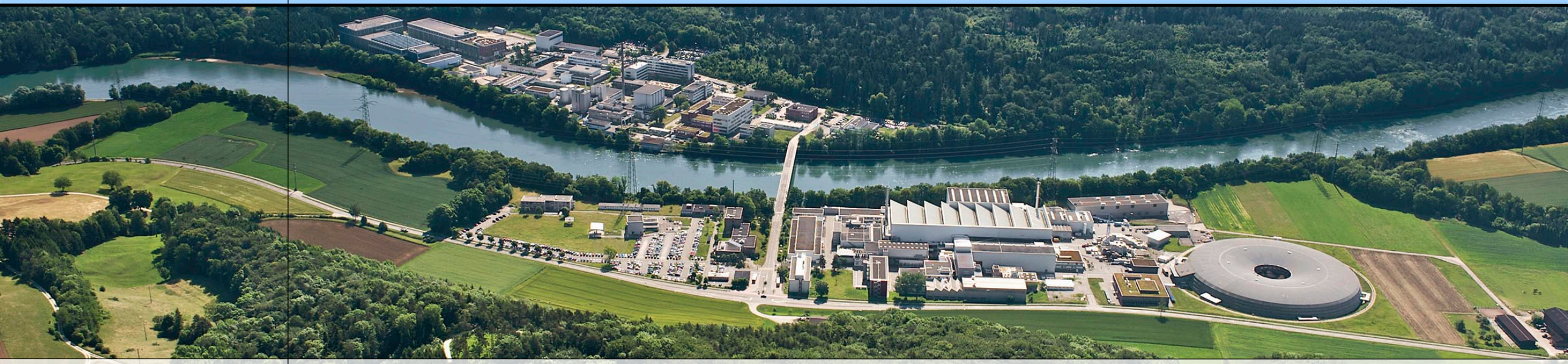
PAUL SCHERRER INSTITUT

PSI



Wir schaffen Wissen – heute für morgen

Paul Scherrer Institut

Thorsten Bartels-Rausch

Parameterizing Trace Gas - Ice Interactions

A look into laboratories

Thorsten Bartels-Rausch, Sepp Schreiber, Thomas Ulrich,
and Markus Ammann
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Adela Krepelova
Paul Scherrer Institut, Switzerland

Fabienne Riche and Martin Schneebeli
WSL Institute for Snow and Avalanche Research, Switzerland

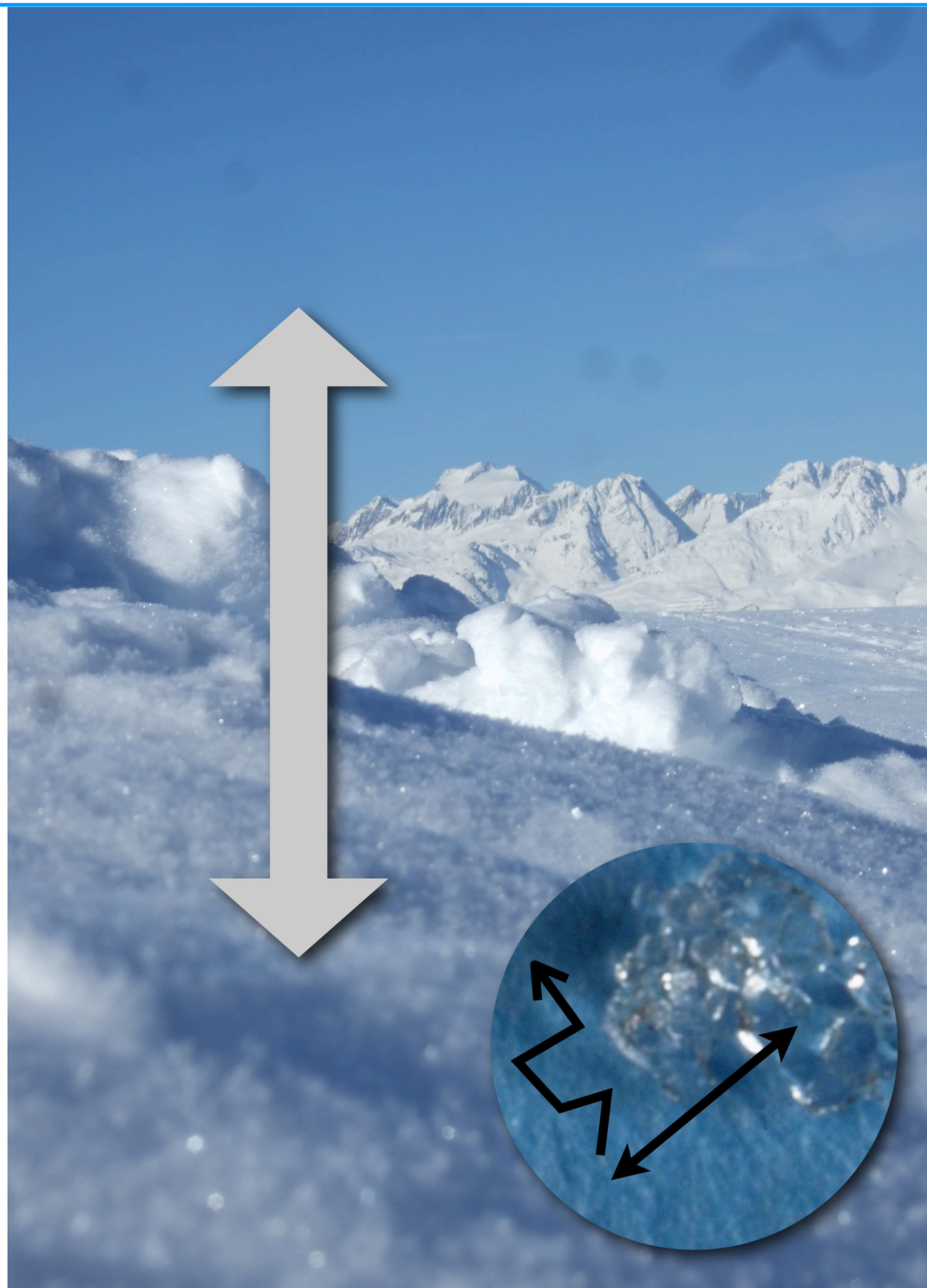
Sumi Wren
University of Toronto, Canada (research group of D.J. Donaldson)

Snow-Pack - Air Exchange

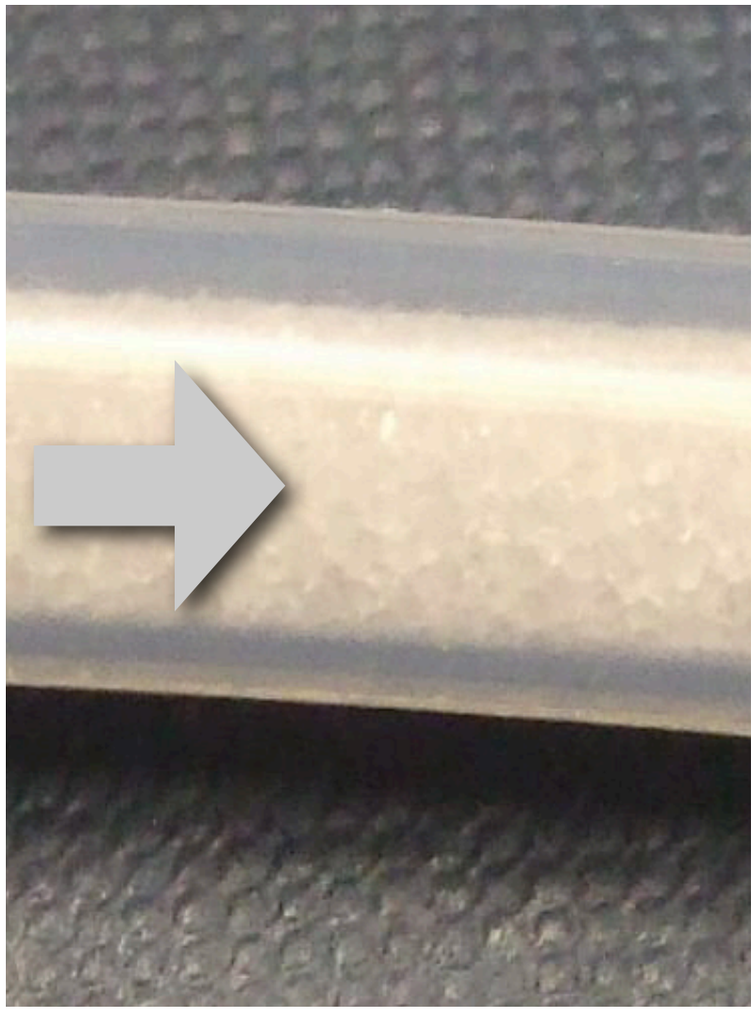
- turbulent transport

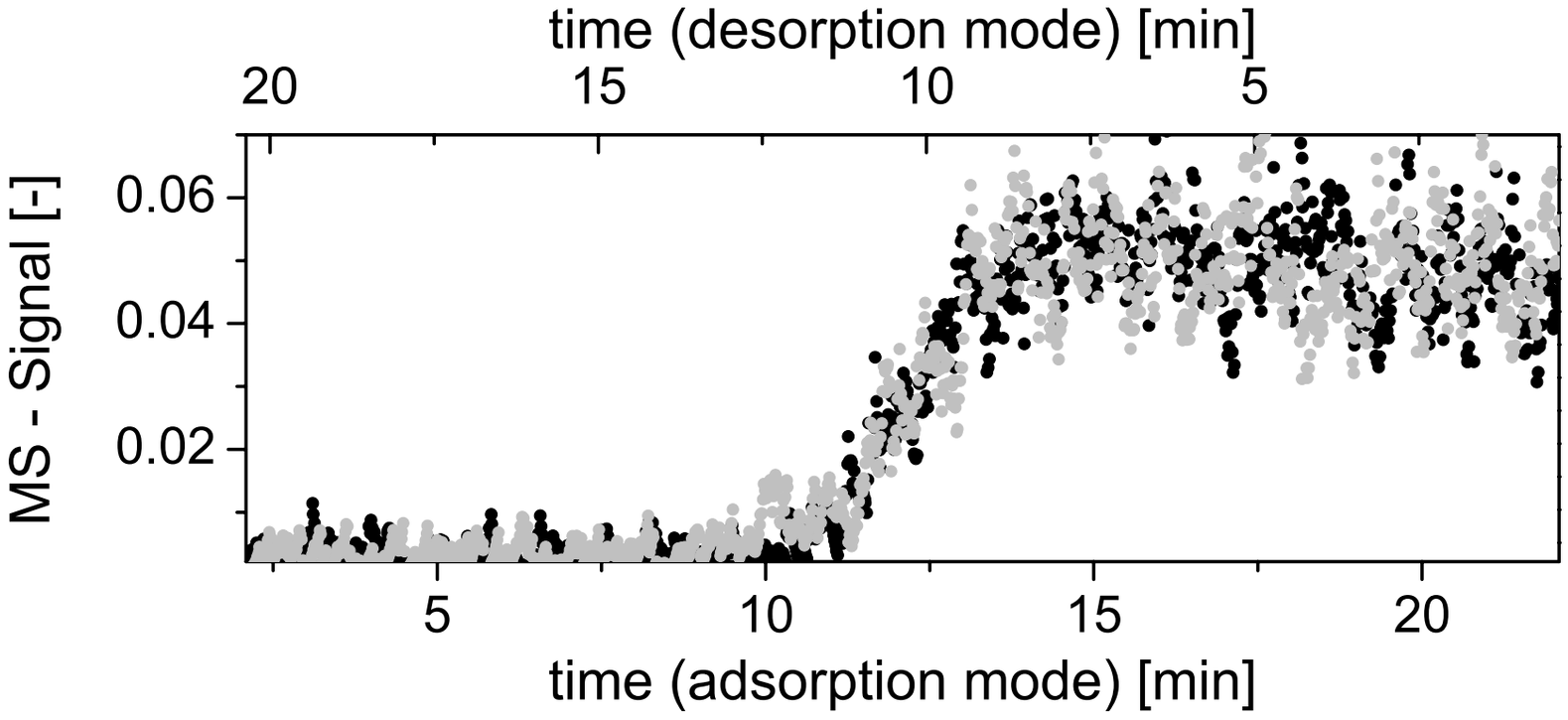
- wind pumping
- diffusion through porous media

- partitioning
- diffusion in gas phase
- diffusion into bulk,qll,etc



Lab Results: Partitioning of trace gases to ice surfaces

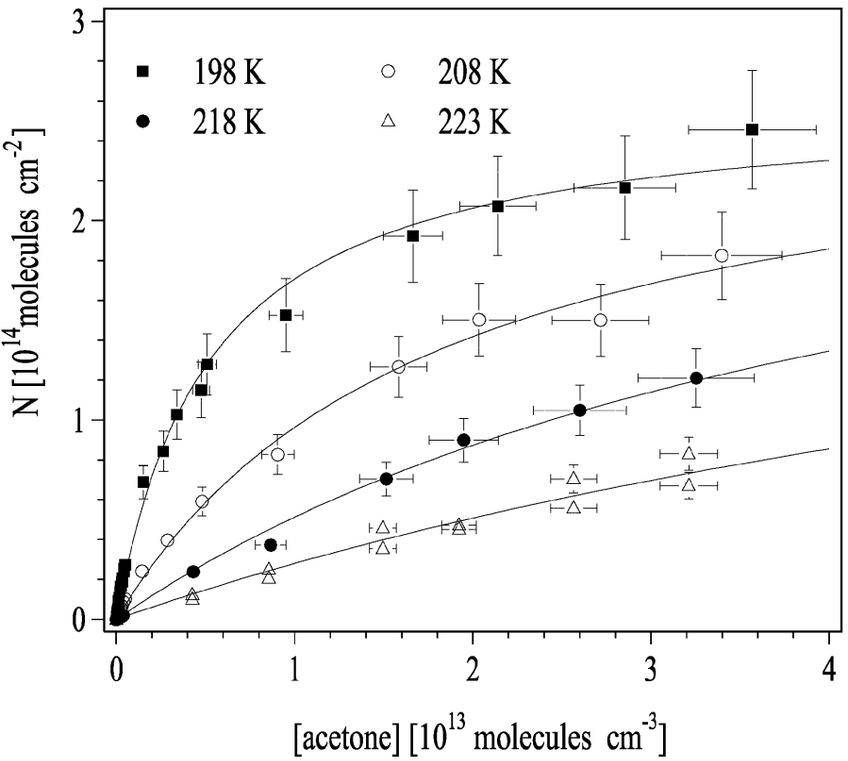


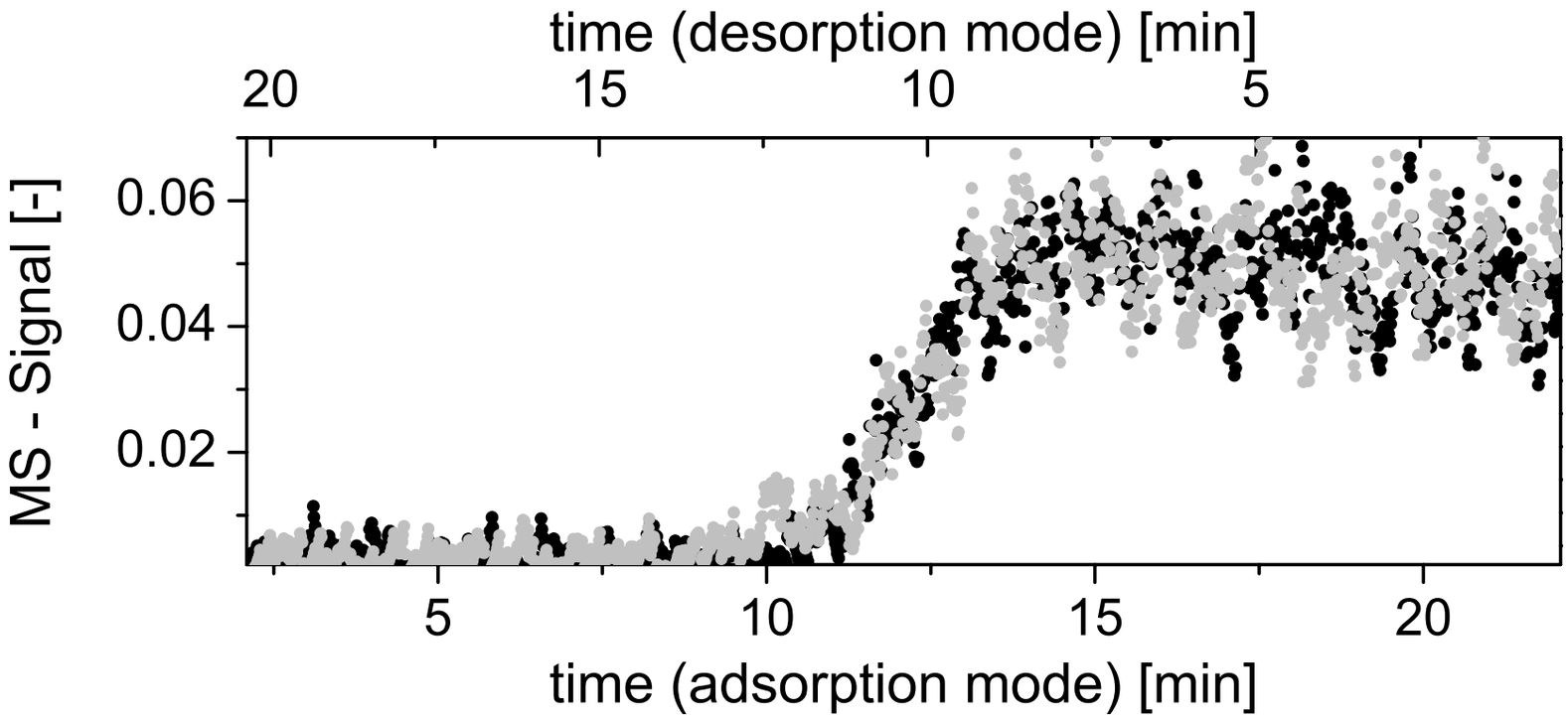


reversible adsorption of acetone

Bartels-Rausch, T. et al., 2004. Geophysical Research Letters, 31, p.L16110.

Lab Results: Acetone





Adsorption - Langmuir

Winkler, A. et al., 2002. Physical Chemistry Chemical Physics.

Bartels-Rausch, T. et al., 2004. Geophysical Research Letters, 31, p.L16110.

Langmuir Adsorption describes Laboratory experiments well

- reversible adsorption to specific adsorption sites
- saturation due to limited number of adsorption sites
- no adsorbate-adsorbate interaction

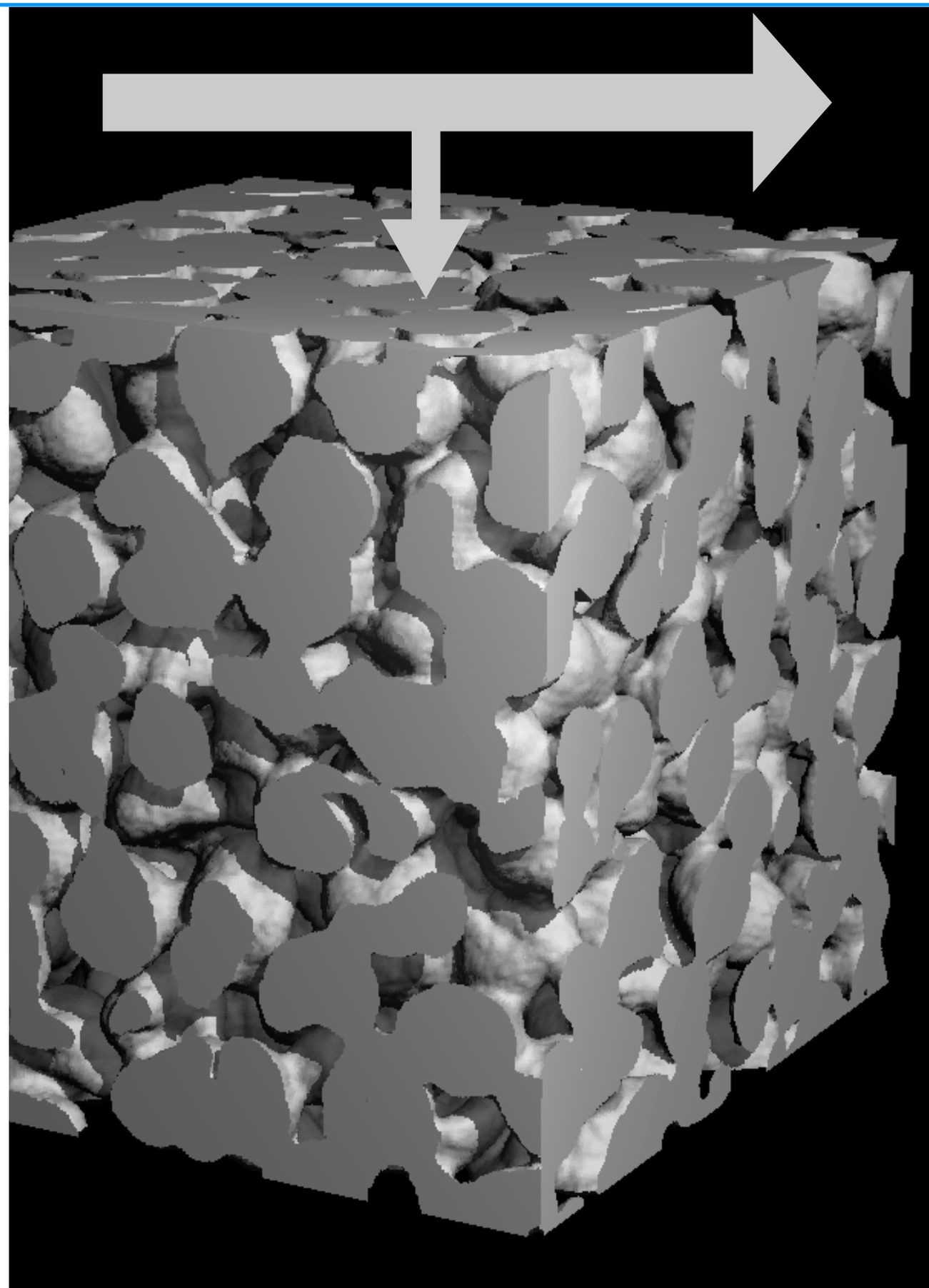
- environmental concentrations: linear range allows extrapolation from lab to field

Analysis: Diffusion through porous of Snow-Pack

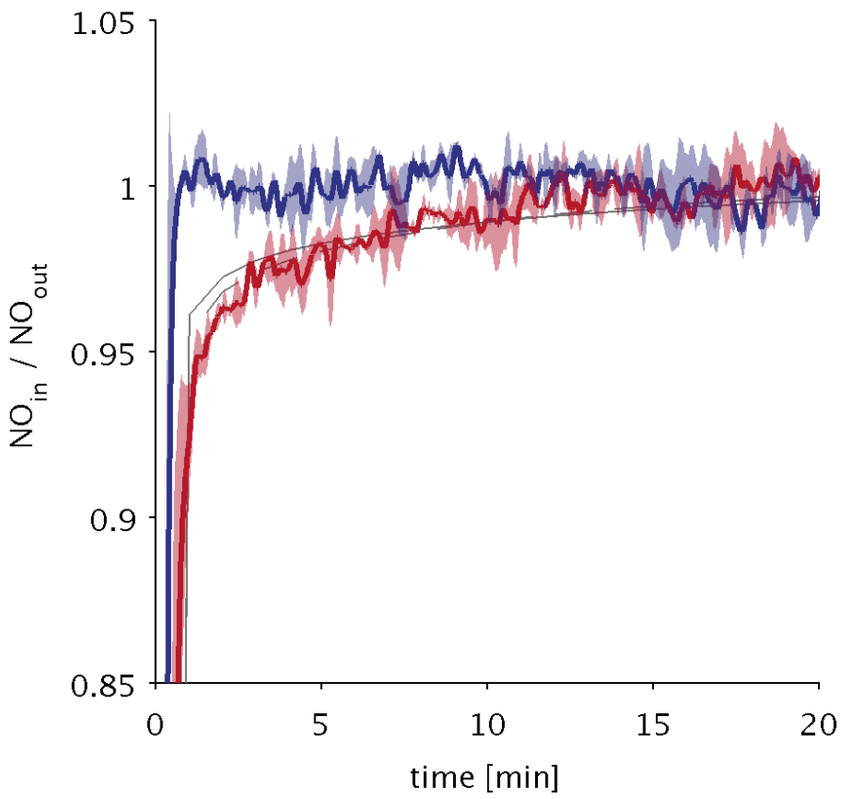
$D_{eff} = D_{air}$
× porosity/tortuosity
× 1/adsorption

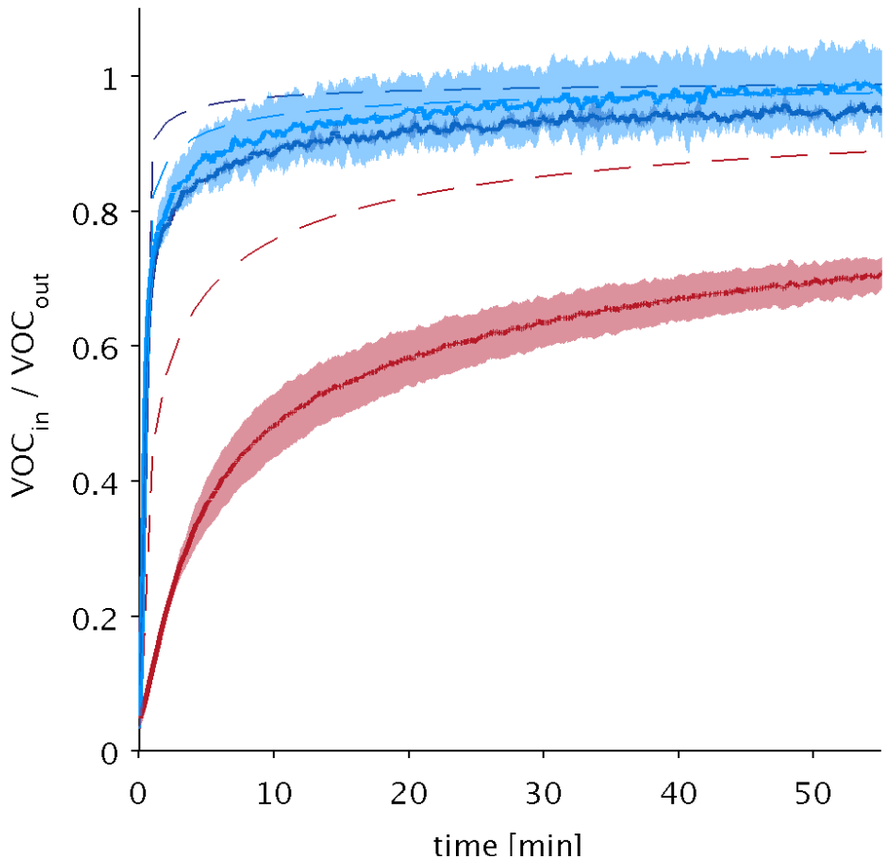
Porosity: 0.6
Tortuosity: 1.5
SSA: 12 m^2 kg^{-1}
diameter: 400 - 500 µm

Partitioning to ice:
acetone ≈ MeOH << acetic acid



Results: Diffusion of NO and VOC





Diffusion slowed by porous medium and by adsorption

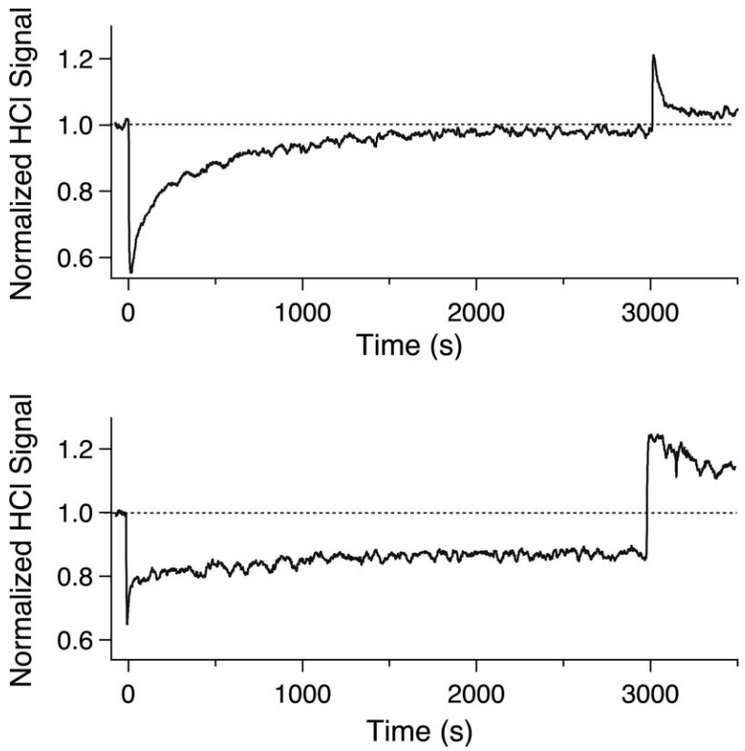
left: NO with and without snow
right: Methanol, Acetone (blue), Acetic Acid (red)

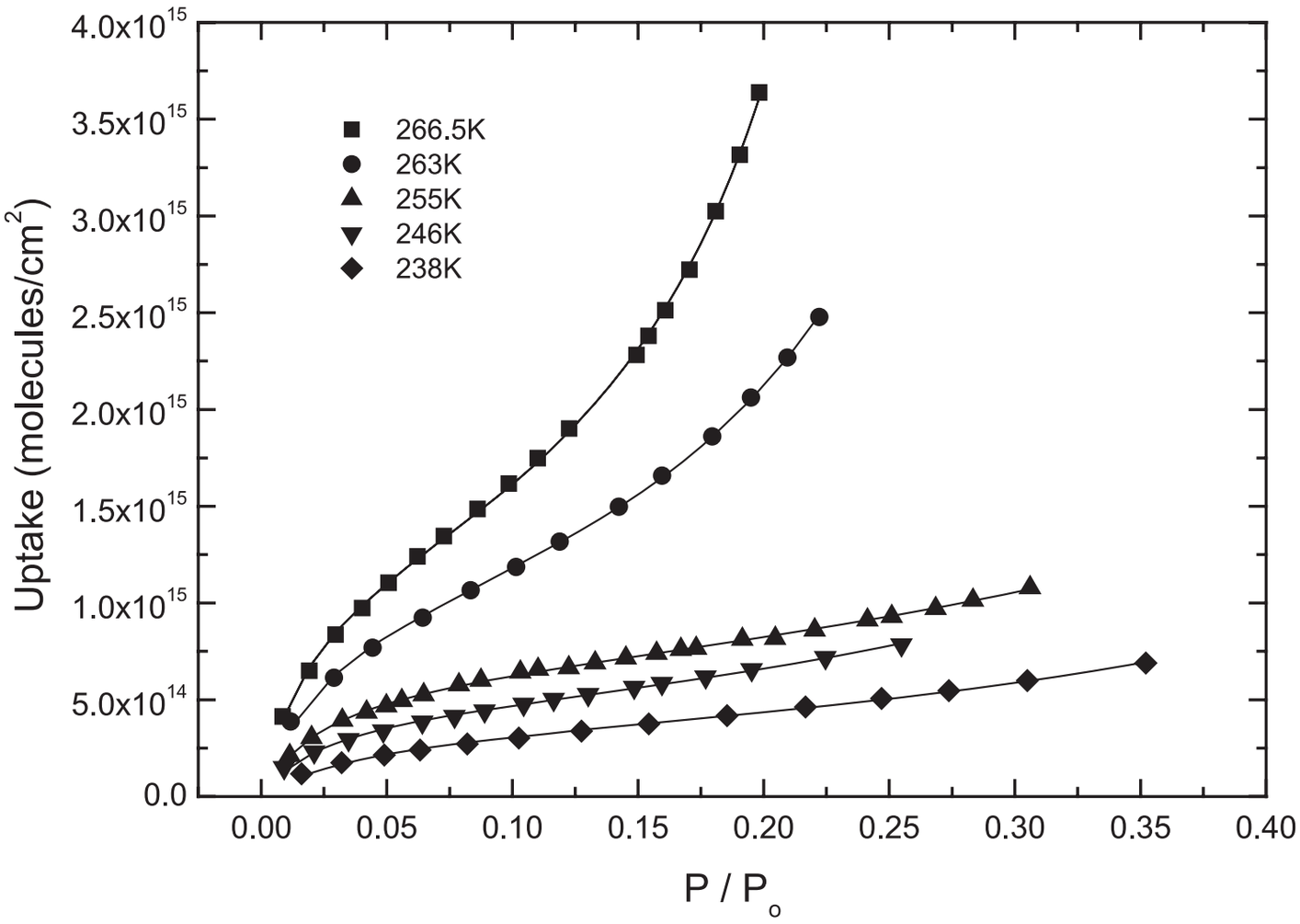
Take Home Message

$$D_{eff} = D_{air} \times \text{porosity/tortuosity} \times 1/\text{adsorption}$$

Diffusion of adsorbing trace gases through snow-pack well described by geometry and Langmuir adsorption

Limits of Langmuir approach



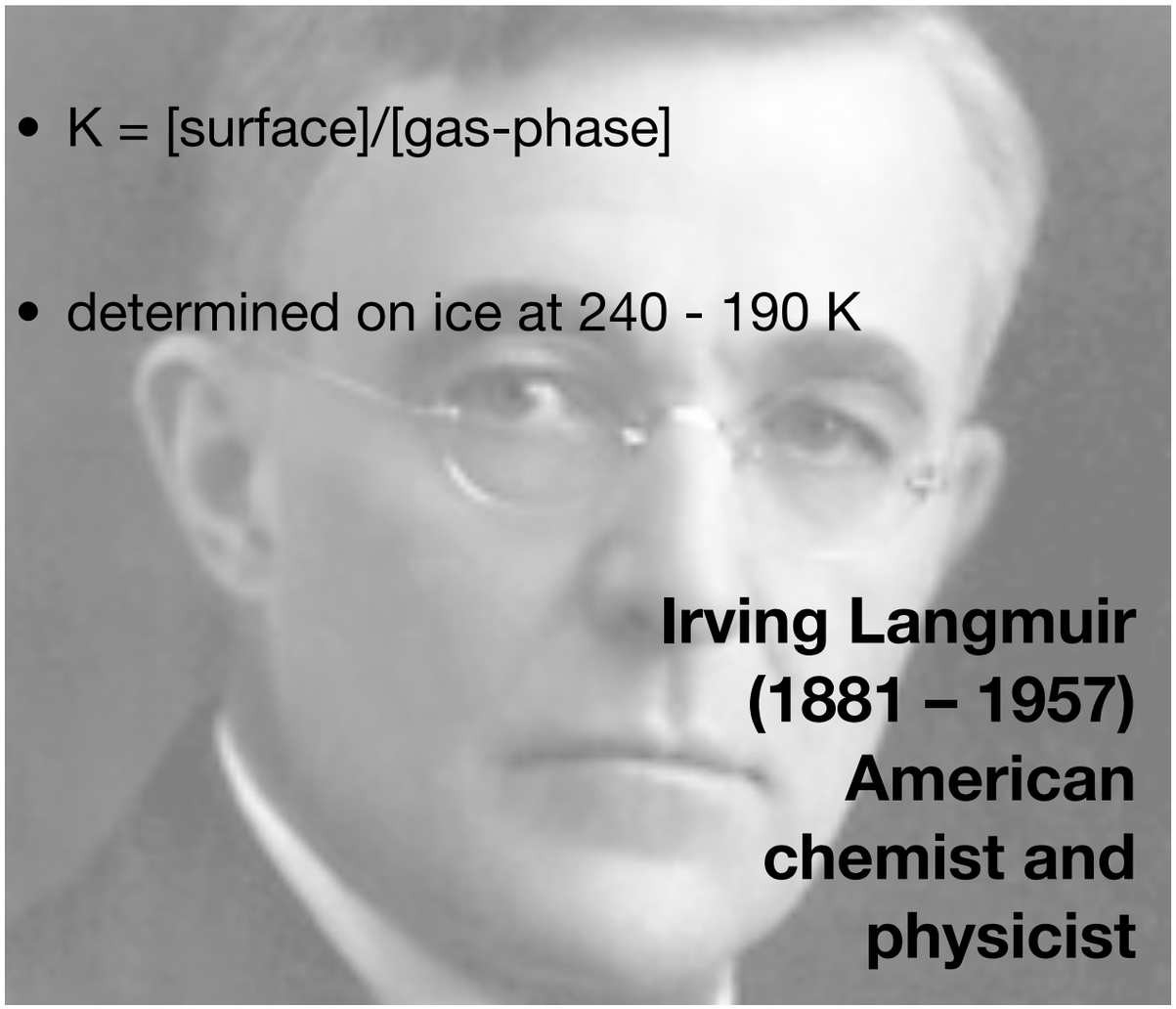


High temperaturs and/or concentrations

Abbatt, J. et al., 2008. Environmental Research Letters, 3(4), p.045008.

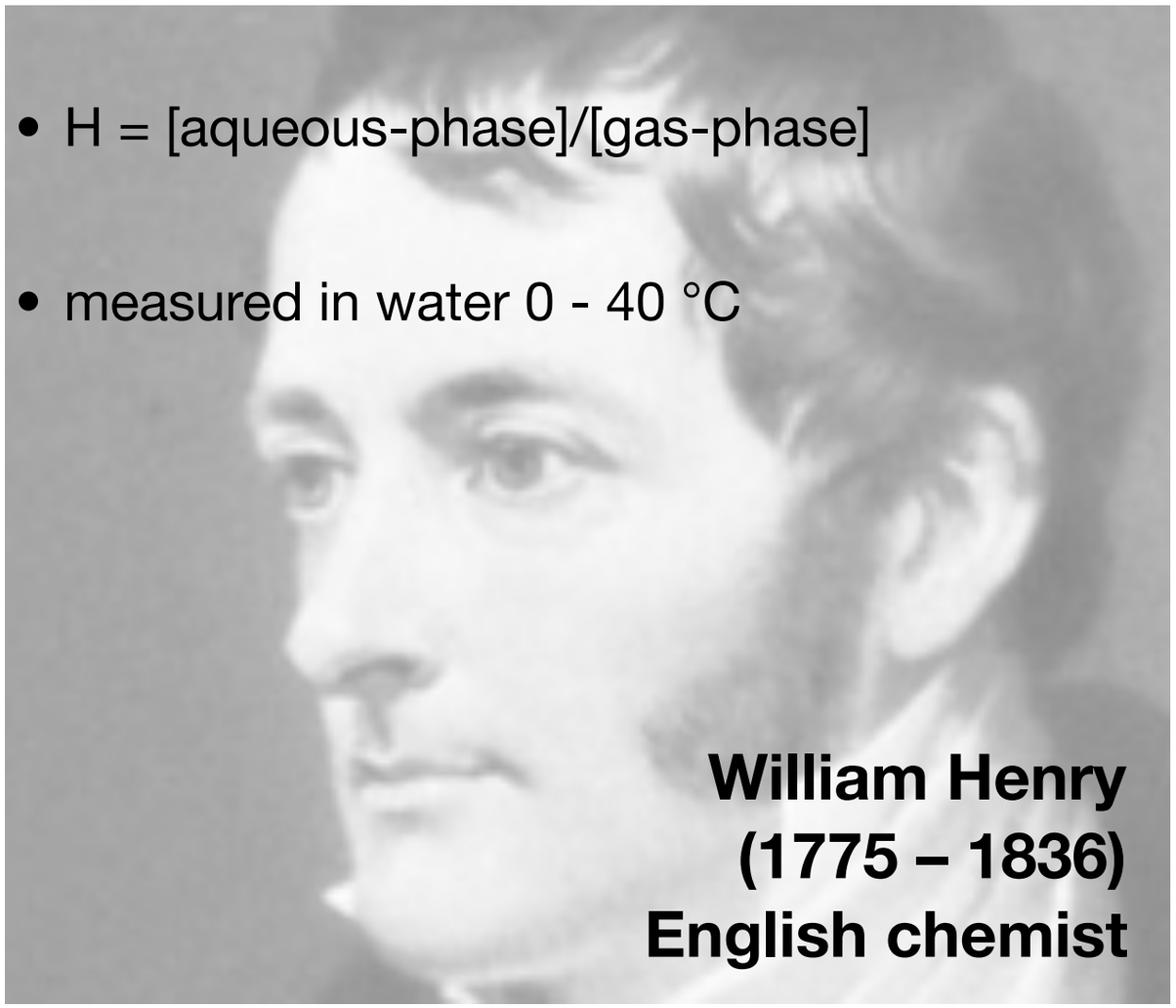
McNeill, V.F. et al., 2006. Proceedings of The National Academy Of Sciences Of The United States Of America, 103 (25), pp.9422–9427.

How to parameterize uptake



- K = [surface]/[gas-phase]
- determined on ice at 240 - 190 K

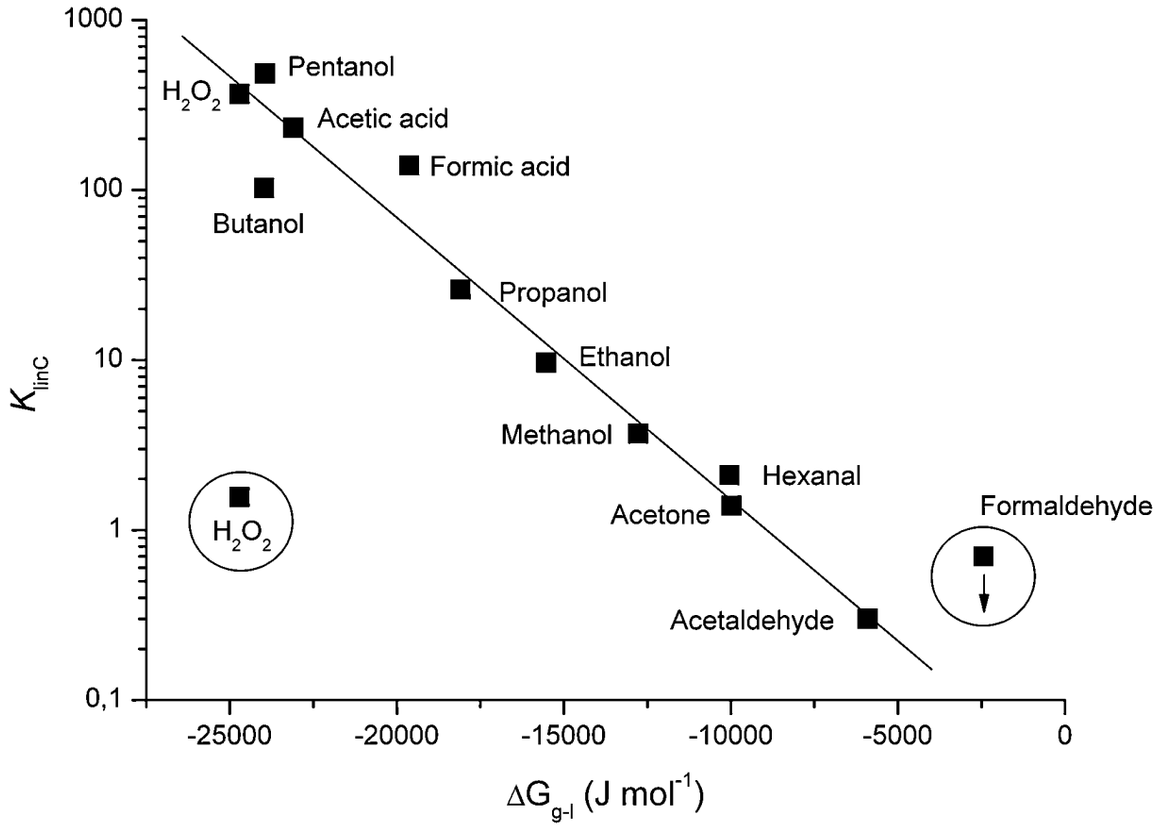
Irving Langmuir
(1881 – 1957)
American chemist and physicist

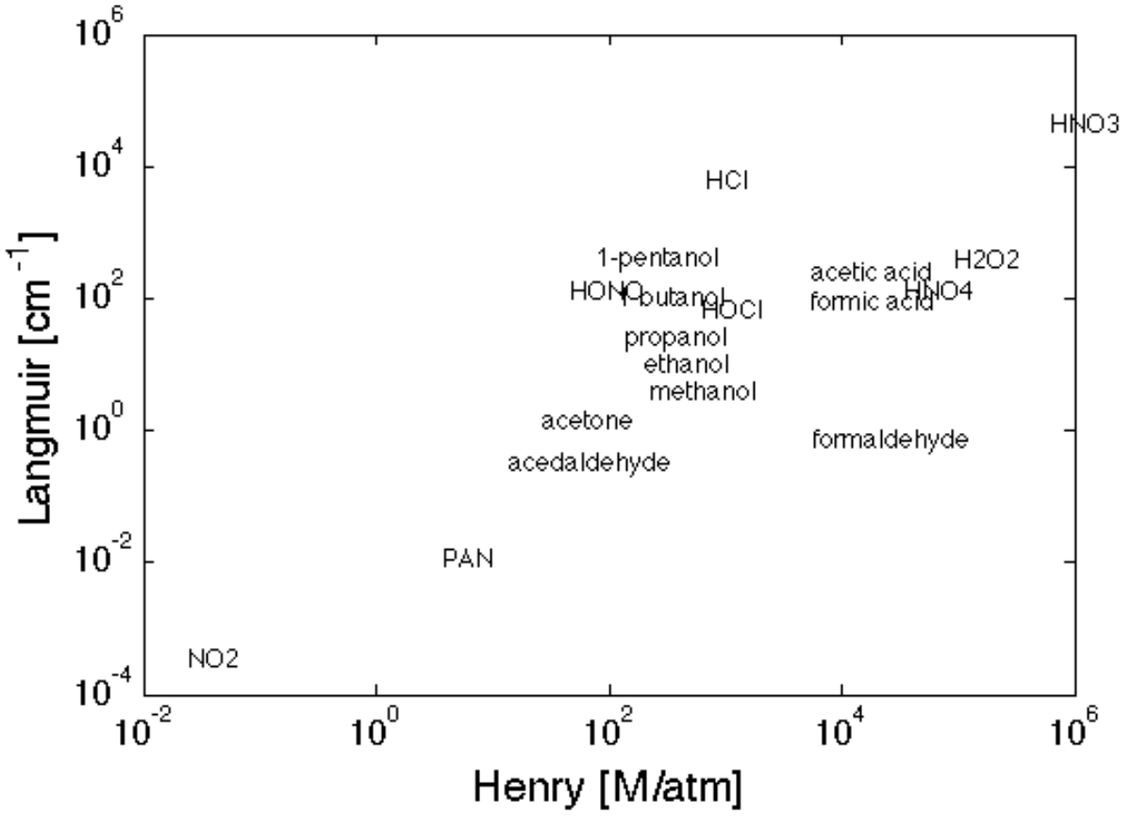


- H = [aqueous-phase]/[gas-phase]
- measured in water 0 - 40 °C

William Henry
(1775 – 1836)
English chemist

Langmuir vs. Henry

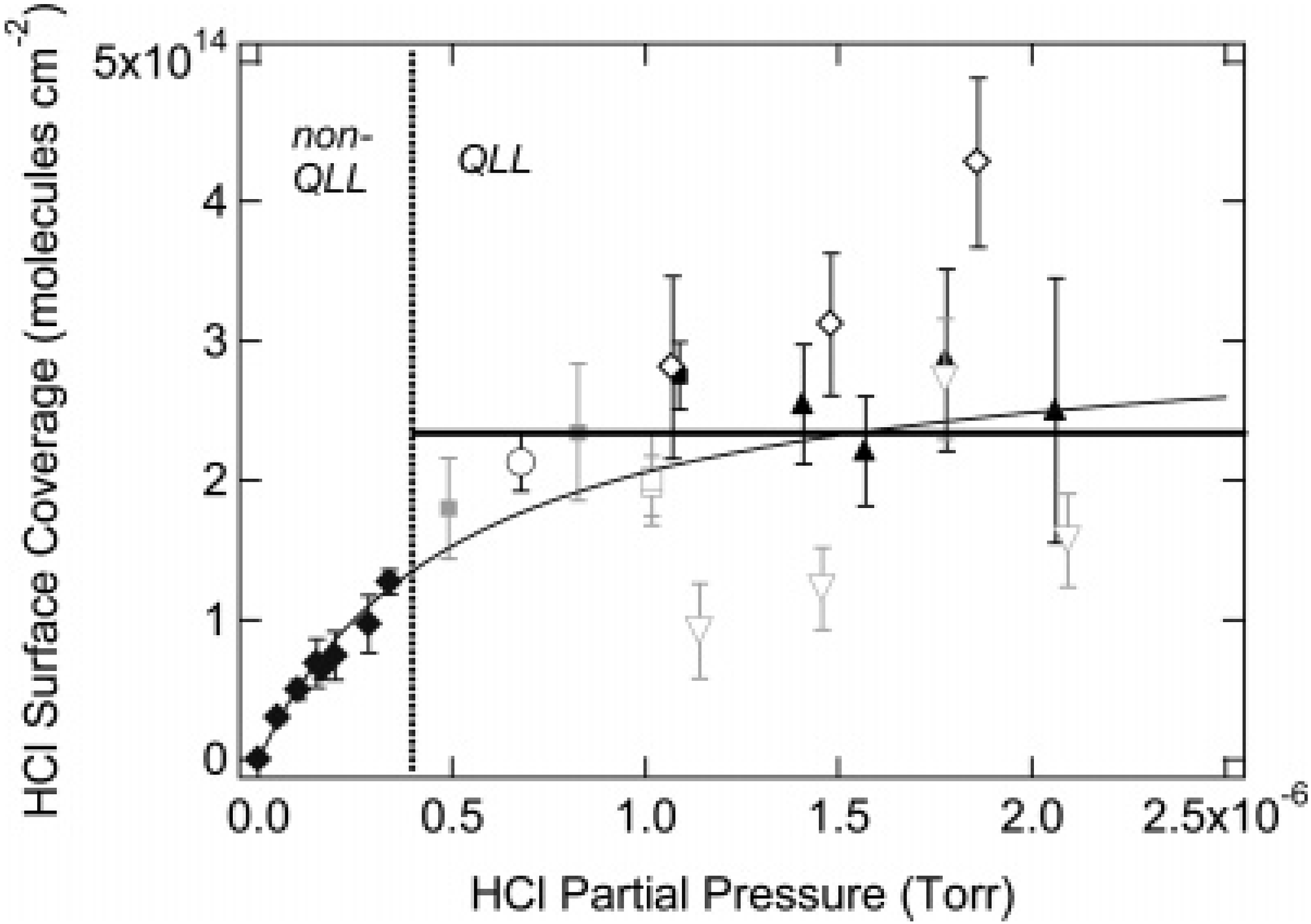




Langmuir correlates with free energy of condensation

Pouvesle, N. et al., 2010. Physical Chemistry Chemical Physics, 12(47), pp.15544–15550.

Who to parameterize non-adsorptive uptake



maximum uptake?

correlation with gas-phase conc.?

time?

McNeill, V.F. et al., 2006. Proceedings of The National Academy Of Sciences Of The United States Of America, 103 (25), pp.9422–9427.

Partitioning to ice

... linear range well described by Langmuir/Henry

... this can be used to model diffusion through porous snow

… non-linear range open to debate