Xenon Acquisition at kTonne Scales: Challenges and R&D

Workshop on Xenon Detector $0\nu\beta\beta$ Searches:
Steps Towards the Kilotonne Scale

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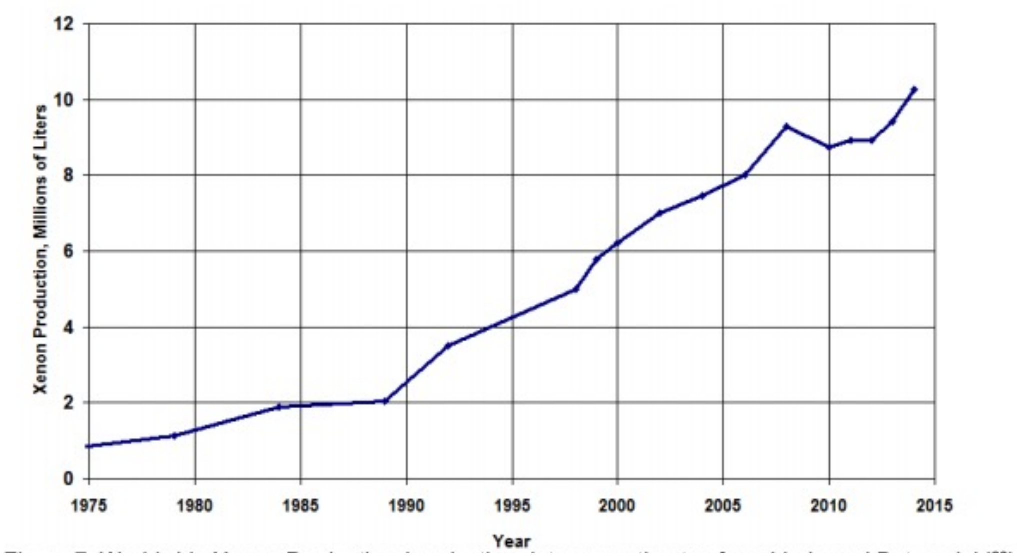
Xenon Global Production

- Xenon is extracted as a parasitic process from the oxygen sump of large air liquefaction plants (mostly for the steel industry)

- About 50-100 tonnes/yr of xenon is produced worldwide
  - Sufficient for upcoming $0\nu\beta\beta$ and DM experiments

Xenon production is tightly coupled to oxygen extraction for steelmaking



From NASA Technical Report GRC-E-DAA-TN23198

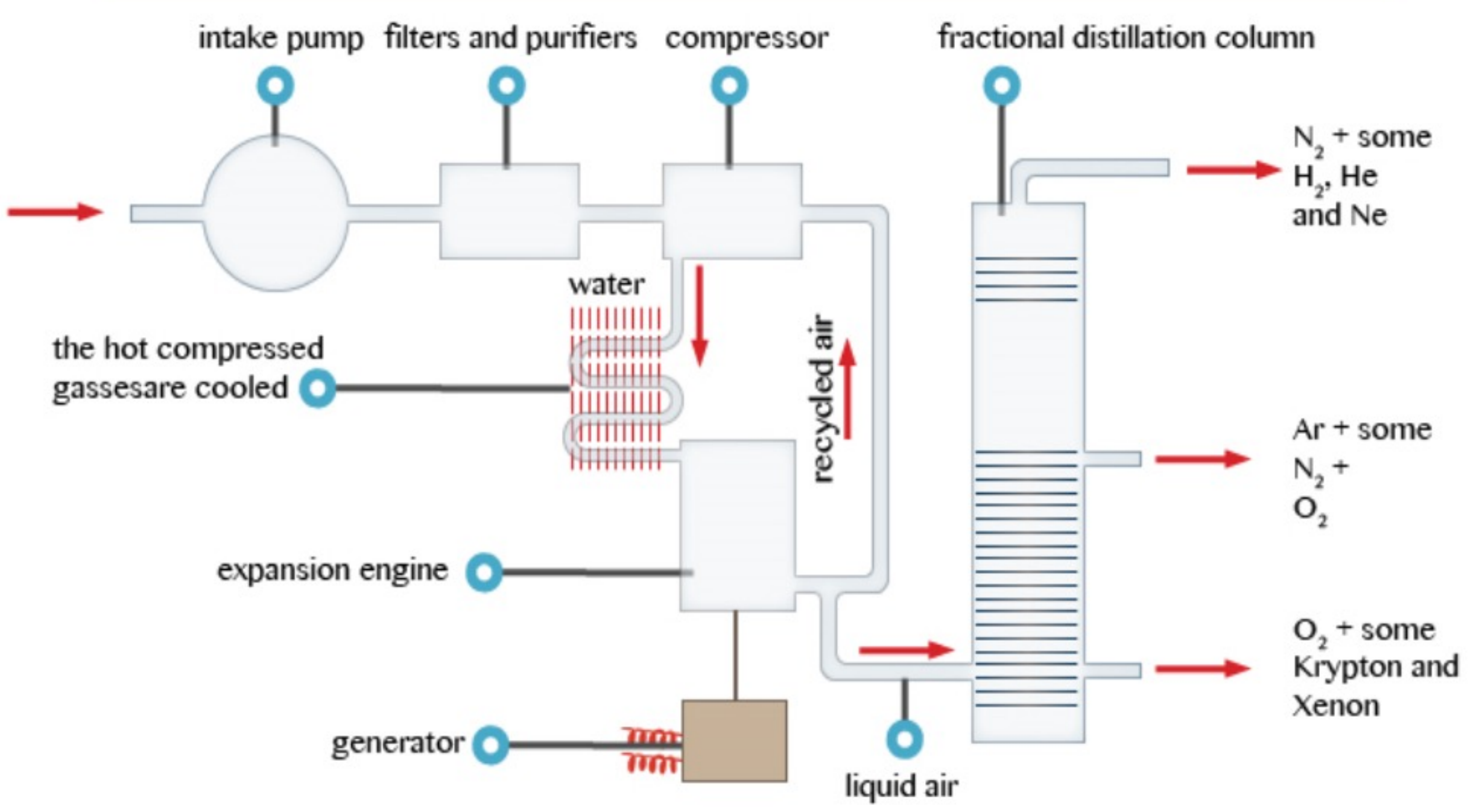
Linde Air Separation Unit in Hungary

Xenon from Cryogenic Distillation

- Commercial air separation via cryogenic distillation
- Efficiency from large size
- Xenon as a byproduct together with other rarer gases

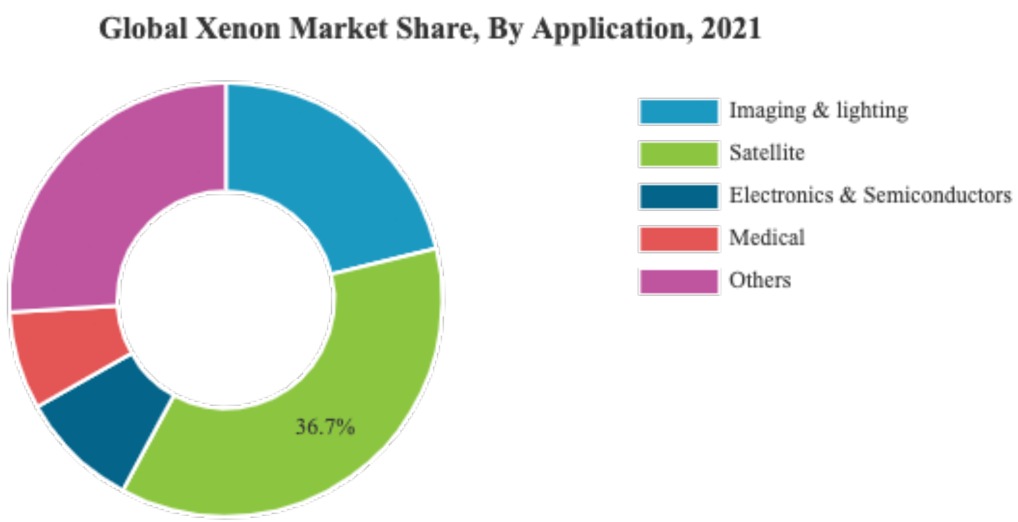
- Cost subsidized:
  - Energy cost to for a plant is around 250 kW.h per gram of Xe
  - $12/g @ 0.05 $/kW.h
  - Compare to >$1/g cost of Xe

- Without the steel industry, xenon would be much more expensive with the current techniques



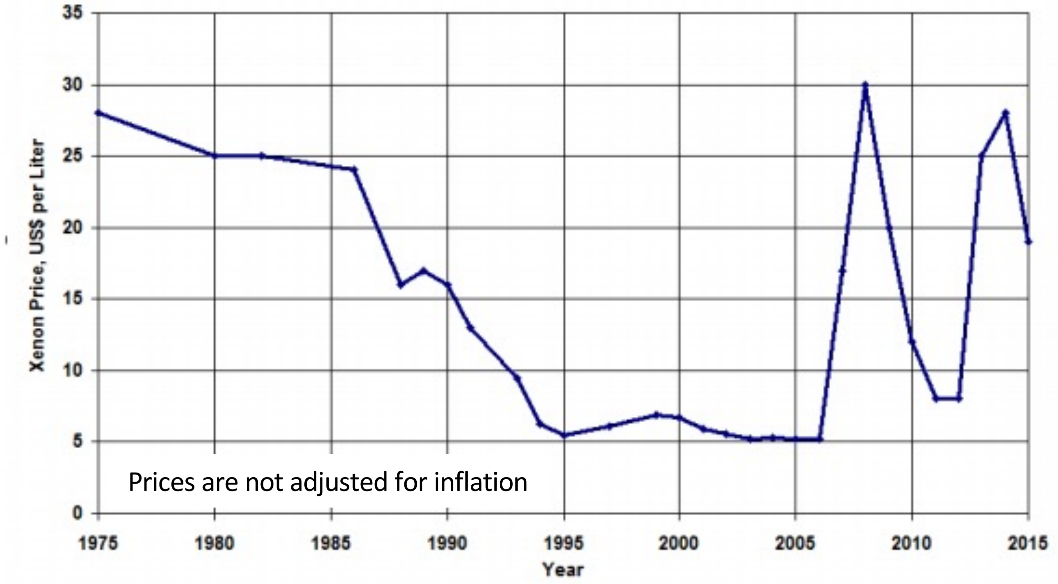
Xenon Global Market

- Cost and availability of xenon is governed somewhat by the steel market
- Inelastic supply
- The xenon market is tight and includes customers that are not price sensitive (aerospace, chip manufactures).
- High volatility



From Fortune Business Insights, Market Research Report, Oct 2023

Bulk Purchase Xenon Market Price



From NASA Technical Report GRC-E-DAA-TN23198

Is it possible to do better?

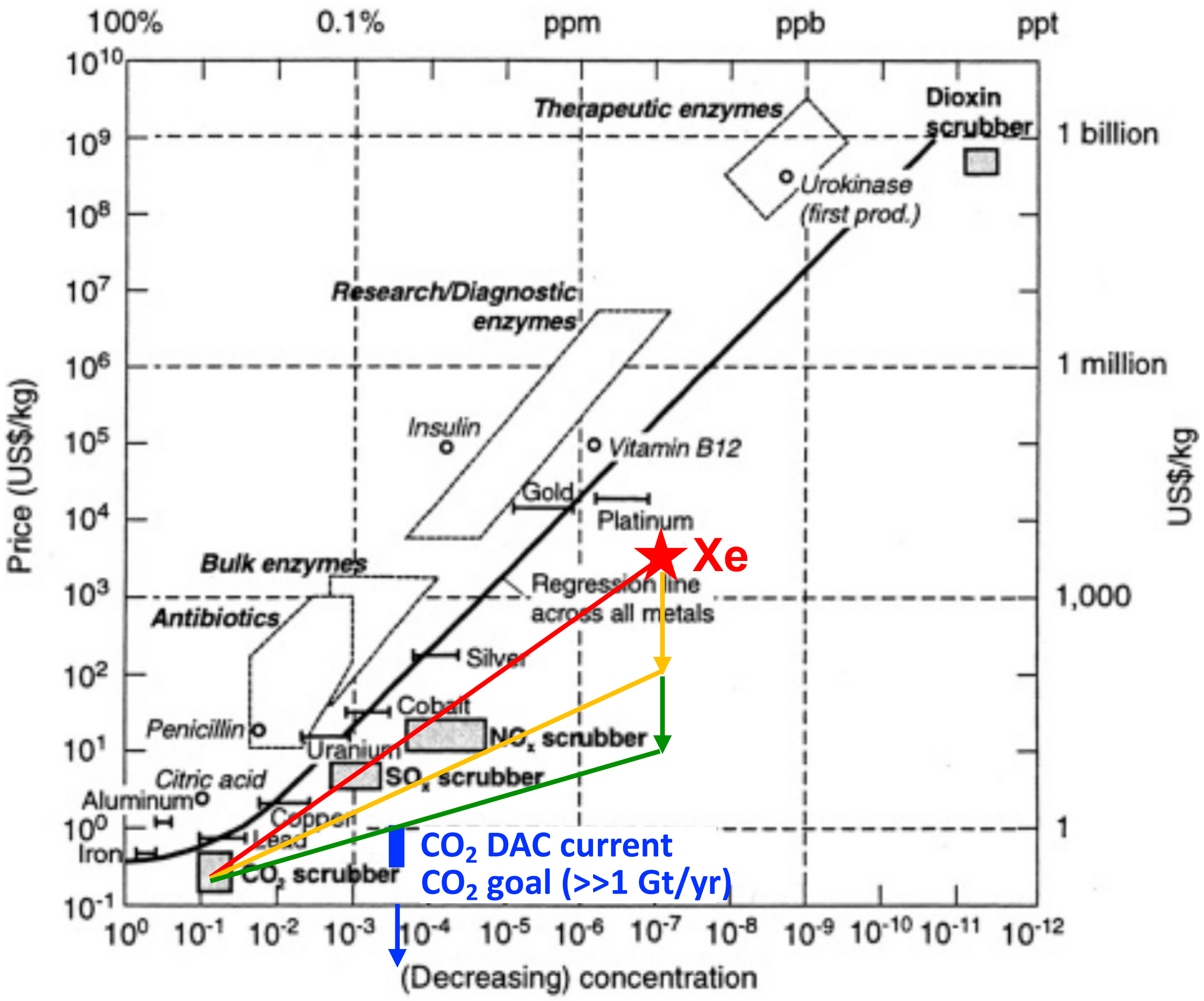
Thermodynamic minimum energy to separate xenon from air: 42.1 kJ/mol

Assuming 5 cents/kWh, that is only $0.004/kg

Methods to increase production and reduce cost would enable greater use of xenon.

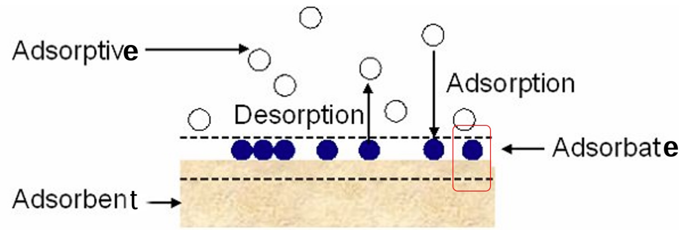
The current production methods are constrained, but there is no fundamental limit to increasing availability by orders of magnitude.

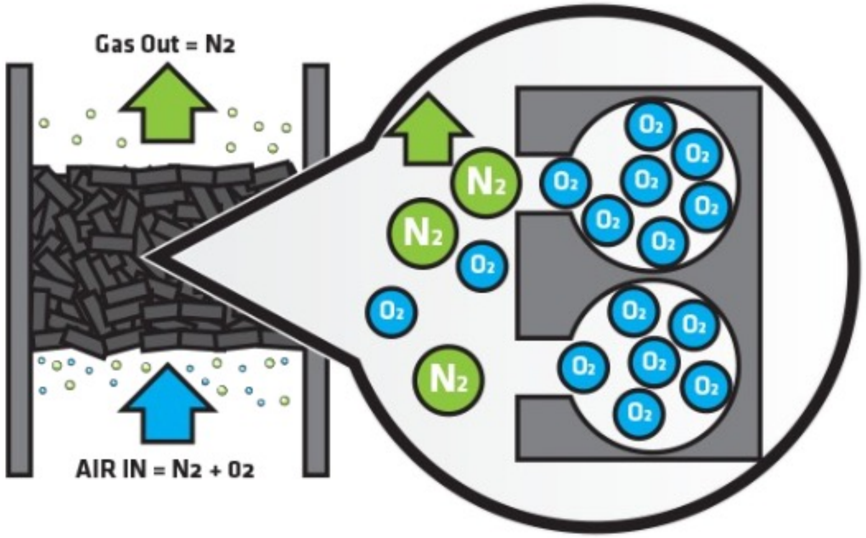
Sherwood plot (separation cost vs concentration)



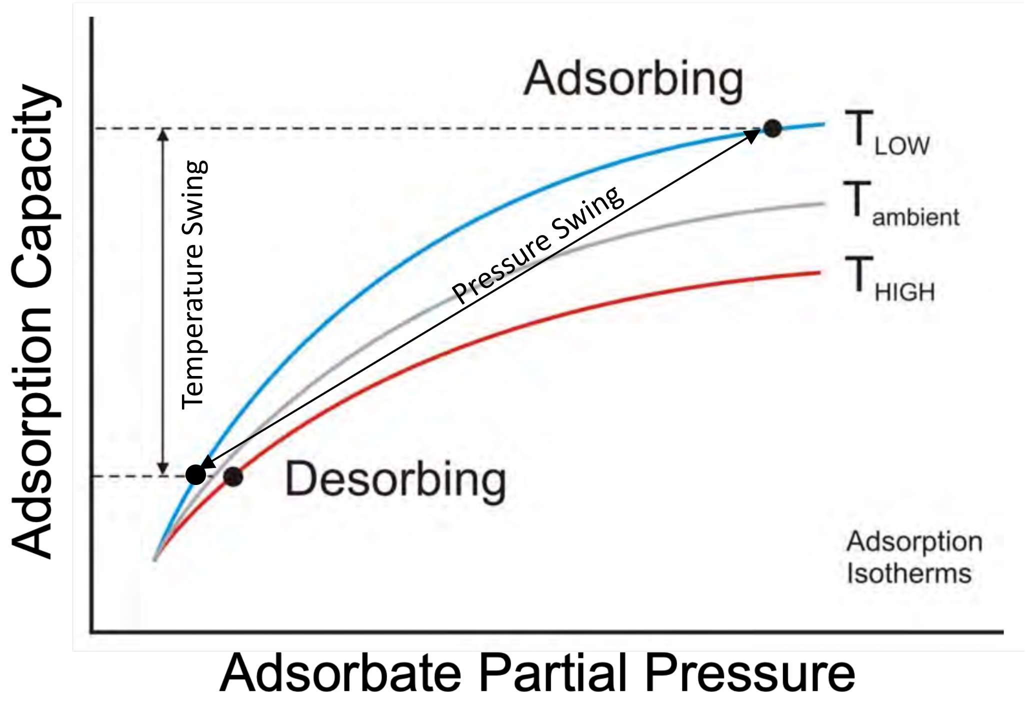
Alternative Noble-Gas Air-Separation Technique

Adsorption processes: gas sticks to the surface of the adsorbent



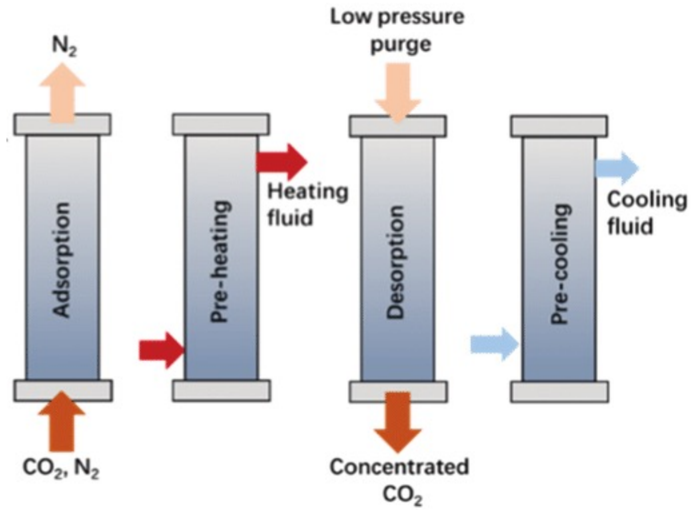


Swing adsorption processes

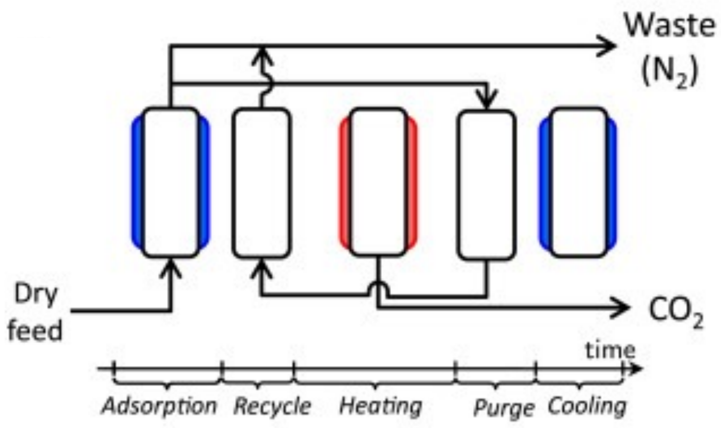


Swing Adsorption Processes

Basic TSA Process Cycle



Complex Multi-step multi-bed process cycle



Pressure swing adsorption requires significant energy

- 1 g of Xe in ~2.5 tonne of air at 100% efficiency
- 1 psi isothermal compression ~ 5 J/g
- 3.4 kWh @ 0.05 $/kWh = ~0.17 $/g of Xe

Temperature swing adsorption can be more efficient

- Use low-grade heating
- Cost of moving air (see later)

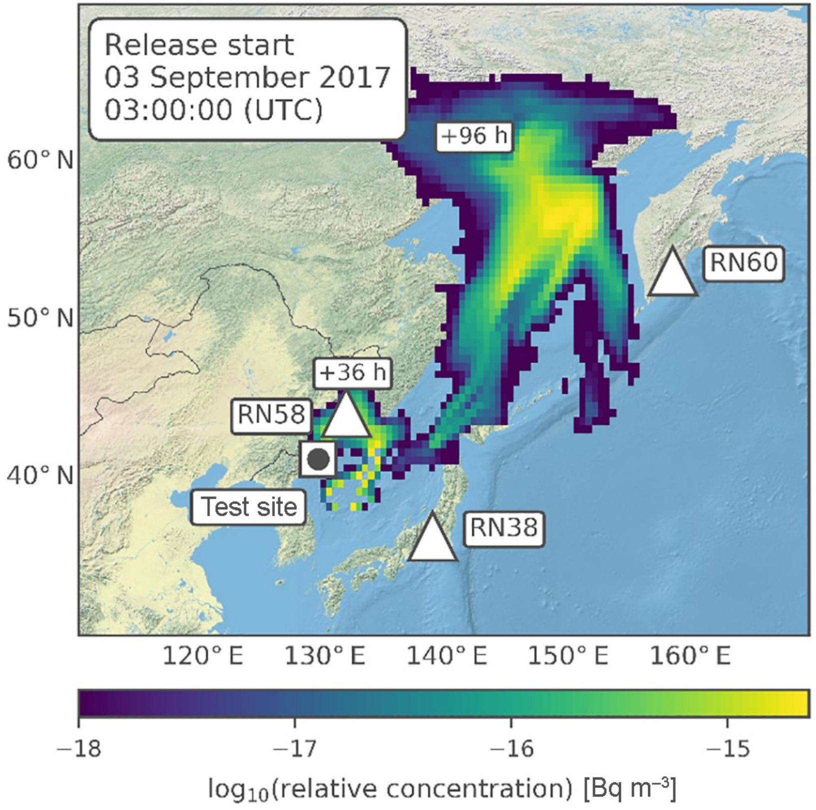
Complicating factors:

- Gas pre-processing (e.g. to remove H_2O)
- Multi-step / multi-bed
- Reflux
- …

Radioxenon Collection Devices

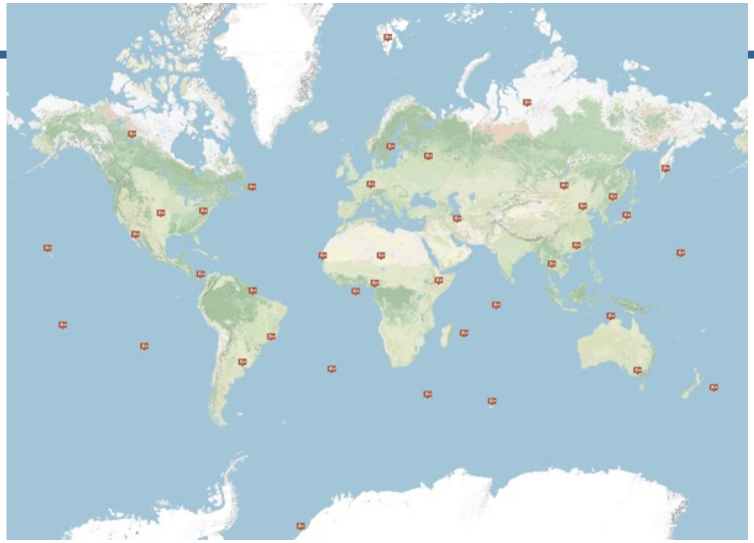
- Radioxenon is a highly-specific telltale of nuclear explosions
- Support of CTBTO mission

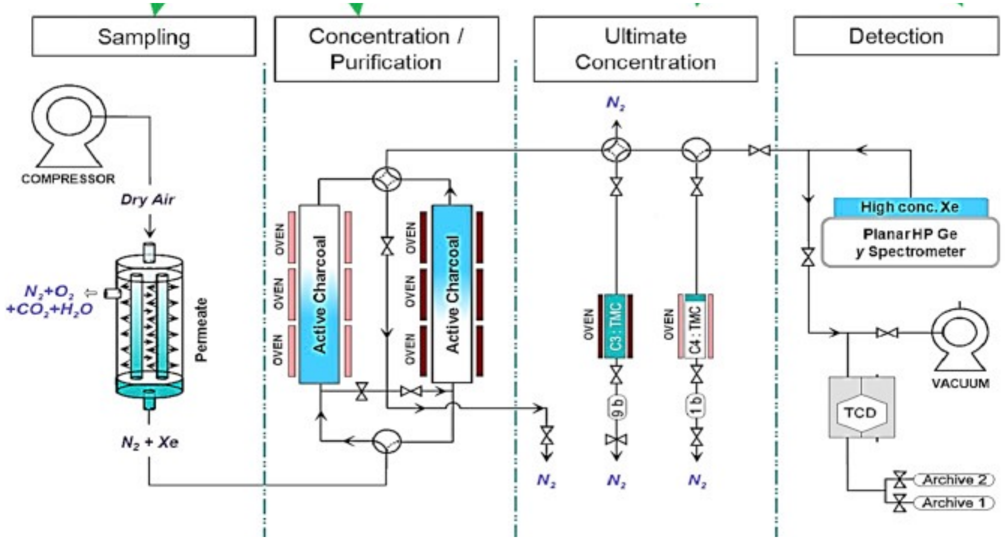
Simulation of RXe transport in the atmosphere following the 2017 DPRK Nuclear Test



From https://doi.org/10.5194/se-10-59-2019

Noble-gas stations around the world as part of CTBTO's International Monitoring System





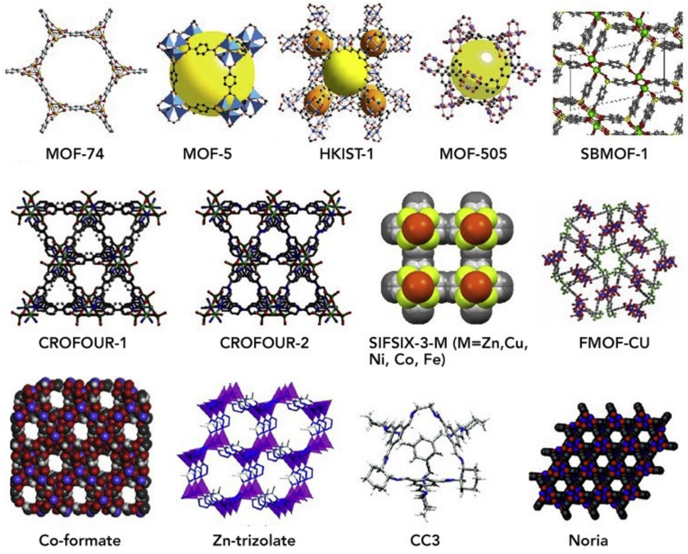
From https://doi.org/10.1016/j.jenvrad.2015.06.027.

Proof-of-principle of xe separation via adsorption

Recent Enabling Technologies

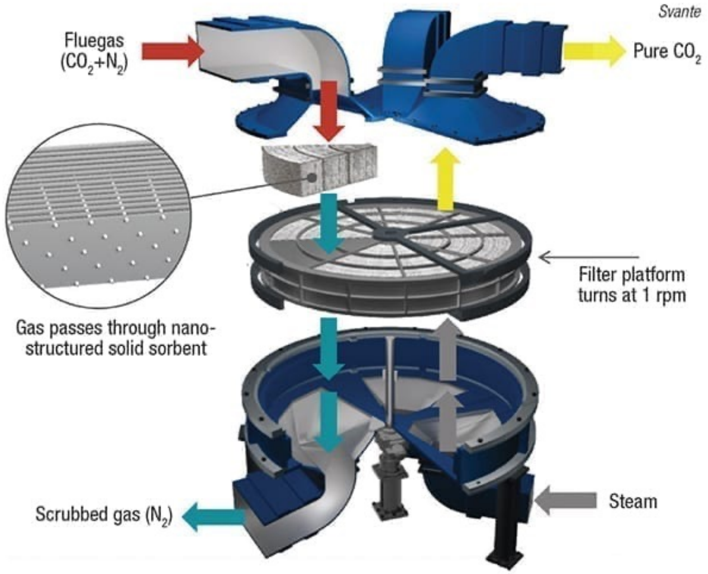
- Recent advancements in gas adsorption technology
  - Novel Adsorbent Materials
  - Structured Adsorbent Beds
  - Advanced Adsorption Cycles
- Significant expertise in the industry sector, less so in academia

Metal-Organic-Frameworks for Xe adsorption



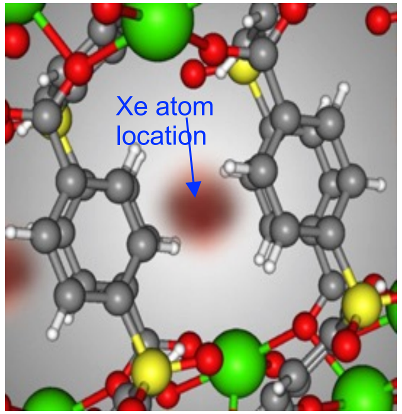
Banerjee, et al, Chem 4, (2018) 466

Example: CO_2 capture by Svante, Inc



Example: oxygen concentrators

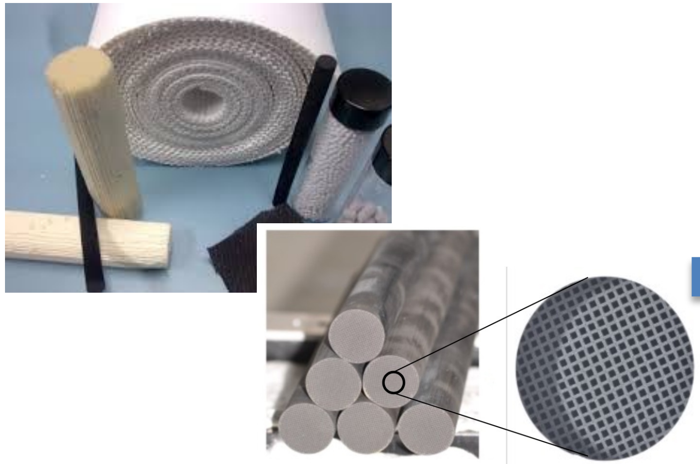
Ingredients for a new Xenon DAC Technology



Highly-selective, stable Xe-adsorbing material

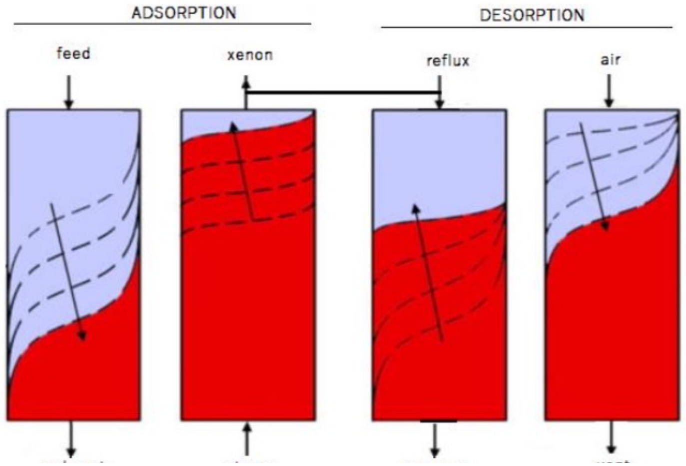
- Metal-organic-Frameworks
- Multiple options available, currently focusing on Ca-based MOF called SBMOF-1

→ See Noelle's talk



Embedded into a structured adsorbent

- Low pressure drop and high mass transfer coefficient



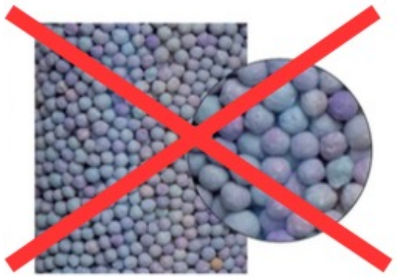
Rapid Intensified Temperature Swing Adsorption (TSA) Cycle

- Adapted from successful CO_2 capture solution

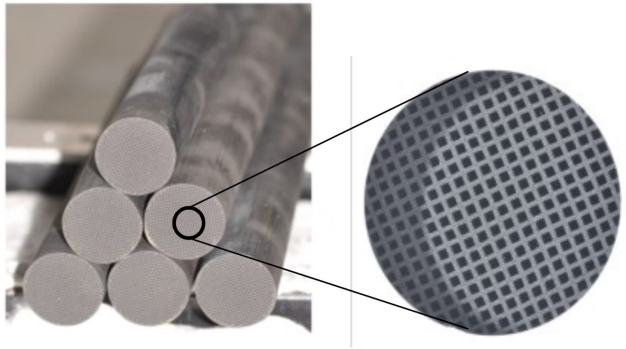
Structured Adsorbents

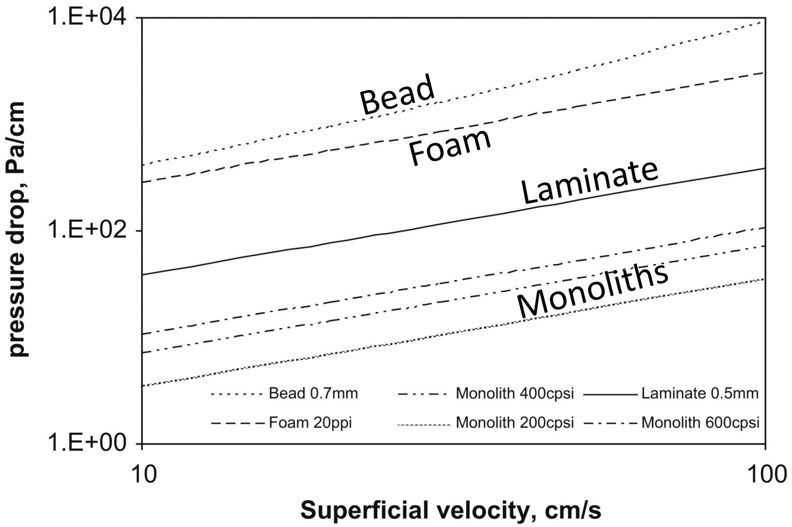
- Typical packed bed incurs high pressure drop
- Structured bed:
  - x10-100 smaller dP than packed beds
  - High surface area/volume, short diffusion, high mass transfer coeff
  - Avoid bed fluidification issues
  - More complicated to build and model

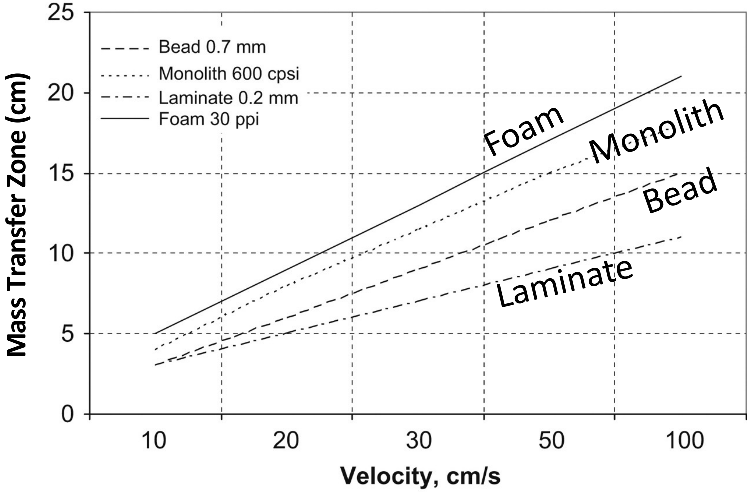
Packed bed



Variety of structured adsorbents





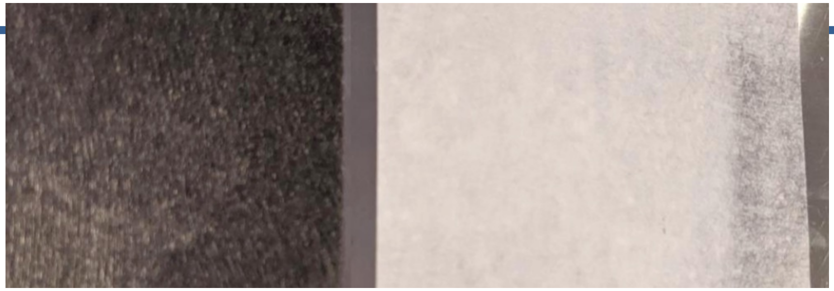


Plots from F. Rezaei, P. Webley, Chem. Eng. Sci., 64 (2009)

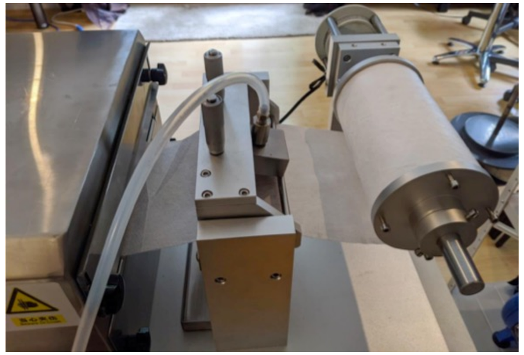
Structured Adsorbent Development

- Successfully prototyped a solutions for laminate adsorbents based on SBMOF-1
- Coating of carbon fiber foil with MOF-loaded slurry (90% MOF, 10% binder)
  - Large area samples produced
- Verified uptake performance of coated sample
- Ongoing:
  - Full-bed performance characterization

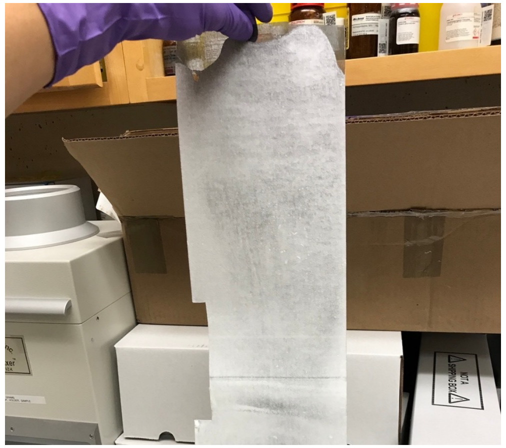
Carbon-fiber substrate | Coated with SBMOF-1



Coating line



Large area sample of SBMOF-1 coated adsorbent foil



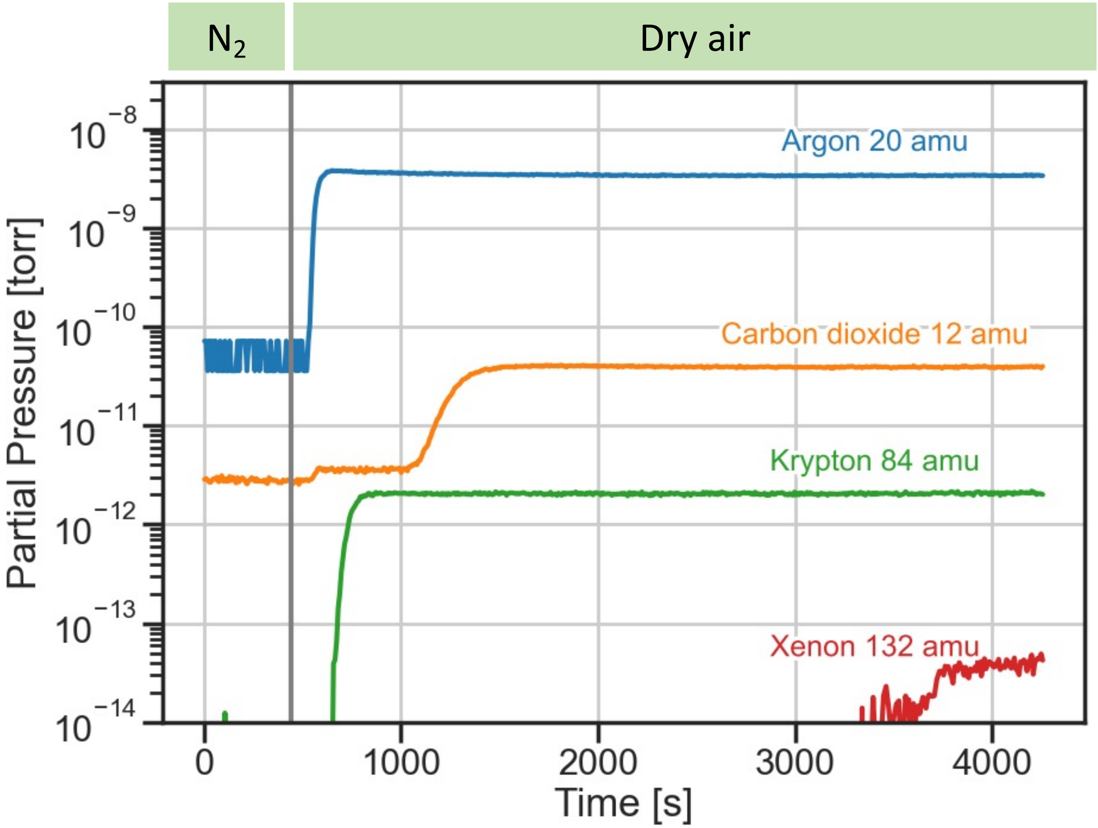
Full-size laminate adsorbent bed with SBMOF-1 adsorbent

Characterization and Testing Station

- Dedicated test setup for automated and reproducible breakthrough curve measurements
- Sensitivity to Xe
- Ability to replicate process steps

LLNL high-sensitivity adsorption testbed

Breakthrough curve with an activated charcoal adsorption bed

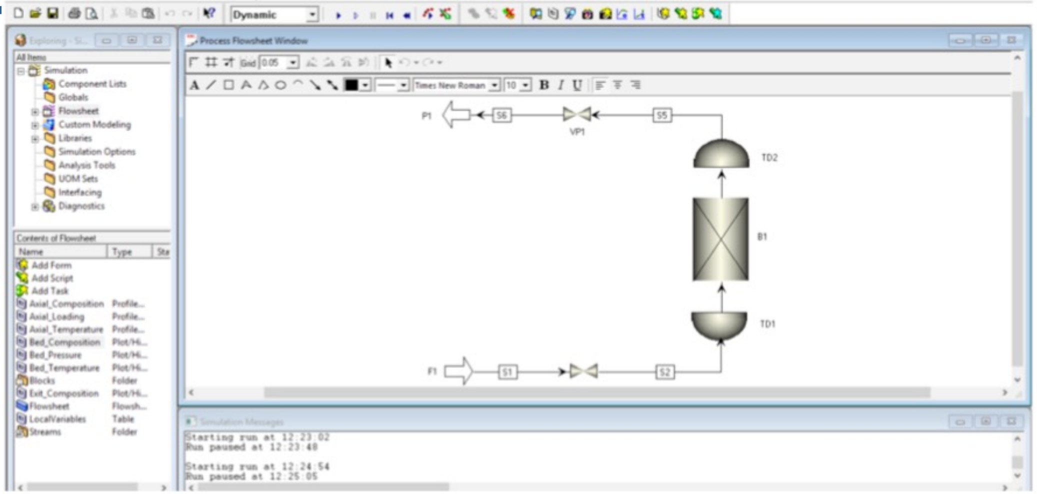


Adsorption Cycle Modeling

- Worked with industry partner to apply their proprietary rapid intensified adsorption cycle to SBMOF-1 laminates for xenon capture from air
- Promising results obtained using ASPEN process modeling software

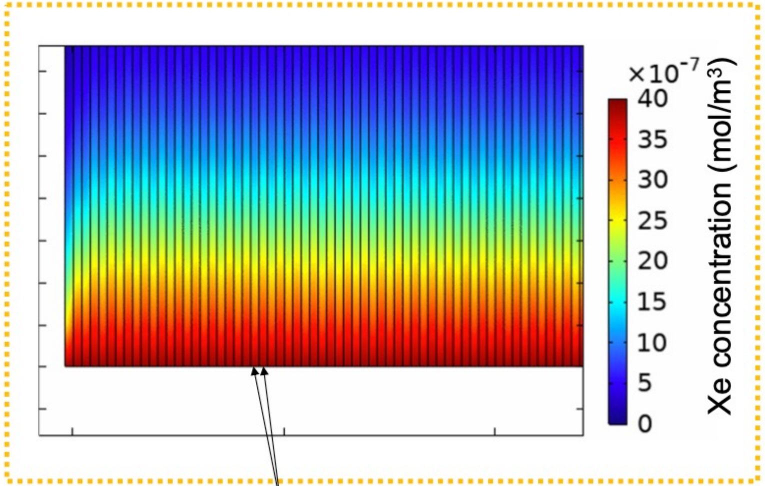
- Ongoing development of COMSOL-based model @ Yale
  - Deeper understanding of the process
  - Validation in progress

Finite element method customized ASPEN model of adsorption process dynamics



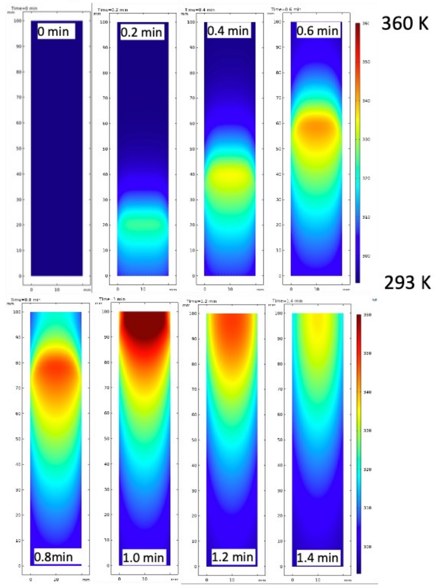
Initial results from COMSOL model

Zoom of concentration vs position (*t* = 6 s):



0.2 mm alternating adsorbent sheets and slots

Temperature profile vs time:



Synergies with CO_2 DAC?

Let's assume perfect efficiency…

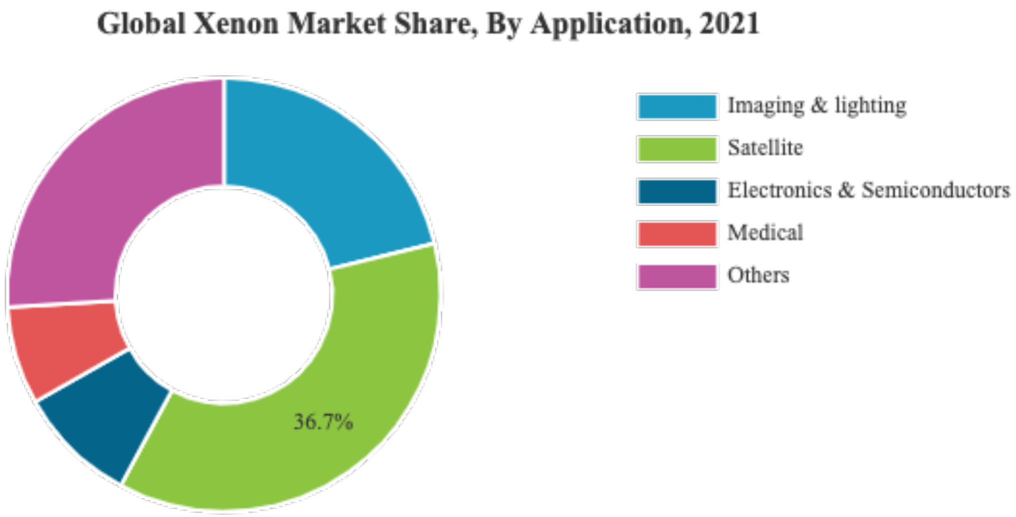
Largest CO_2 DAC plant ~ 4 ktonne CO_2/y
which means moving 8.5 km^3/y of air
(for scale this is ~8000 the volume of the Empire State Building processed per year)

Plants with capacity > 250 ktonne CO_2/y are under construction

To meet climate change goals, goal is to remove 5 - 10 x 10^6 ktonne CO_2/y!

For comparison, to obtain 1 kton of Xe in 10 years requires moving 330 km^3/y of air or the equivalent air of ~150 ktonne CO_2/y
(i.e. almost 1 Empire State Building/min)

Applications that benefits from cheaper & larger Xe supply



From Fortune Business Insights, Market Research Report, Oct 2023

- Several applications, many growing
- Potential for partnership with industry
- Considerations for “storage” of xenon in a underground physics facility
- Coordination across different gov agencies unlikely

Aerospace Industry

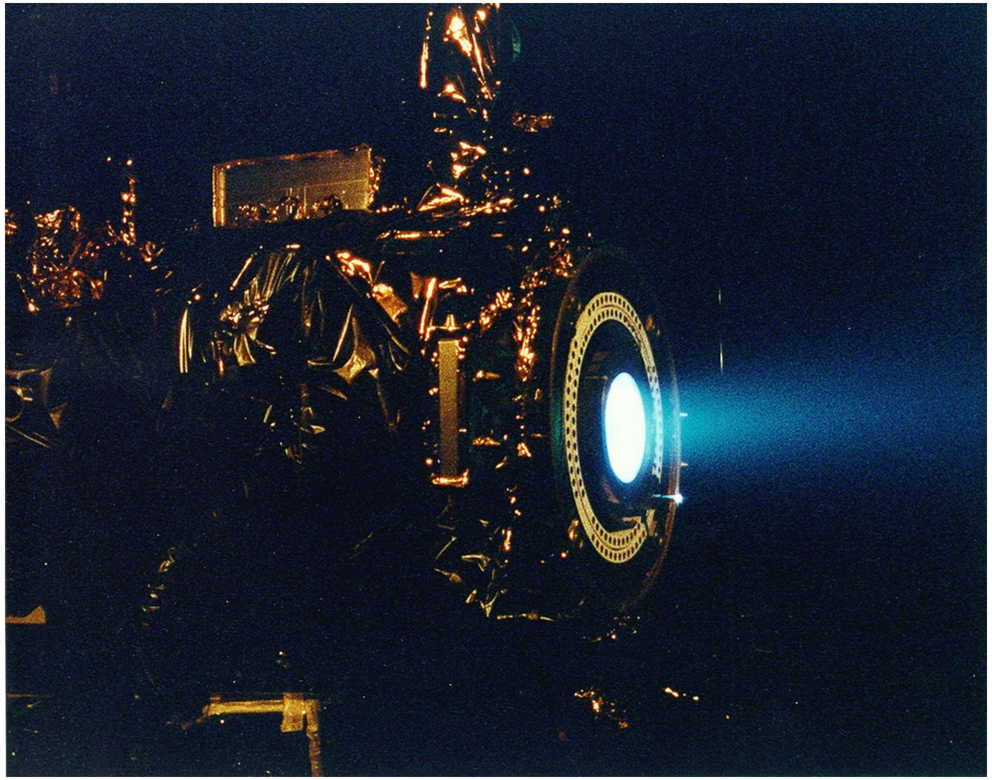
The primary space application is Ion thrusters.
Xenon is the best propellant and these thrusters can produce much higher specific impulse than chemical systems, but at a lower instantaneous thrust.

Two areas that greatly benefit from these thrusters are:

- NASA deep space missions
- Satellite station keeping

Single mission xenon requirements vary from 100's of kg to 10 tonnes.

Large growth in recent years driven by commercial sector for satellite megaconstellations (think Starlink)



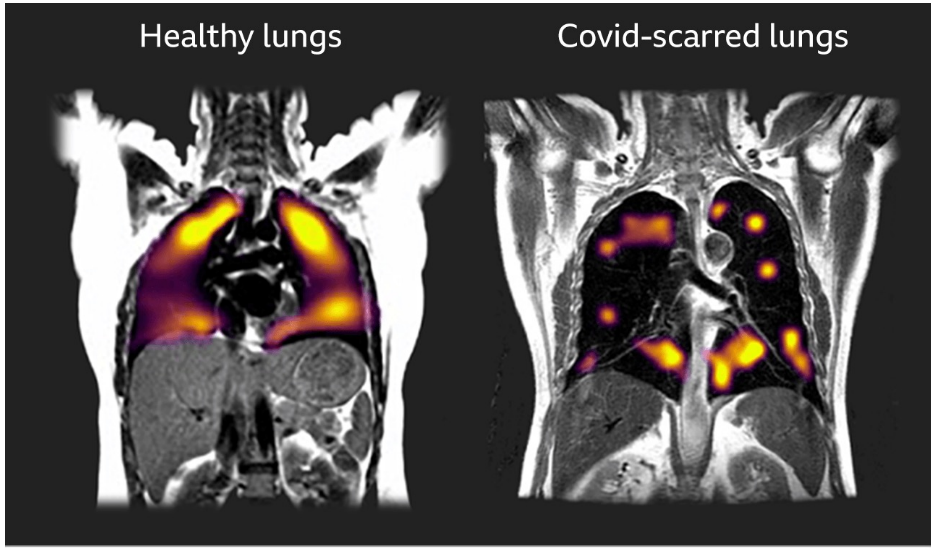
The 2.3 kW Xenon-based ion thruster of NASA's Deep Space 1 spacecraft

Application in Medicine

Xenon has been used as an effective and extremely safe general anesthetic, but it is not widespread due to availability and high cost.

Both natural Xenon and enriched Xenon is needed

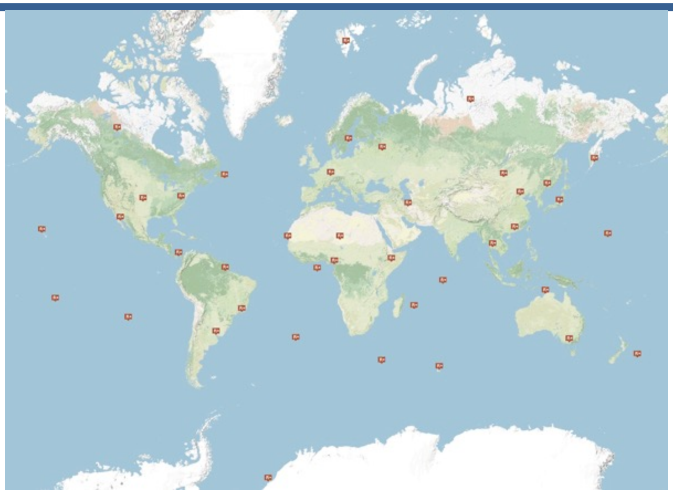
Hyperpolarized Xe-129 is an excellent contrast agent for magnetic resonance imaging (MRI), in particular for lungs studies



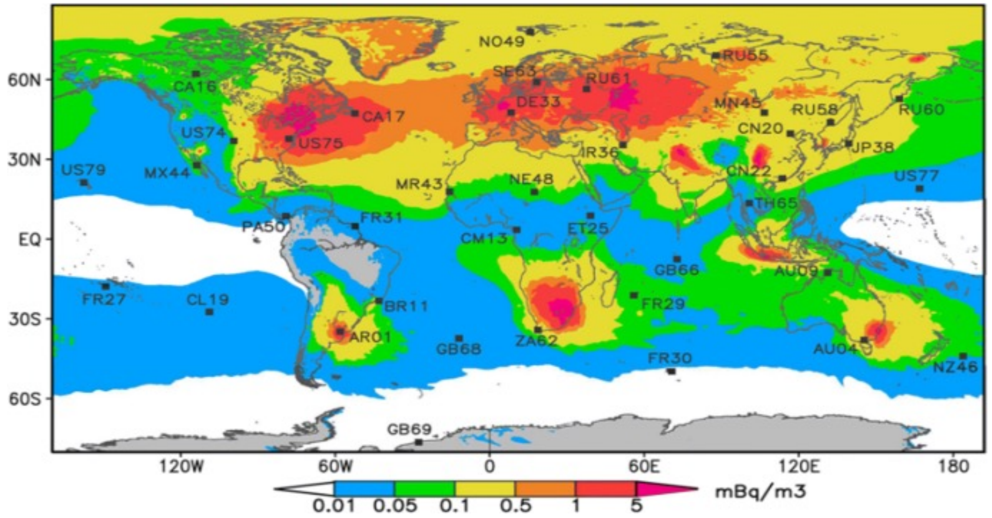
Source: Oxford University BBC

Specialized Nuclear Applications

- Radioxenon detection for nuclear explosion monitoring
- Reduction of radioxenon emission from man-made isotope production facilities
- Xe/Kr separation at nuclear reprocessing facilities



Radioxenon stations around the world track radioxenon as part of CTBT Nuclear Explosion Monitor programs



Average global concentration of Xe-133 from anthropogenic sources

(from Achim, P., et al. (2016), J. Geophys. Res. Atmos., 121, 4951)

Conclusions

- Current technology for Xe separation does not scale to meet the need of ORIGIN-X
- Swing adsorption technology using novel materials, structured adsorbents, and advanced cycles could be a viable alternative

- Promising initial efforts:
  - Development of a Xe-specific structured adsorbent
  - Ongoing modeling with measured adsorbent characteristics

- Key challenges:
  - Materials (scale-up, cost, stability, … >> see Noelle’s talk)
  - Process cycle efficiency
  - R&D Funding
  - Avoiding the innovation valley of death

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