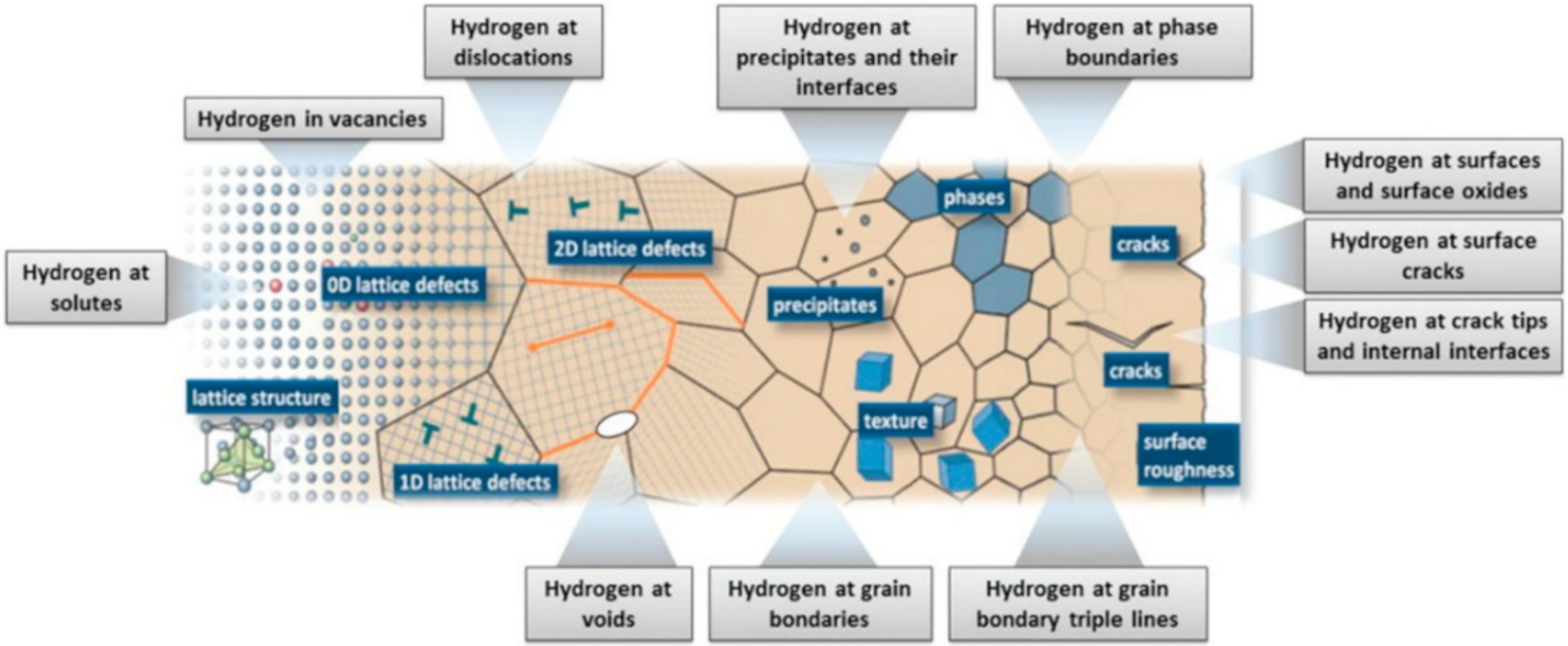


Figure 14: Illustrative representation of different hydrogen trapping mechanisms due to lattice defects in steels. Picture adapted from [Koyama 2017].

Steel, hydrogen desorption

Thermal desorption measurements (rapidly heating a thin sample) and spectroscopy can find activation energies.

Outgas measurements (spinning rotor gauge) can measure time-dependent outgasssing

- Study of mild steels, including weldability, coating effects, Thermal Desorption spectroscopy and analysis, and outgassing measurements are ongoing.

- We aim to combine the material studies in the simulation package so that measurements can be compared to model and predictions for ET/ETpathfinder can be made.

Table 3: Grade compositions, in wt%.

	IF	DP600	DP980
C	< 0.003	0.08	0.07
Si	< 0.010	0.26	0.27
Mn	0.12	1.83	2.54
Cr	0.02	0.19	0.30
Mo	/	/	0.11
Al	0.06	0.03	0.16
Nb	/	/	0.03
Ti	0.06	/	0.02
Thickness (mm)	1.5	1.5	1.6

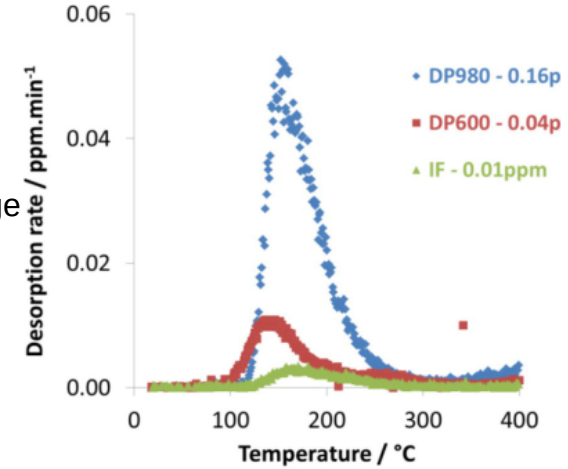


Figure 19: Diffusible H-content in different steel grades afte typical continuous annealing process.

Georges SAE Int. J. Mater. Manf. 9(2), 2016

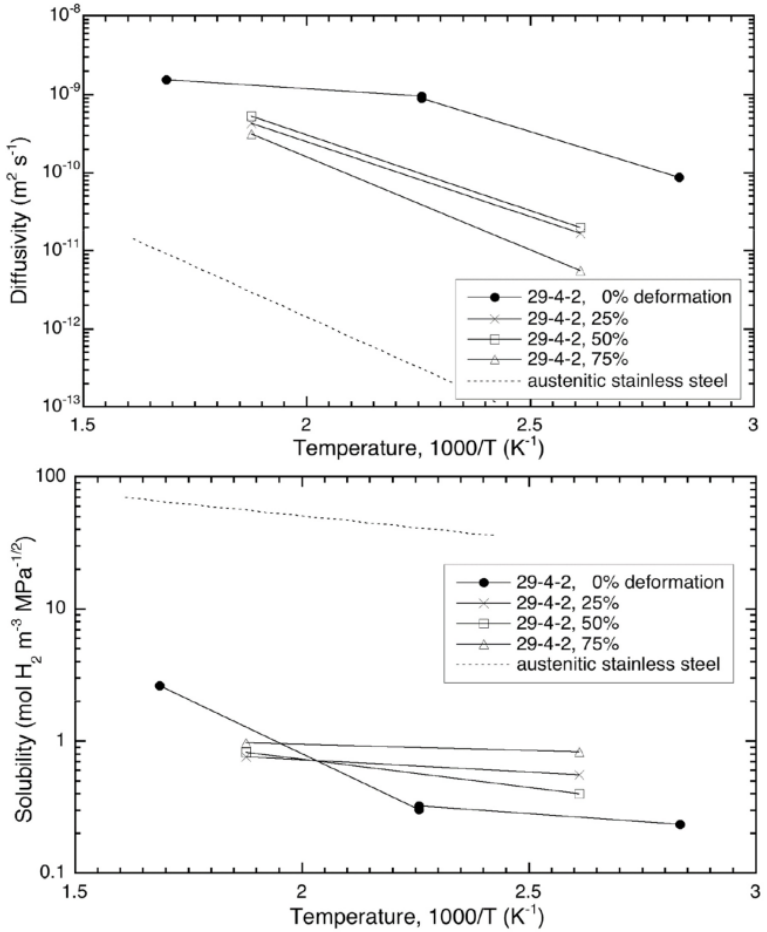


Figure 13: Diffusivity (top) and Solubility (bottom) for austenitic stainless steel (dotted lines) and ferritic stainless steel (solid line with solid symbols (29-4-2, 0% deformation). Figures from p95 of [San Marchi 2012]. Data from [Perng 1986] and [Perng 1989]. The curves for 25%, 50% and 75% deformation can be ignored within the present context.

Hydrogen from steel

- ETT-WP2 Vacuum: Tata steel, VDL and Nikhef research beampipe ET
  - Austenetic steel : lower diffusion speed. Much higher initial hydrogen concentration – around 1.7 ppm weight for SS304
  - Mild steel – low Carbon content, high diffusion speed, and typically ~ 0.02 ppm weight dissolved.
  - Park paper: mild steel without firing has similar performance as fired stainless steel, around 10^{-13} mbar/(s cm^2)

- However detailed modeling needed to describe bake-out results: what for thin-walled pipes, what for baking cycles at moderate temperatures (350 deg. C)?

- With recombination-limited model it is possible to get qualitative agreement with data sets at different baking cycles

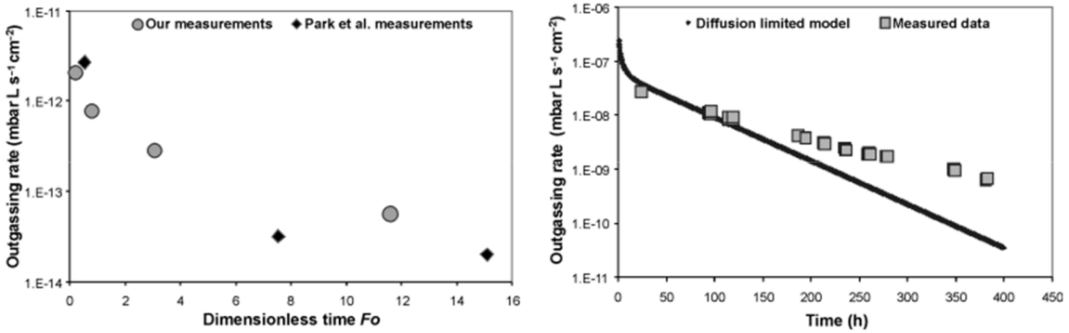
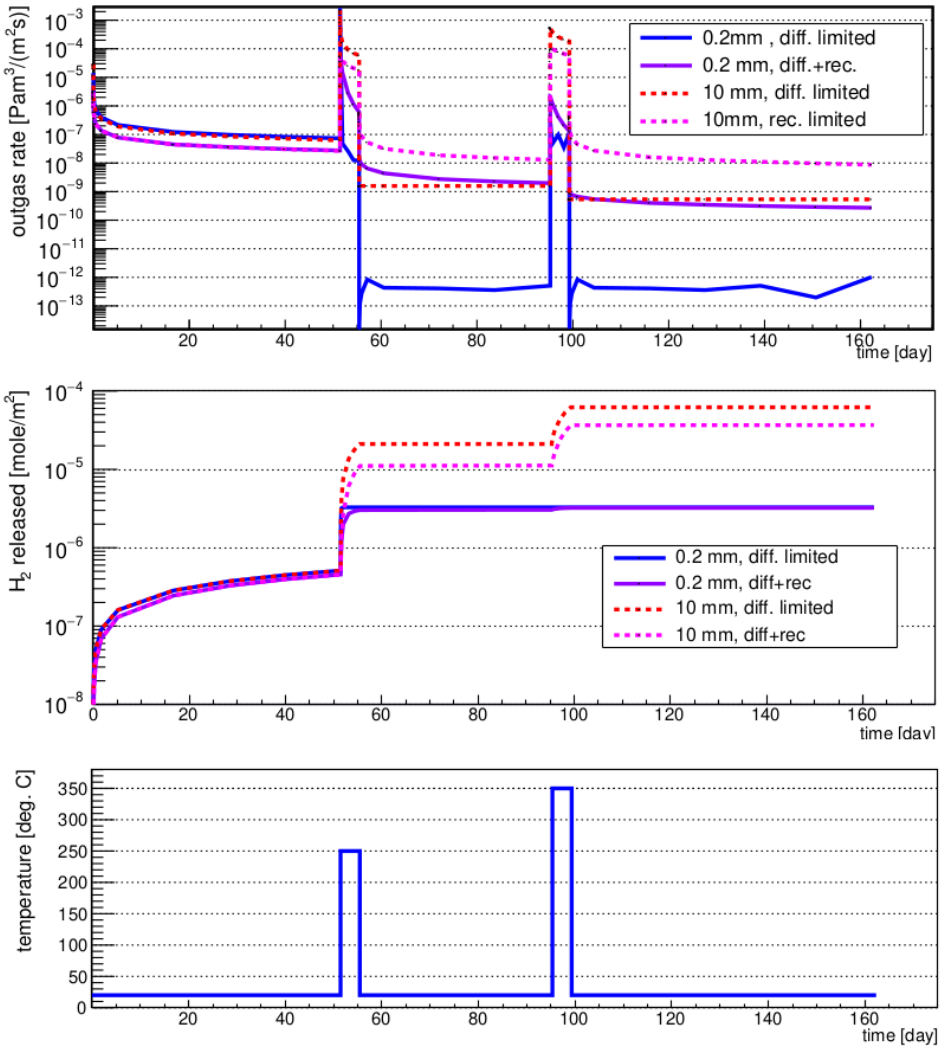
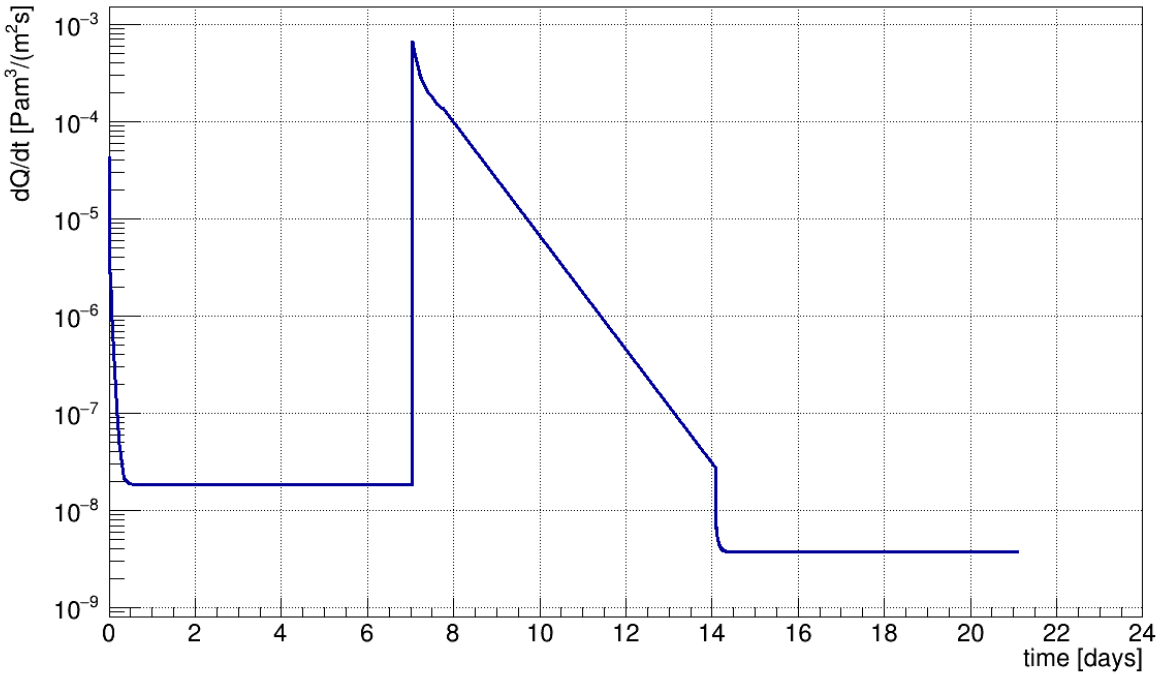


Figure 22: Observed outgassing rates from a stainless-steel chamber for different dimensionless pumping times F_0 (left) and outgassing rate as a function of time for a temperature of 250 °C (right). Figure from [Avdiaj 2012].



Hydrogen, mild steel or SS beampipe

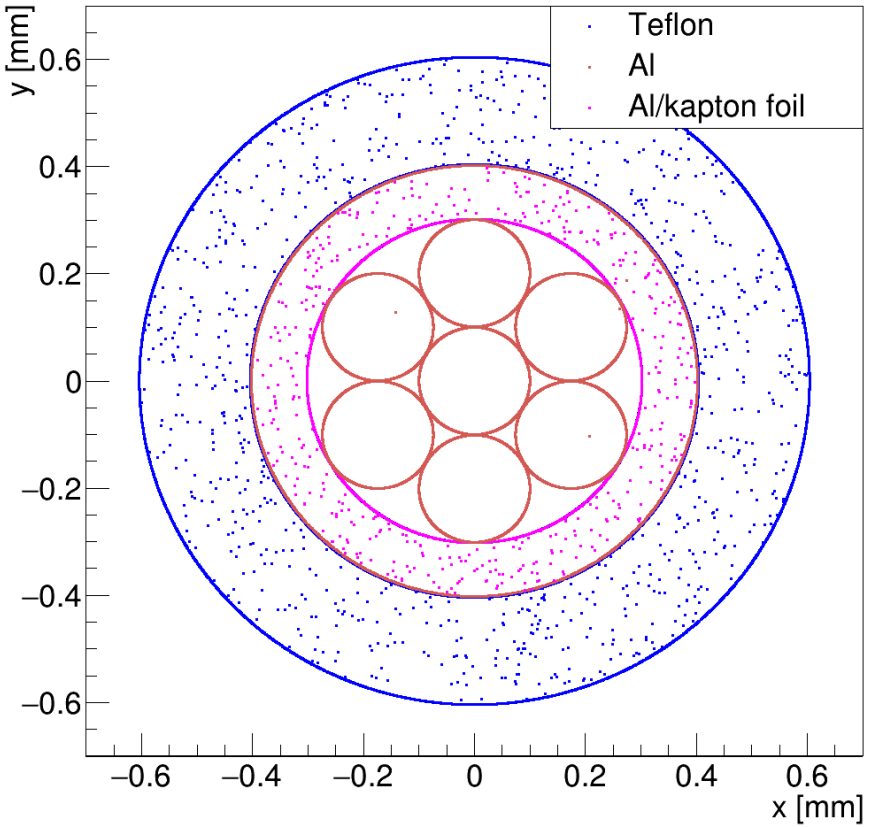
- Outgassing for fresh stainless steel, assuming a week bake-out at 250 deg: 3e-9 $Pam^3/(m^2s)$
- Conductance of a 250 long cylinder with 1 m diameter for hydrogen at room temperature: 1900 l/s
- Leads for unfired SS to about 1e-8 Pa; too high
  - Either vacuum-fire stainless steel
  - Or increase pumping speed
    - NEG coating every 50 m or so
  - Or make a very thin beampipe (dual system)
  - Or use mild steel



Example: Teflon-coated wire

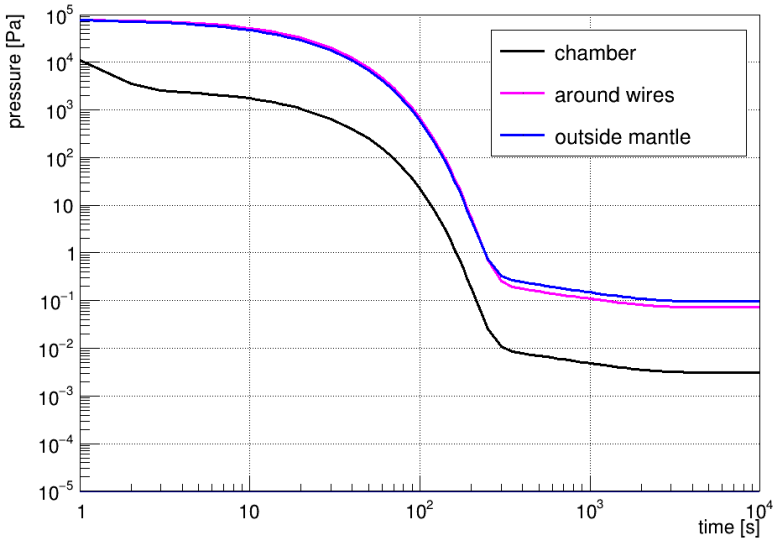
- Typical wire: multi-strand twisted pair, a polymer insulation around the strands, a ground layer around the pairs (e.g. DAK layer) and again a polymer insulation.
  - Gas, most notably H2O, is dissolved in the polymers (0.1-0.5% weight).
  - H2O adsorbed on the metal parts
  - Very little vacuum conductance
  - You want to know how the outgassing proceeds as a function of time and temperature, and also how quickly water adsorbs/dissolves into the cable when vented.
  - This should come from outgas measurements, but it is nice if your model can reproduce it

- Tracking calculated for 2m wire length. Average distance until pump and average amount of hits inside the wire scale with length-squared. Average track length around strands ~ 55 micrometer. Average track length between ground mantle and shielding 10 micrometer (equal to gap)



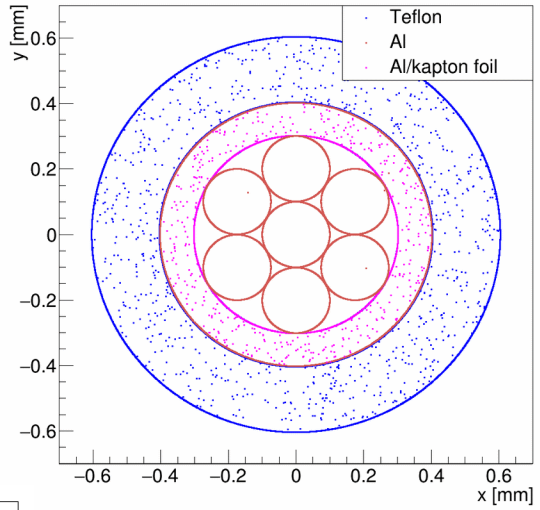
Wire: strands have 0.1mm diameter, distance between strands/mantle 0.01mm, distance between ground layer and outer insulation 0.01.mm
On average a molecule starting from a strand hits 16million times before exiting the wire at the end, a molecule starting between ground layer and outer insulation hits 235 million times.

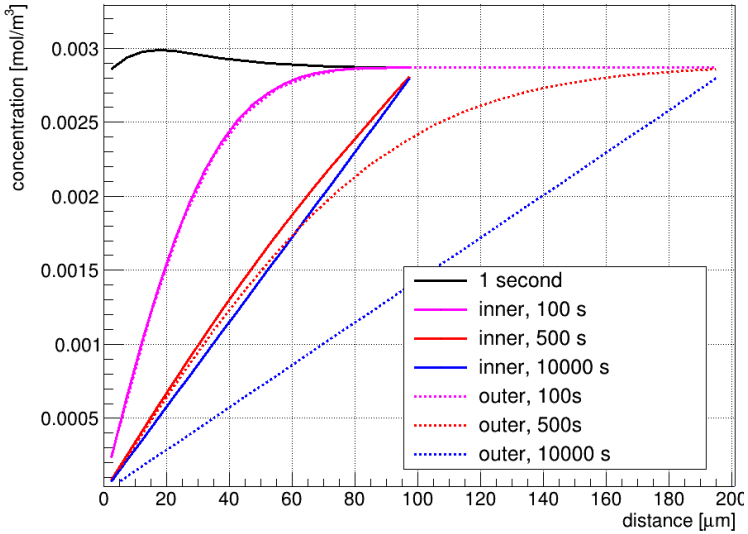
Example: Teflon-coated wire

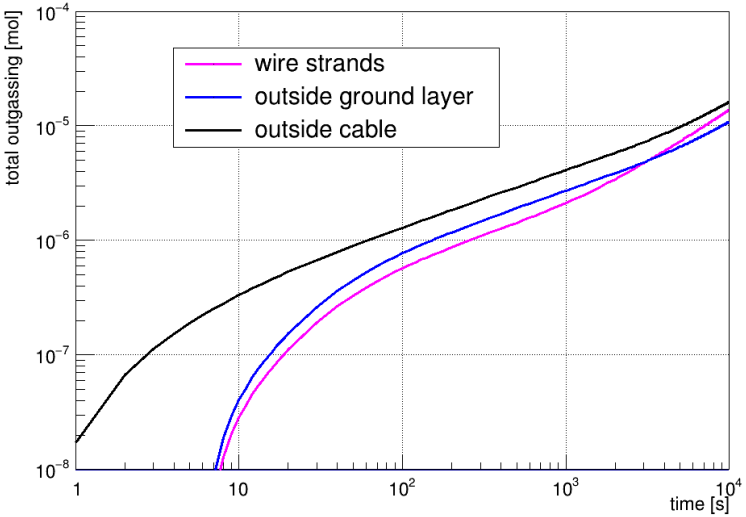


Pressure (left), concentration in wire isolation (bottom left) and net desorption (bottom right) of Nitrogen from 2 m of cable, starting with a cable that had been in air for a long time.

The pressure in the chamber is a complicated function of time. Water outgassing decreases much less rapid in time, since a monolayer of water can bind on the mantle and wire strands; water dissolves easier in the Teflon coating.







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summary

- Vacrysim – vacuum and cryogenic modeling
  - Divides tracking from time evolution – saves time
  - Exact coverage of pre-defined shapes – much less elements so better speed
  - 6th-order Runge Kutta – faster in time evolution
    - Can still be problematic
  - Includes different models for scattering, adsorption, dissolved gases
  - Can give detailed predictions for cool-down curves, accumulated gas/ice layers, etc

Our aim for Etpathfinder is to test this model: include data for materials and composite objects, e.g. LVDTs, cables

- Measure outgasssing as a function of temperature in an outgas chamber
- Expose to air for a week, repeat
- Try to characterize what happens with a mild bake, and with venting.

- Code is documented and in git – can be distributed if someone has interest
  - Still materials need to be added, and some tuning to be done on the time integrations

- I am also willing to perform calculations for the community (henkjan@nikhef.nl)