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VOC injection into a house reveals large surface reservoir sizes in an indoor environment

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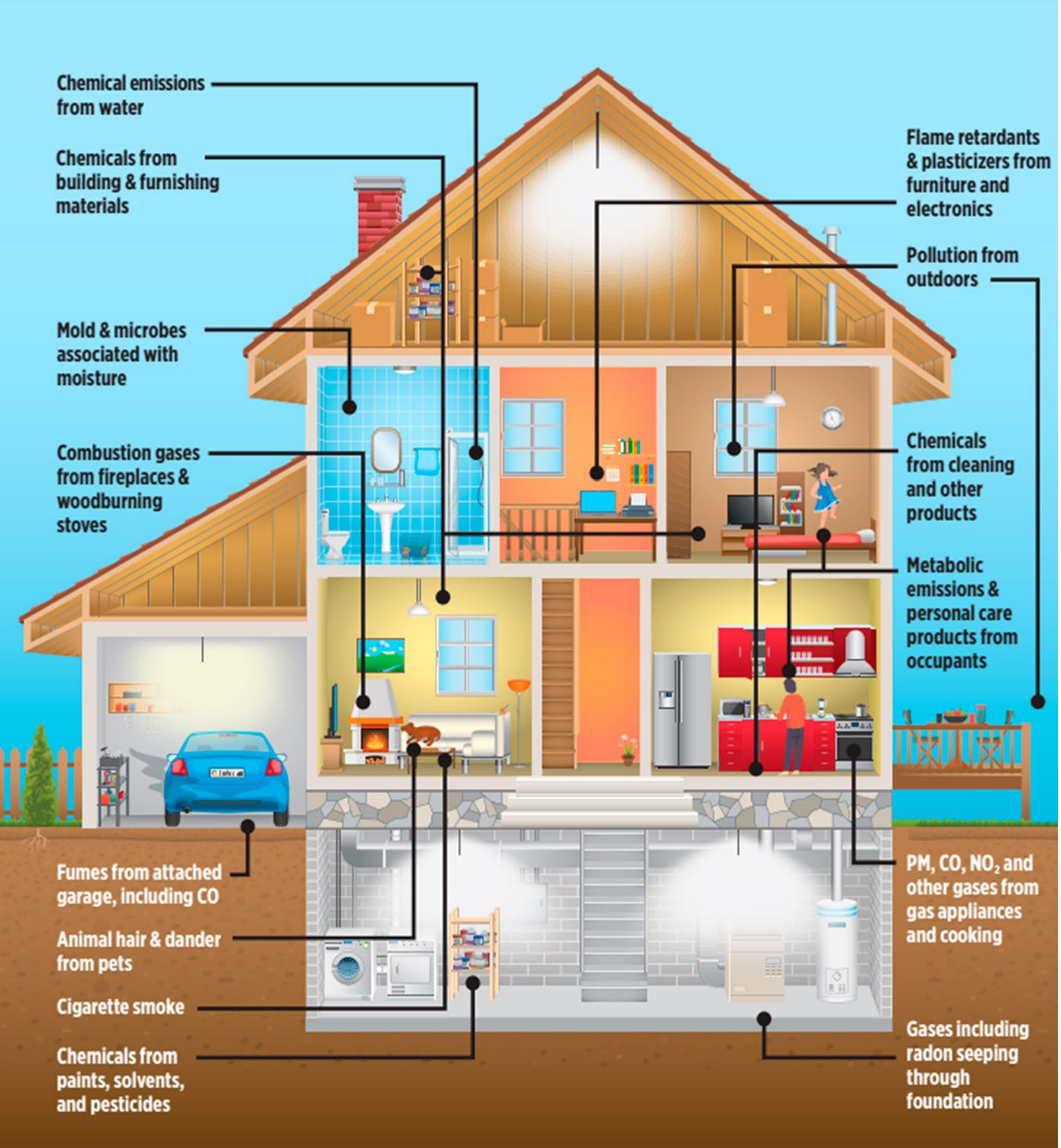
ALFRED P. SLOAN
FOUNDATION

CASA: Chemical Assessment of Surfaces and Air Study

- State-of-the-art instruments from 13+ institutions
- Spring 2022
- NIST Net Zero Energy Residential Test Facility
- Goal: investigate how indoor and outdoor pollutants transport and transform across gas, aerosol, and surface phases in a house

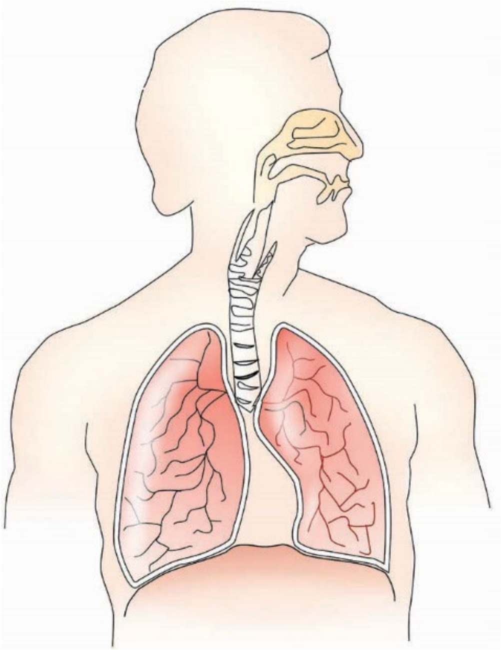
[Farmer et al. Env Sci:Proc Imp. 2025]



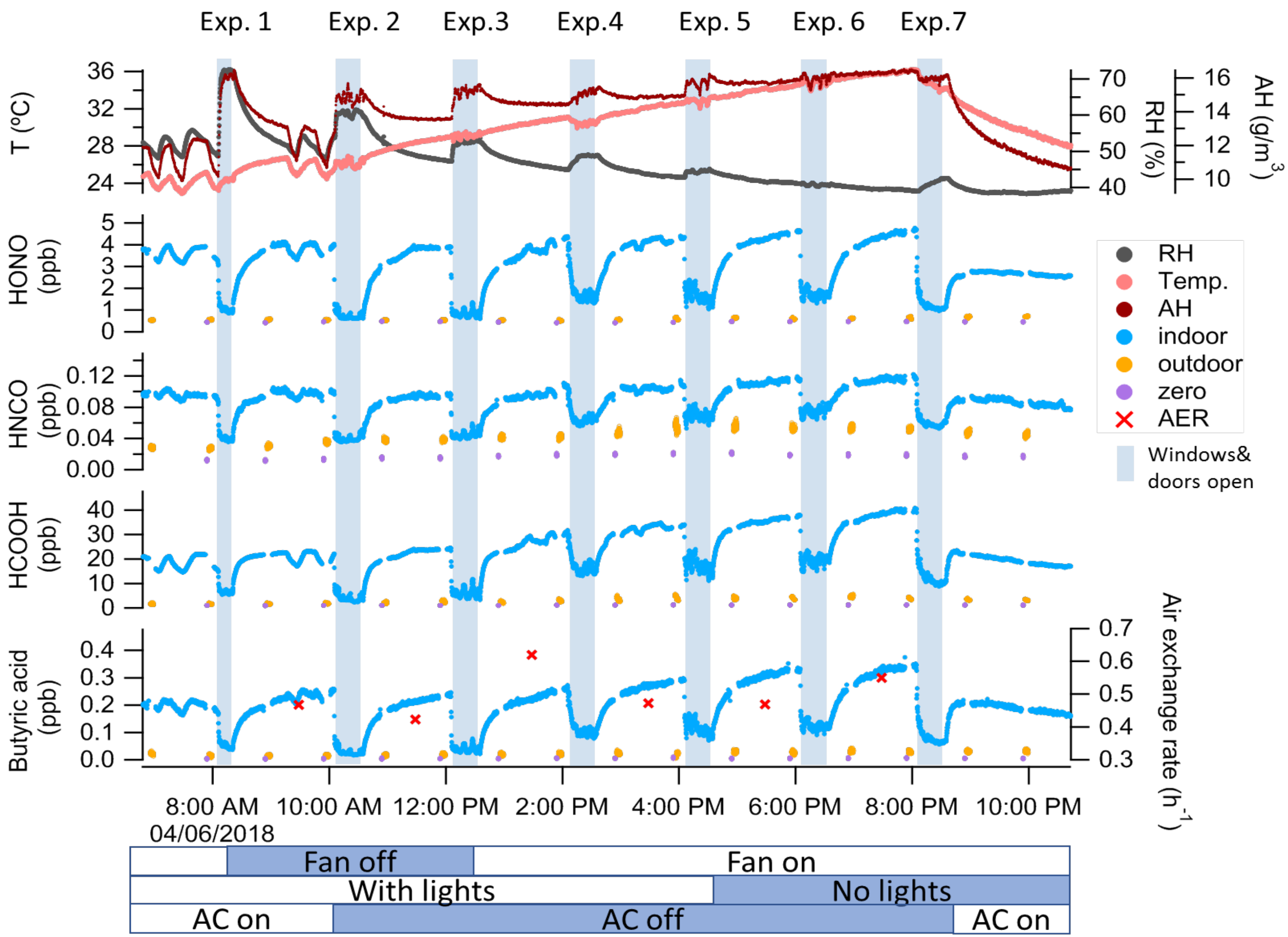
There are many chemicals around indoors

National Academy of Sciences, “Why Indoor Chemistry Matters”, 2022

We get most of our non-dietary chemical exposure indoors

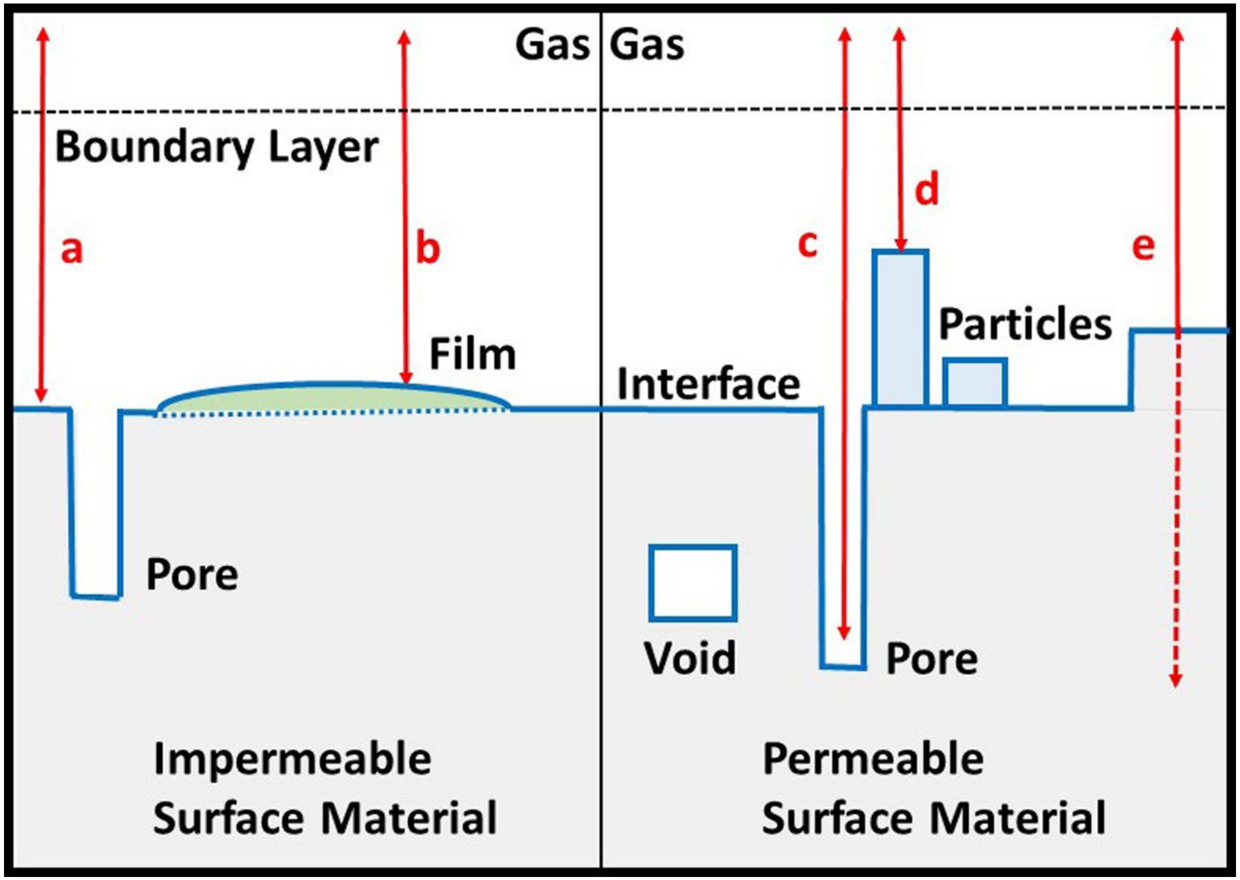


Enhanced Ventilation experiments at HOMEChem (2018)



Wang et al., Science Advances, 2020

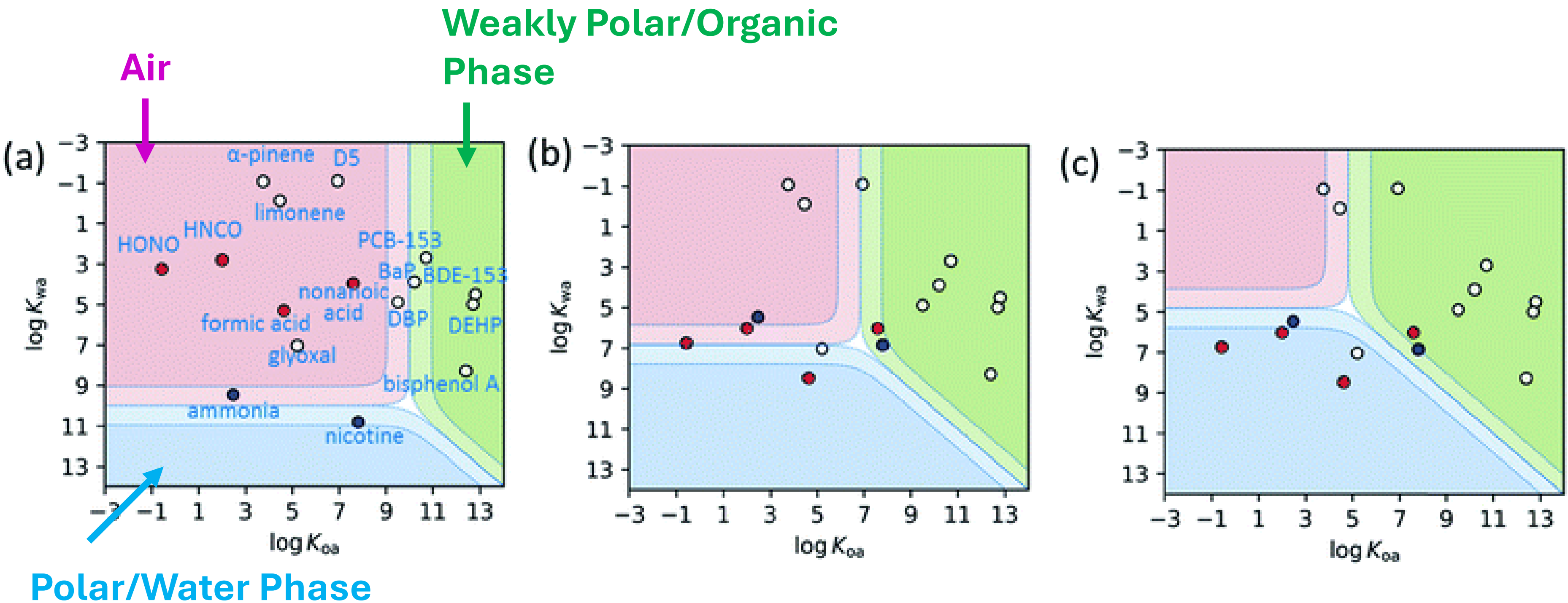
Indoor surfaces, gas-surface partitioning



There are many components of indoor surface reservoirs that interact with the gas phase

Abbatt, Morrison, et al., Indoor Air, 2022

In what phase do molecules reside indoors?



Partitioning in a polluted outdoor environment

Partitioning to thin films indoors (50 nm thick, pH 7)

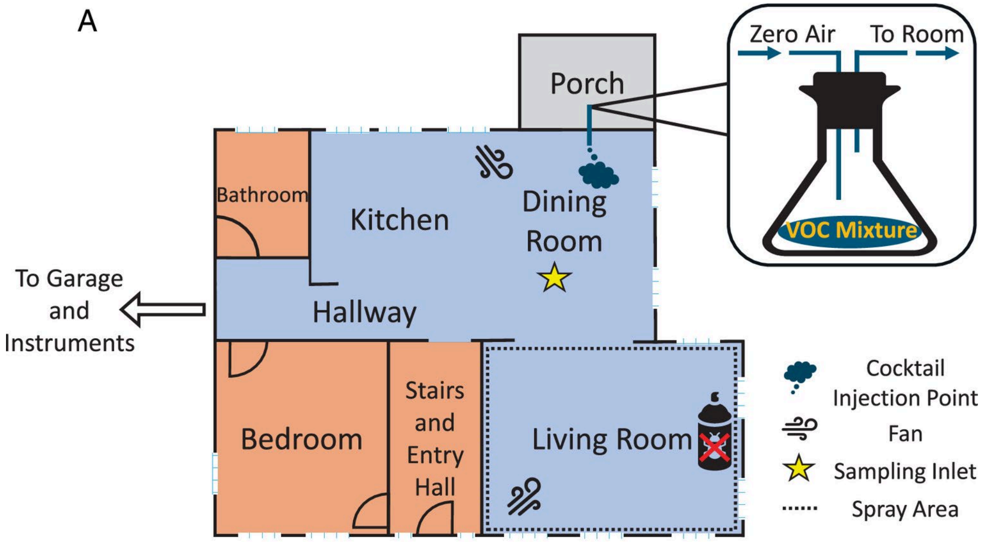
Partitioning to much larger surface reservoirs (5 μm thick, pH 7)

Molecules that are predominantly gaseous outdoors undergo considerably more surface partitioning indoors

Abbatt and Wang, RSC Env Sci, 2020

VOC emissions into a NIST test house during CASA

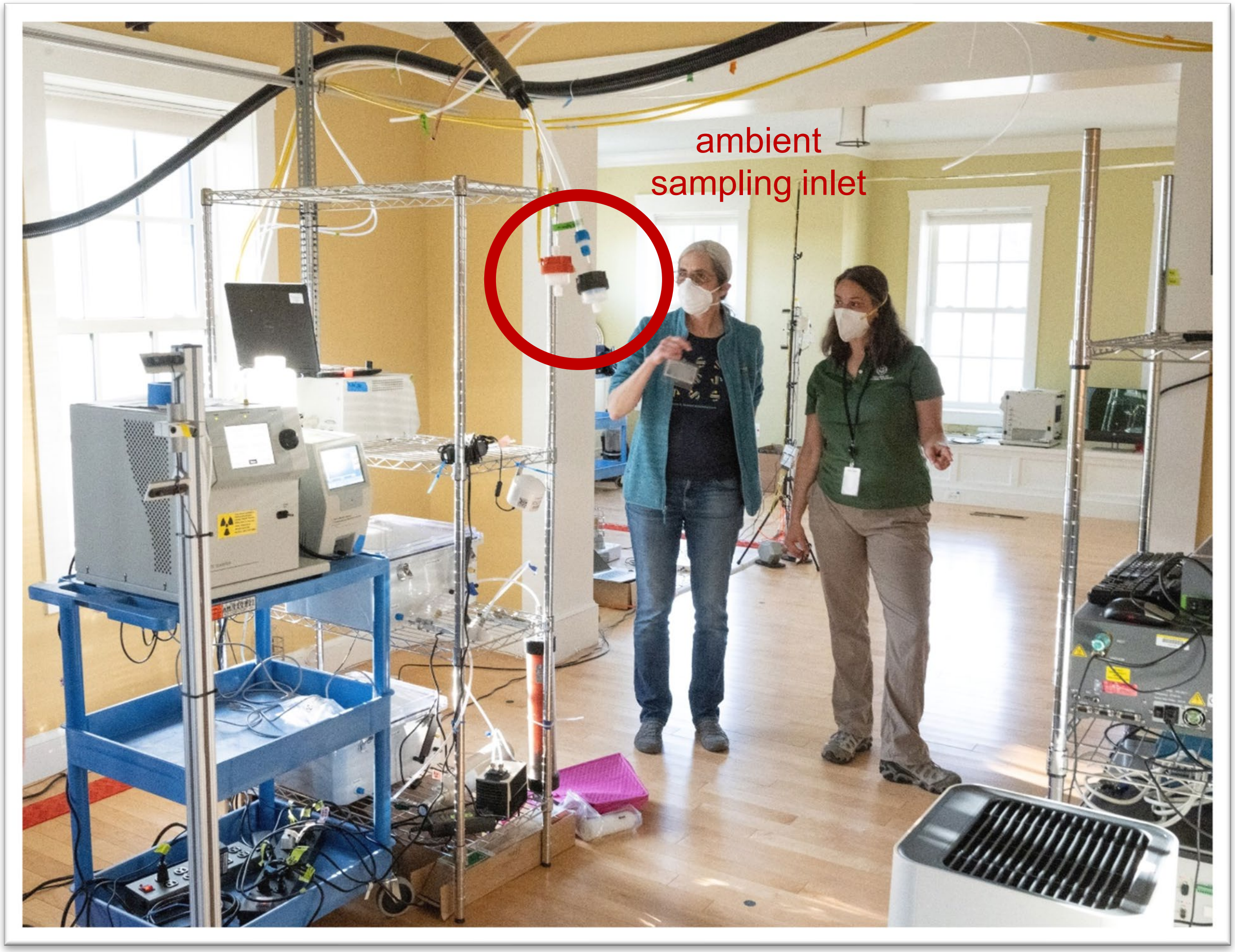
<u>Goal</u>: *To determine the VOC partitioning capacity of indoor surfaces*



<u>Method</u>: *Time-resolved measurements of VOCs injected into a house are used to constrain a gas-surface partitioning model*

Online measurements at CASA

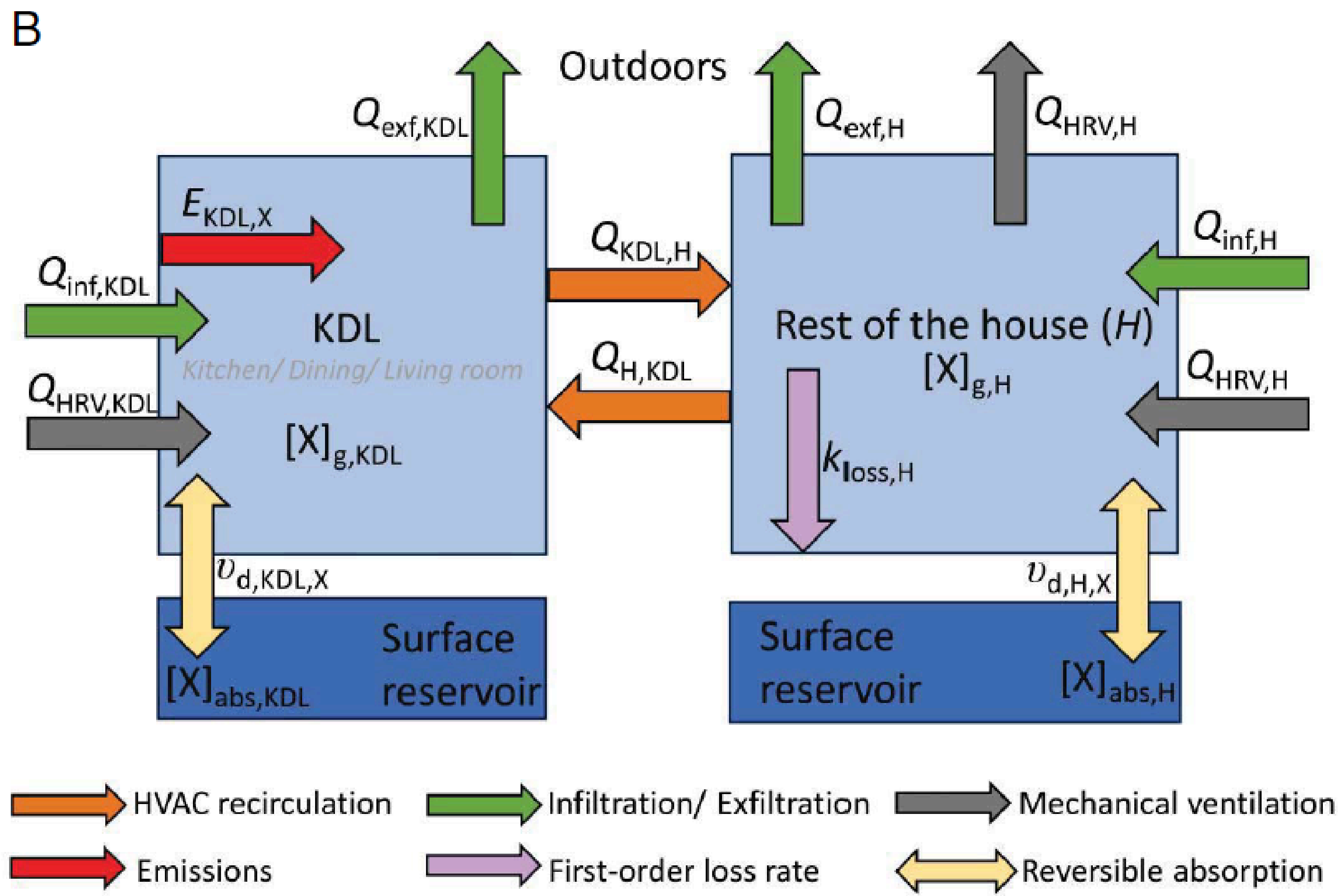
GC-Vocus PTR-ToF-MS



CASA PIs: Delphine Farmer, Nina Vance, Dustin Poppendieck

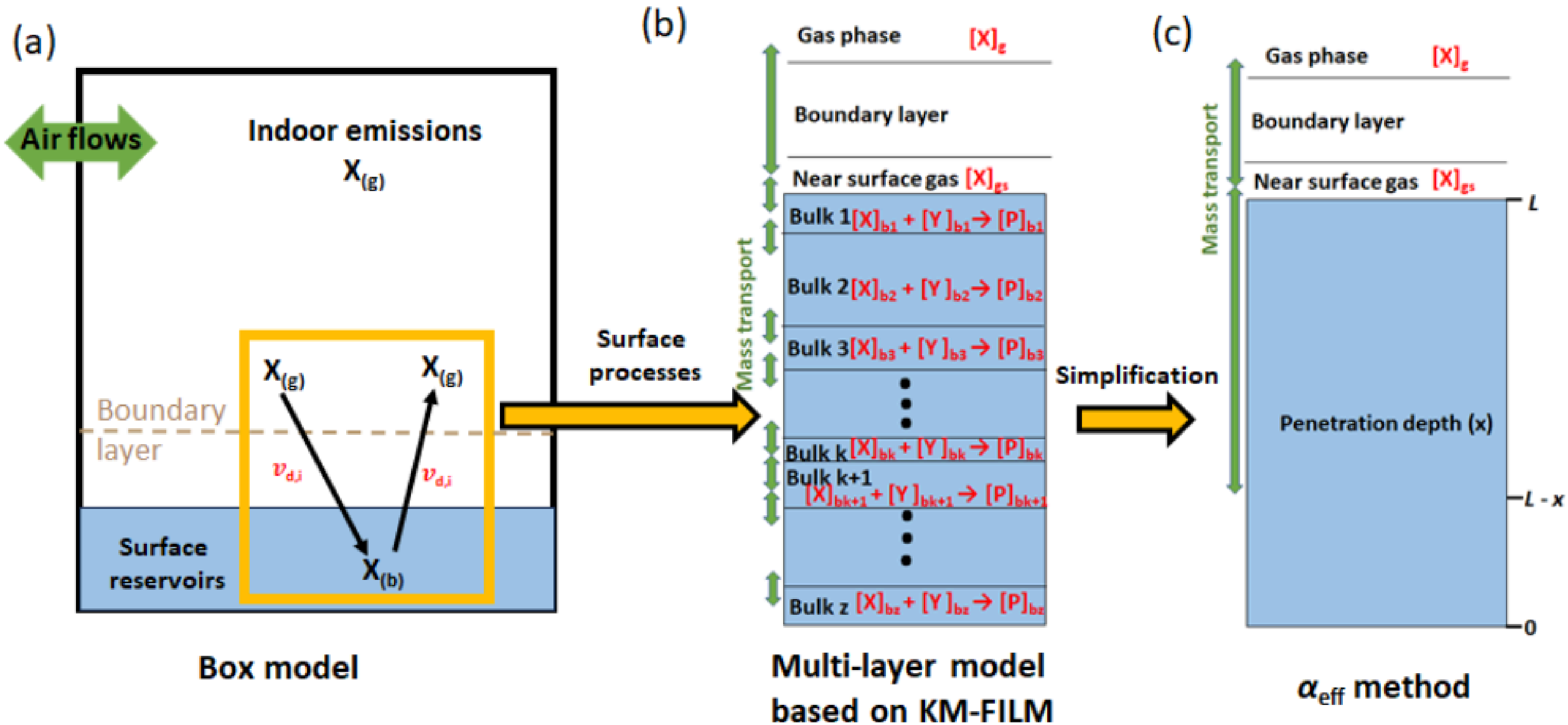
Jenna Ditto, Han Hyunh, Jie Yu

Indoor Two-Box Model



Two boxes: KDL (where VOCs were injected) & the rest of the house
Flows are measured/calculated or estimated based on CO_2 decay

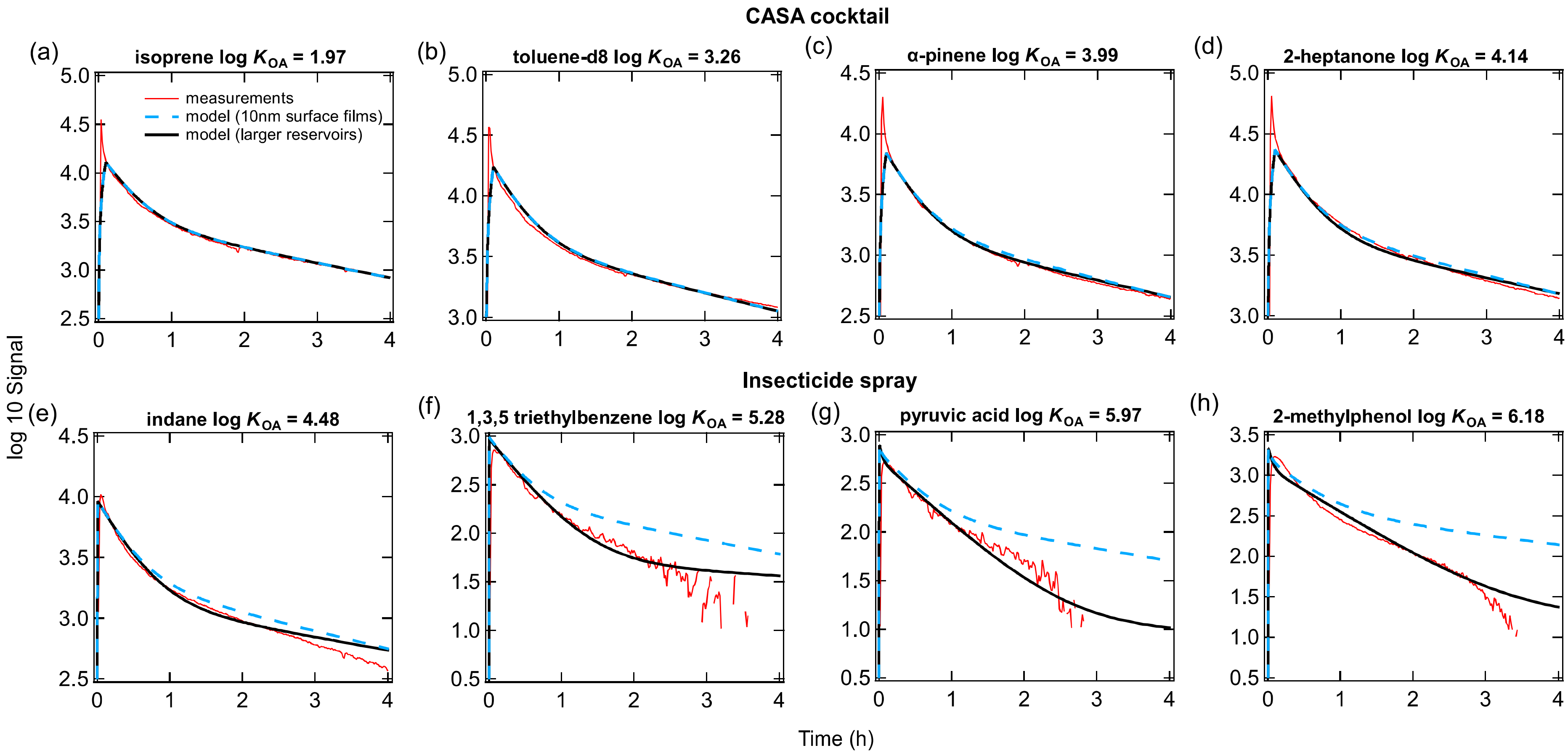
Modeling Partitioning to Surface Reservoirs



Surface partitioning of indoor compounds is treated as fluxes, either by explicitly treating bulk diffusion or by applying effective mass accommodation coefficient.

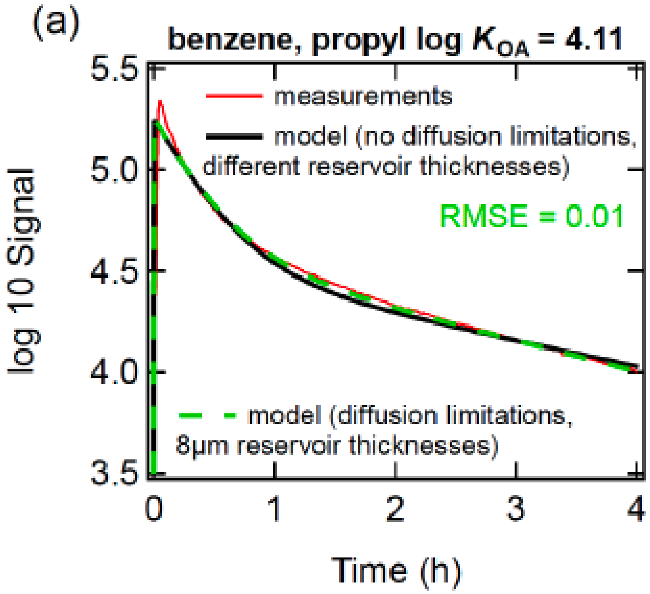
Surface organic films are ubiquitously present with 10's of nanometer thick (Weschler & Nazaroff, 2017). Is this major surface reservoir?

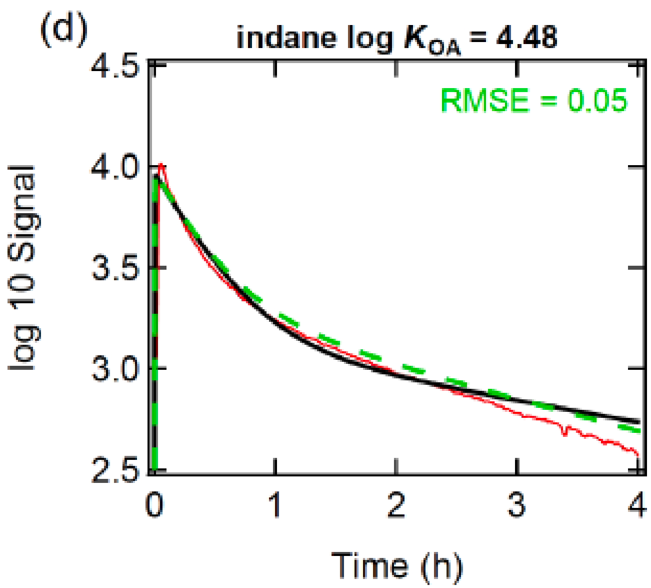
Measured vs. Modeled VOC Decay

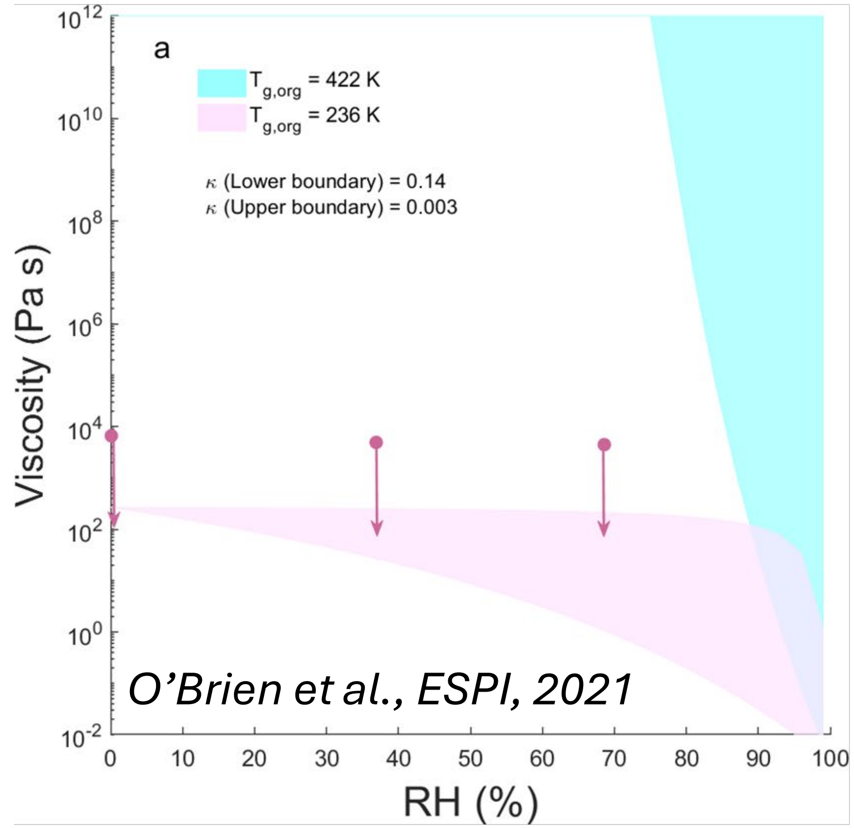


VOCs (log K_{OA}~2-4) do not partition significantly to indoor surfaces.
Decay of SVOCs (log K_{OA} ~4-6) reproduced with large surface reservoirs with large thickness (200 nm in KDL, 8 μm), indicating that permeable/porous materials such as painted surfaces/wood are likely the major surface reservoirs.

Potential Bulk Diffusion Limitations?



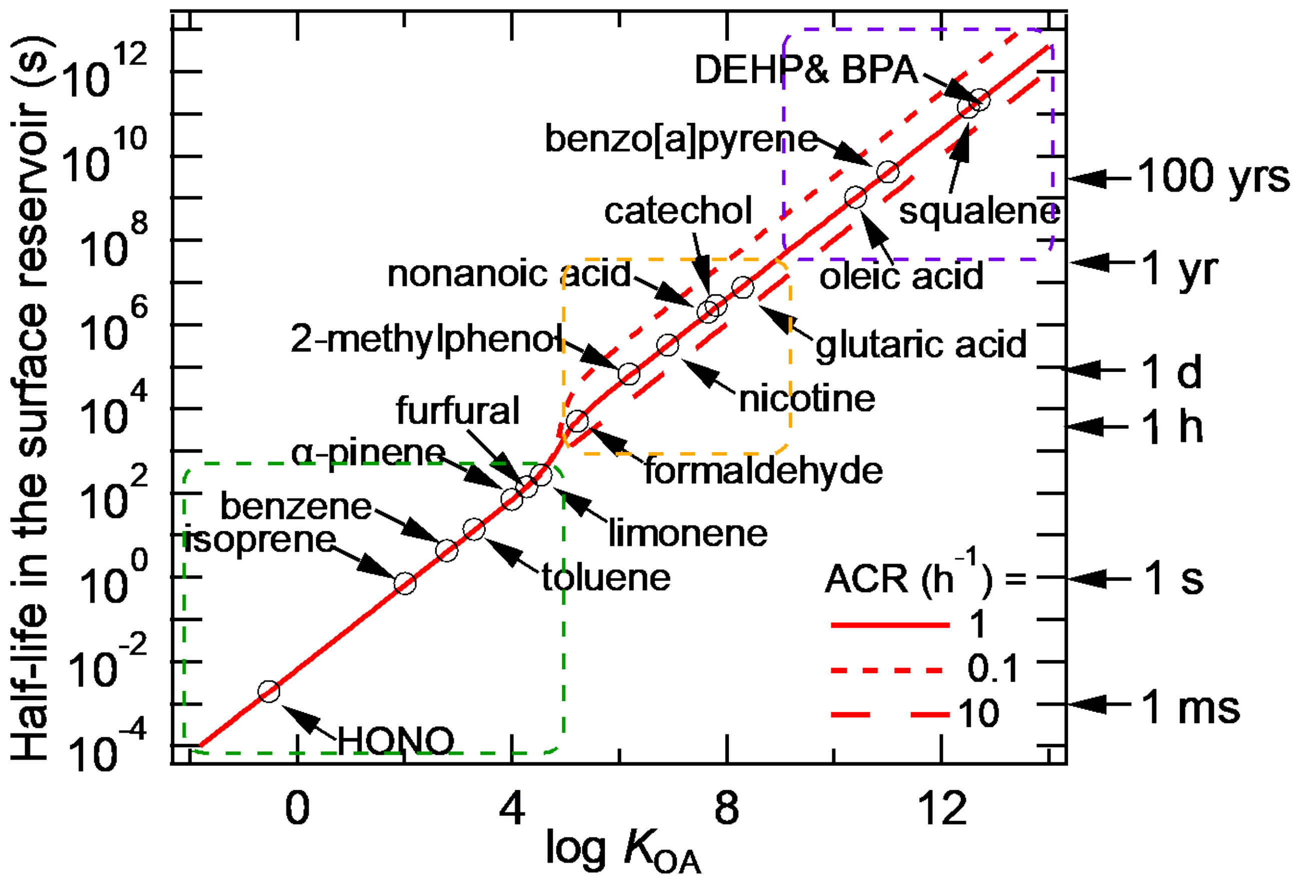




Data can be fitted with an thickness of 8 μm throughout the house with bulk diffusivity of 10^{-13} cm^2 s^{-1} (consistent with HOMEChem) in KDL and $>10^{-11}$ cm^2 s^{-1} in the rest.

Take Home Messages

With a large partitioning capacity, organic contaminants will have much longer indoor residence times. Enhanced ventilation may not be sufficient to remove some of them.



log K_{OA} < 4.5 : predominantly in the gas phase or exist in polar reservoir

4.5 < log K_{OA} < 9: Significant lifetime in reservoirs, as modulated by ACR

9< log K_{OA} : Practically impossible to remove with ventilation