



Active photocatalytic air cleaners

**Alfred T. Hodgson, Hugo Destailats,
William J. Fisk**

Lawrence Berkeley National Laboratory
Environmental Energy Technologies Division
Indoor Environment Department

Berkeley, June 29th 2007



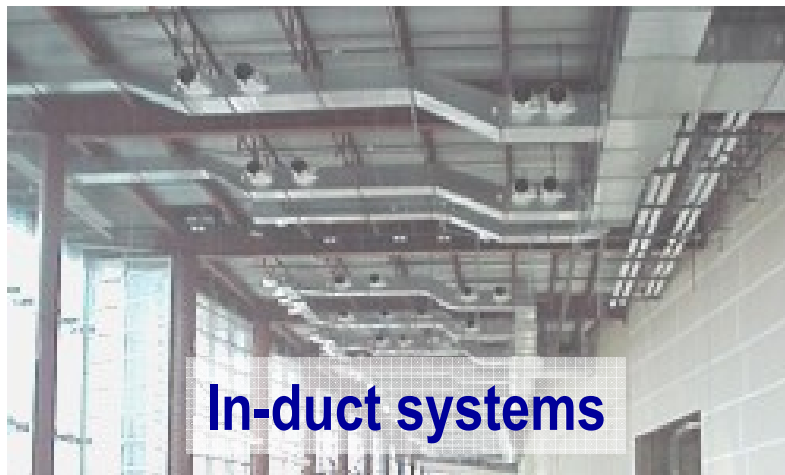
Indoor air cleaning technologies

UV photocatalytic oxidation (UVPCO)

Outdoor or recirculated indoor air with VOCs

UVPCO

“Clean” air with lower VOCs





Goals of our study: performance evaluation of UVPCO

Main questions:

Can we eliminate airborne pollutants from indoor air?

Are air cleaning technologies energy-efficient and safe?

How do we define performance?

Removal efficiency of target pollutants

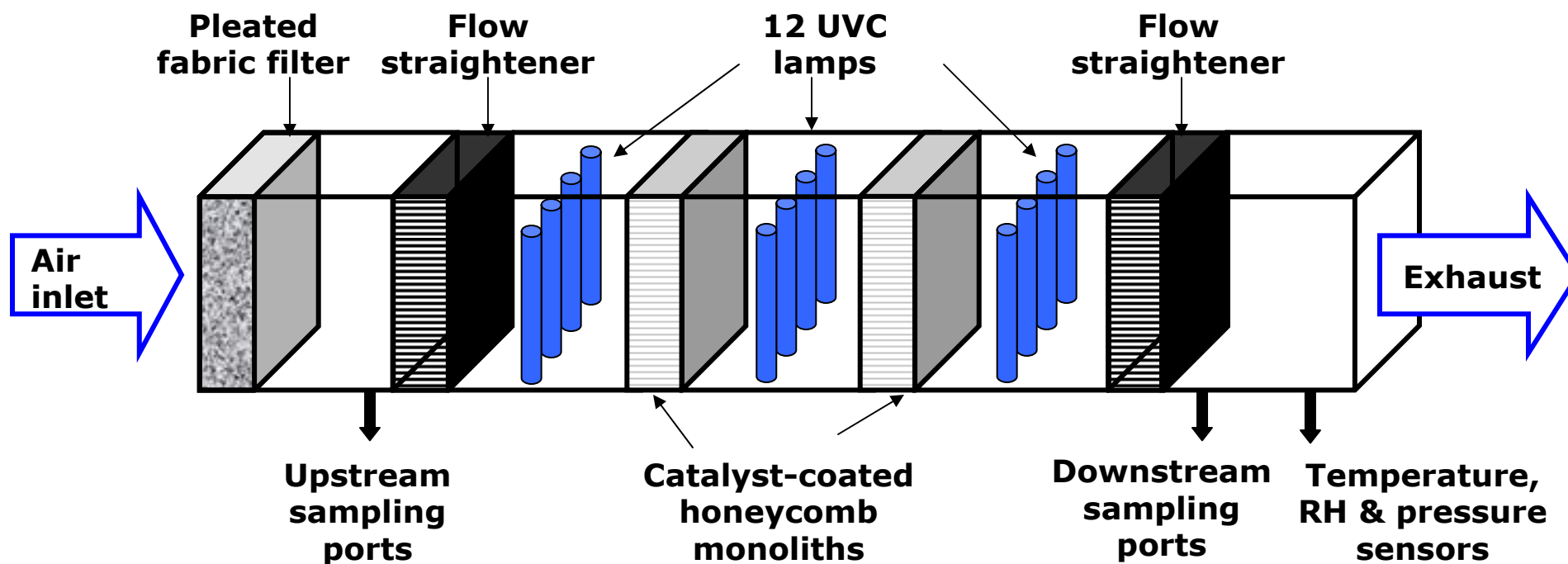
Formation of undesired oxidation byproducts

Catalyst inactivation



UVPCO reactor schematics

In-duct, single pass, plug-flow reactor



UV irradiation: 254 nm, 5 Watts/lamp

Flow range: 150-600 m³/h

Max pressure drop: 35 Pa

Total VOC concentration: 54-780 ppb

Face velocity: 0.5–1.8 m/s

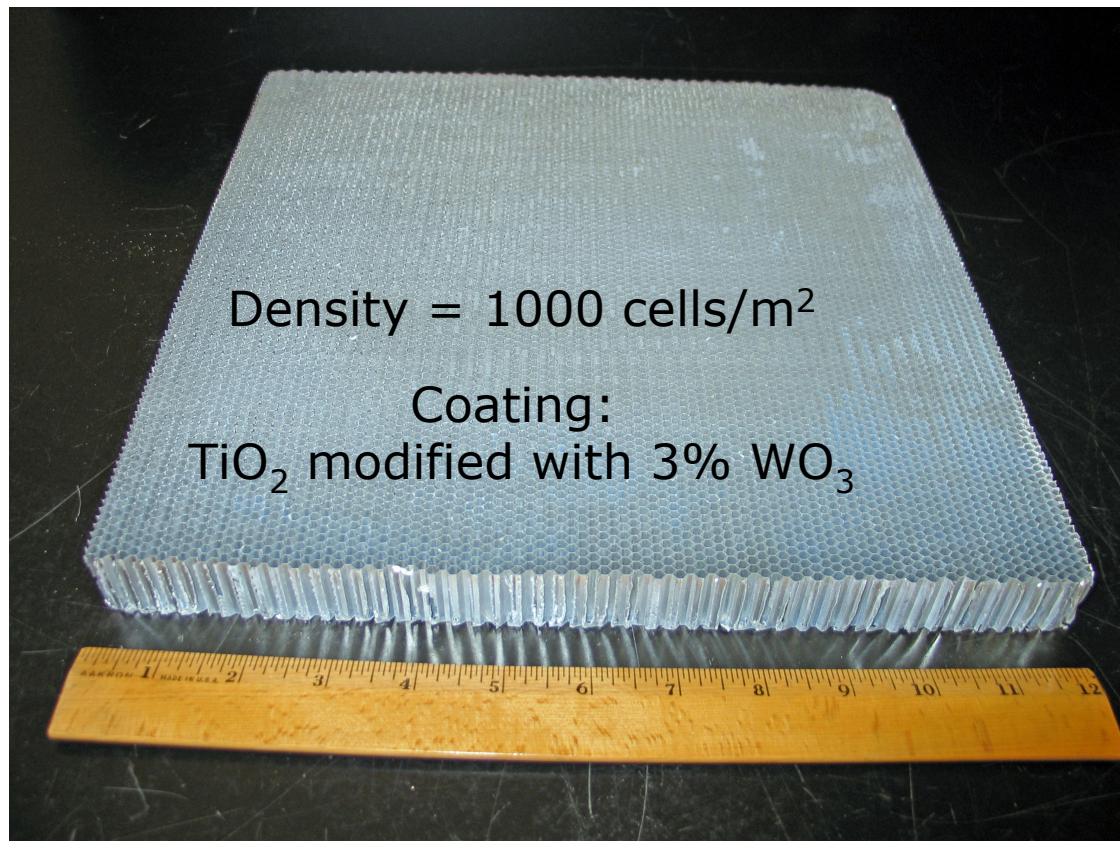
Residence time: 0.03-0.1 s

Temperature: 20-25 °C

Relative humidity: 42-65 %

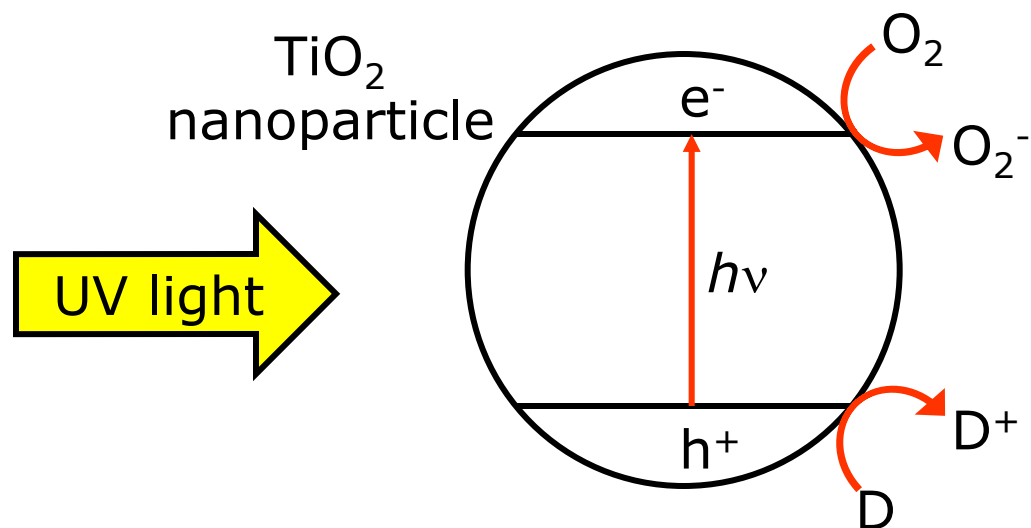


Honeycomb monolith

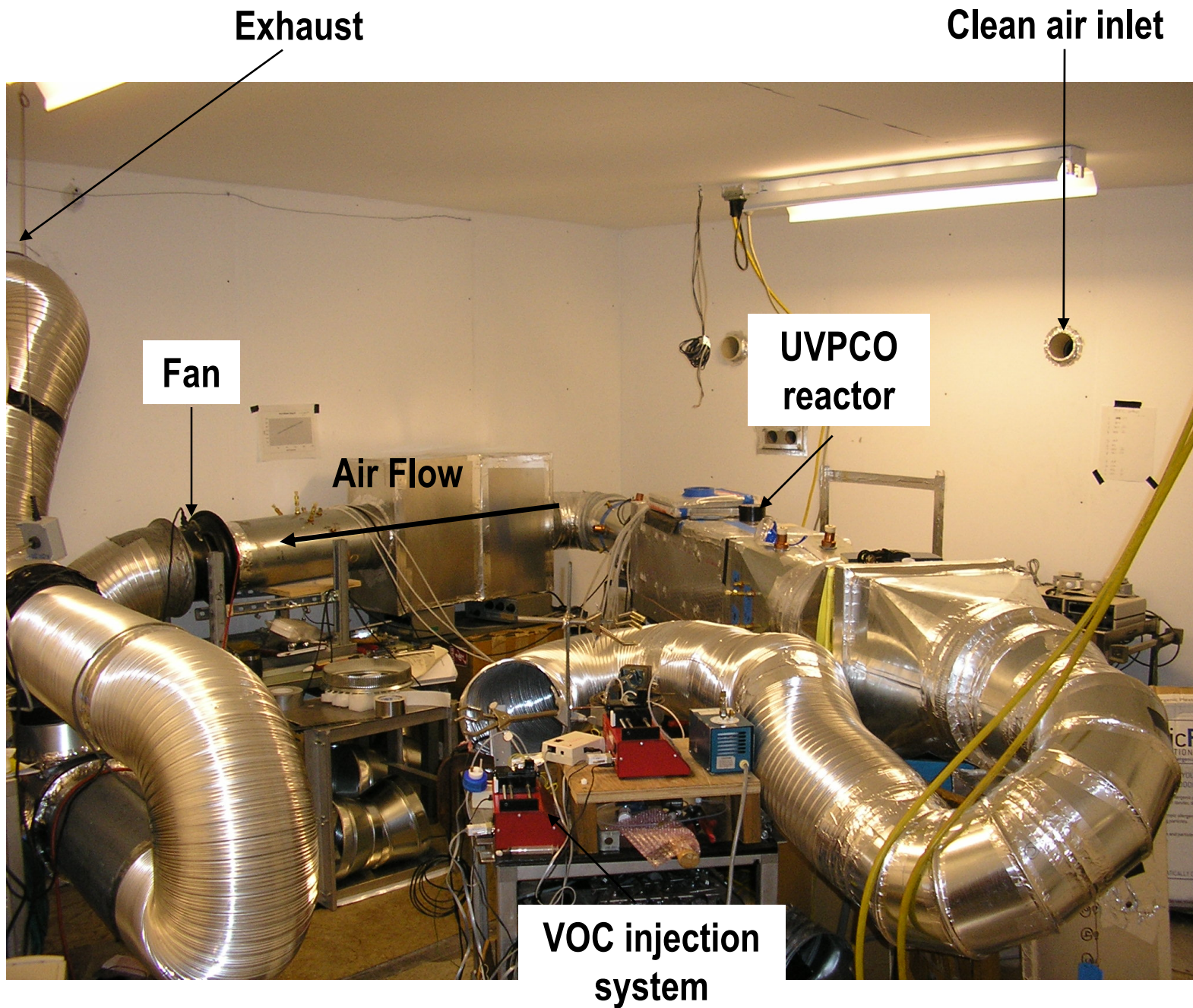


Density = 1000 cells/m²

Coating:
TiO₂ modified with 3% WO₃



D: a volatile organic compound (VOC)



Exhaust

Clean air inlet

Fan

UVPCO
reactor

Air Flow

VOC injection
system



Realistic VOC mixtures

① 28 VOCs typical of office buildings

OB



<chem>CCO</chem> Alcohols	<chem>CCCCC=O</chem> Carbonyls
<chem>CCCCOCCO</chem> Glycol ethers	<chem>CCCCCCCCCCCC</chem> Alkanes
<chem>CC1=CC=CC=C1C=C</chem> Terpenes	<chem>CC1=CC=CC=C1C(C)C</chem> Aromatics
<div> <chem>ClCC(Cl)CC(Cl)Cl</chem> <chem>ClC1=CC=CC=C1Cl</chem> </div> Halogenated VOCs	

② Mixture of common cleaning products

CP



<chem>CC1=CC=CC=C1C=C</chem> Terpenes	<chem>CC1(C)C(O)C=CC=C1</chem> Terpenoids
<chem>CCCCOCCO</chem> Glycol ethers	<chem>CC(C)O</chem> Alcohols
<chem>CC1=CC=CC=C1C(C)C</chem> Aromatics	



Realistic VOC mixtures

① 28 VOCs typical of office buildings

OB

Ethanol
Isopropanol

1-Butanol
Phenol
Ethylhexanol

Acetone
2-Butanone
MIBK
Hexanal

CS₂ Trichlorofluoromethane (R-11)
1,1,1-Trichloroethane
MTBE 1,2-Dichlorobenzene

2-Butoxyethanol

Toluene
m-Xylene
1,2,4-Trimethylbenzene

n-Nonane
n-Decane
n-Undecane
n-Dodecane

TCE
PCE

DCM
Trichlorofluoromethane (R-11)
1,1,1-Trichloroethane
1,2-Dichlorobenzene

Limonene

Decamethylcyclopentasiloxane (D₅)

② Mixture of common cleaning products

CP

Isopropanol

2-Butoxyethanol

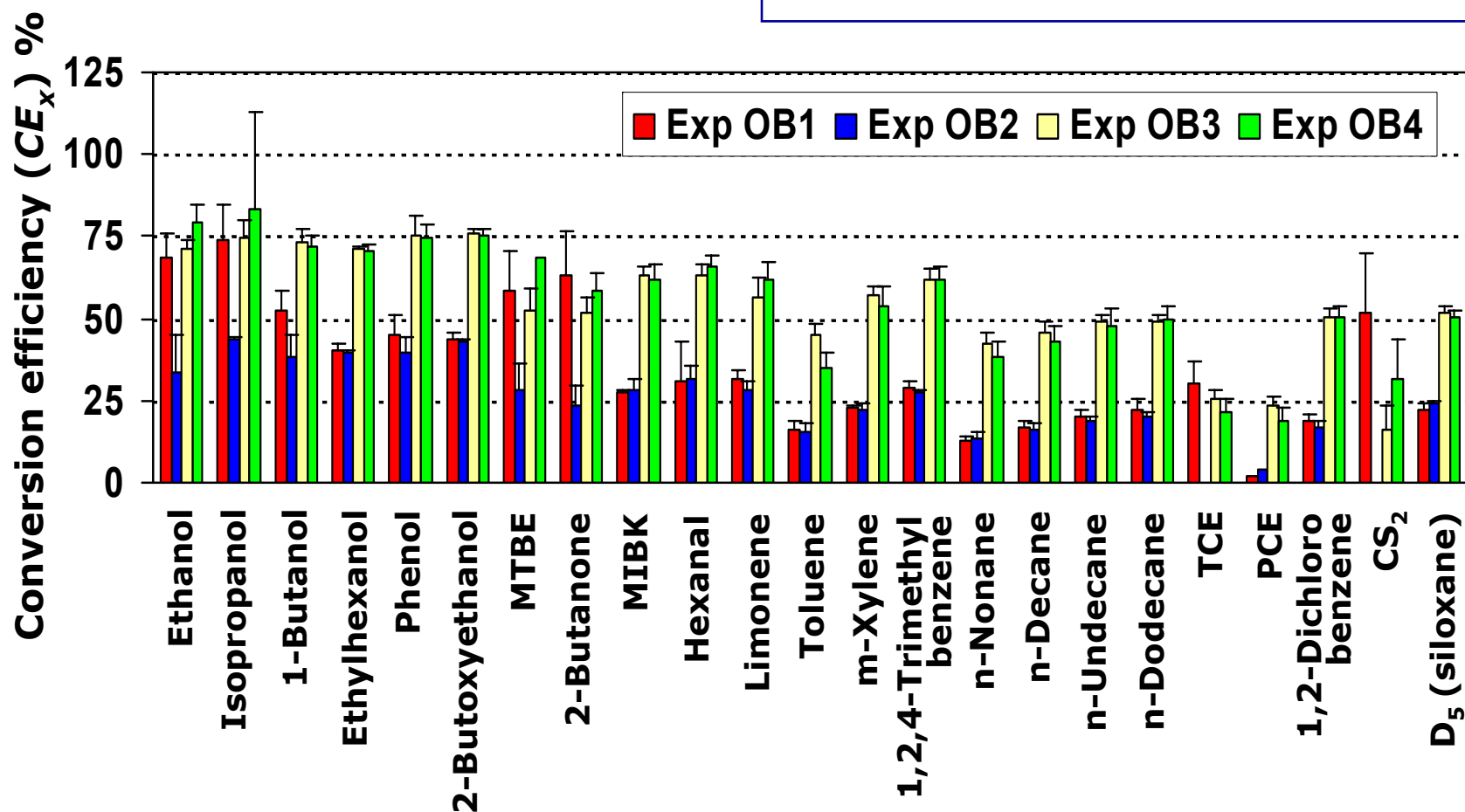
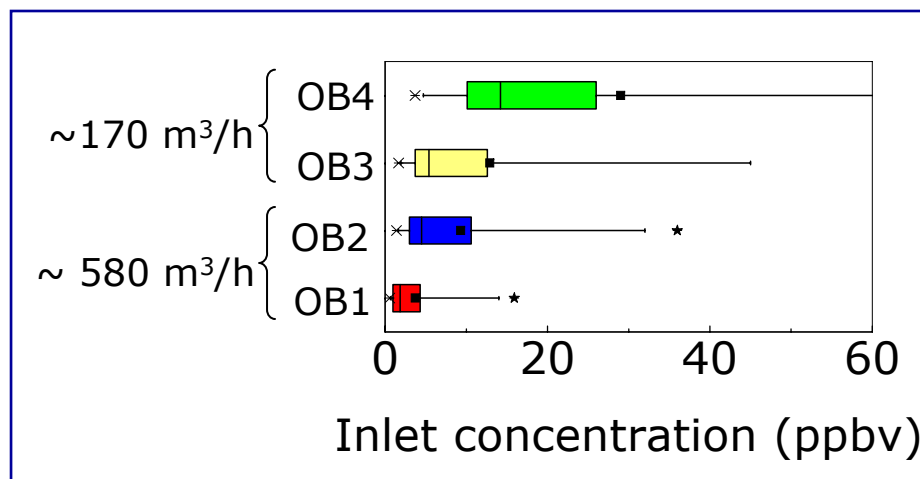
α-Pinene
Limonene
Camphene
γ-Terpinene
Terpinolene

γ-Terpineol
α-Terpineol

p-Cymene

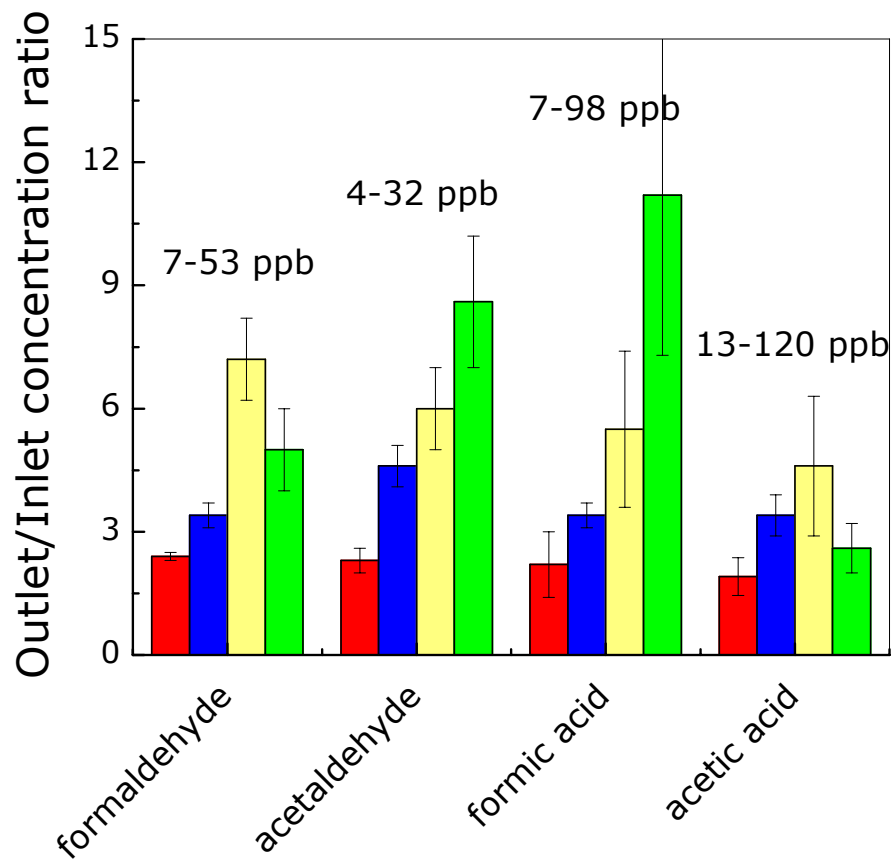
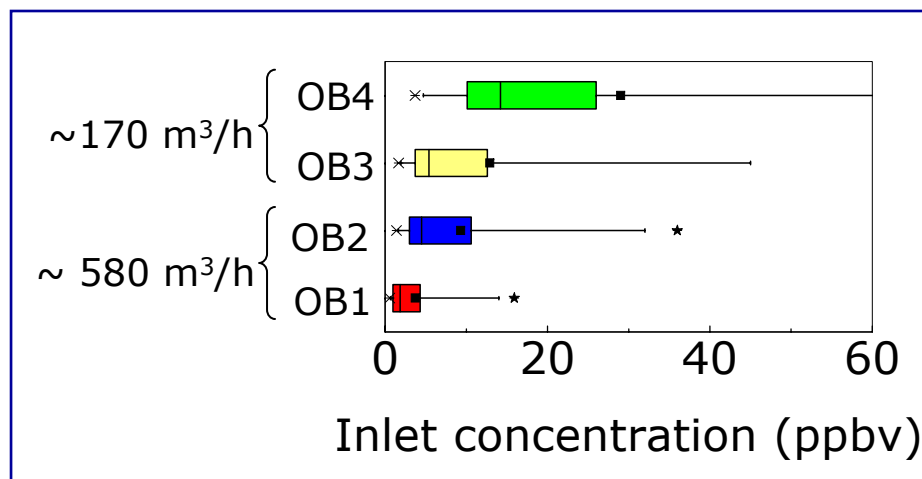


Office building (OB) mixture



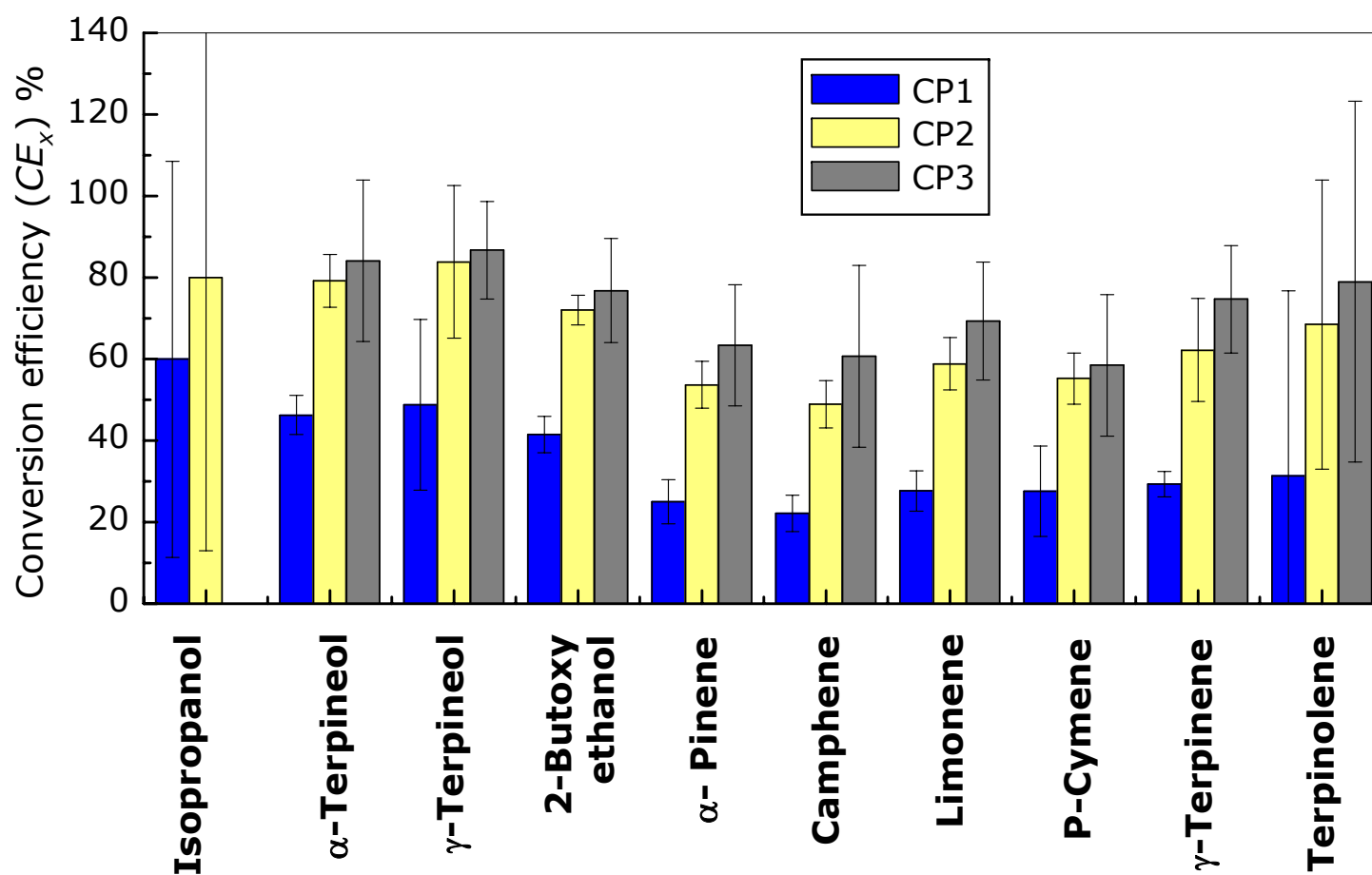
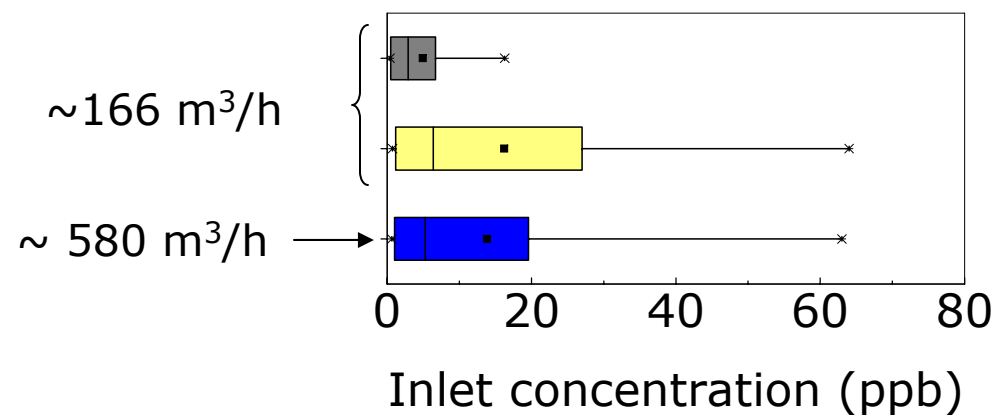


OB mixture: oxidation products



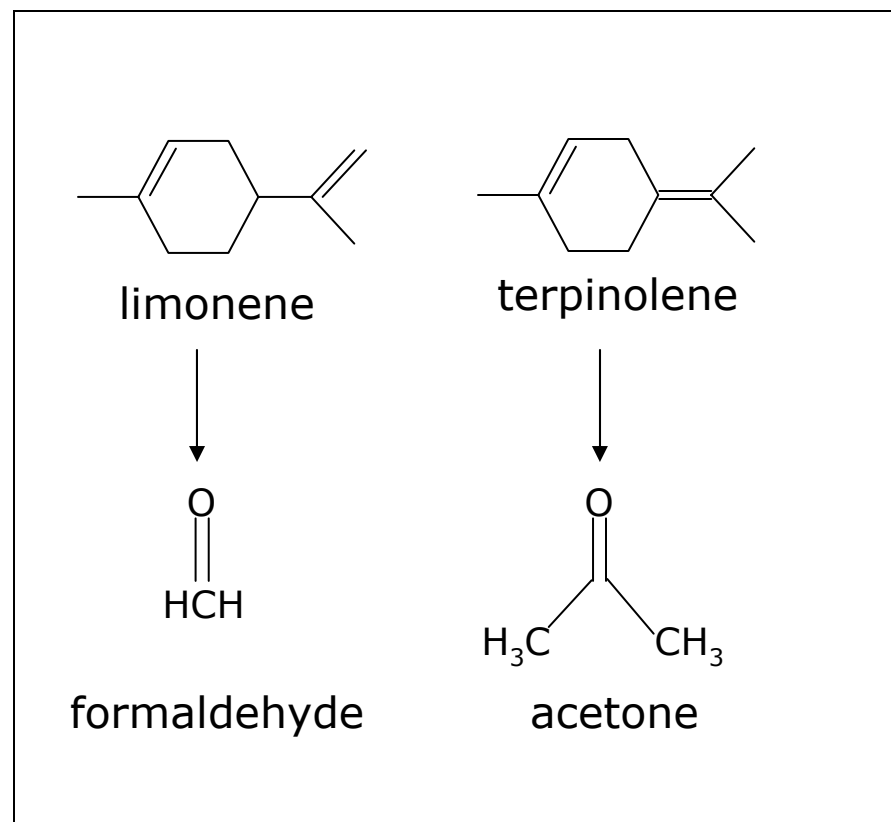
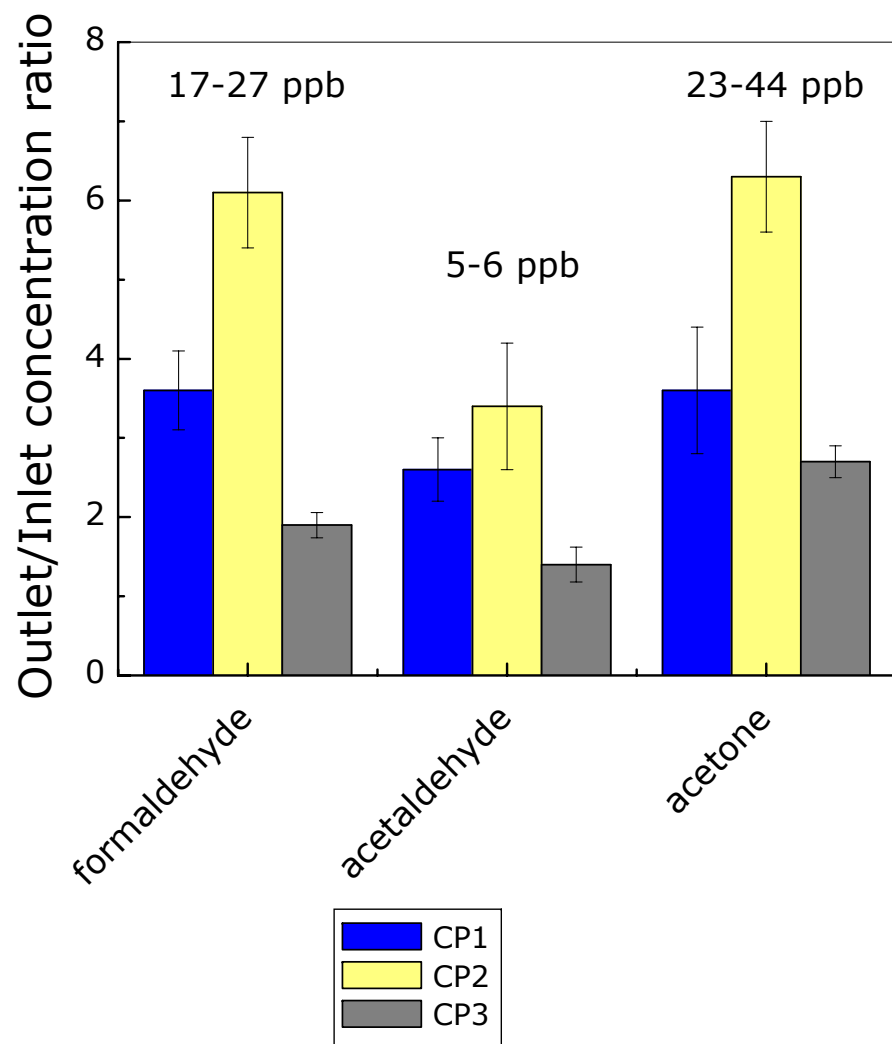


Cleaning products (CP) mixture:





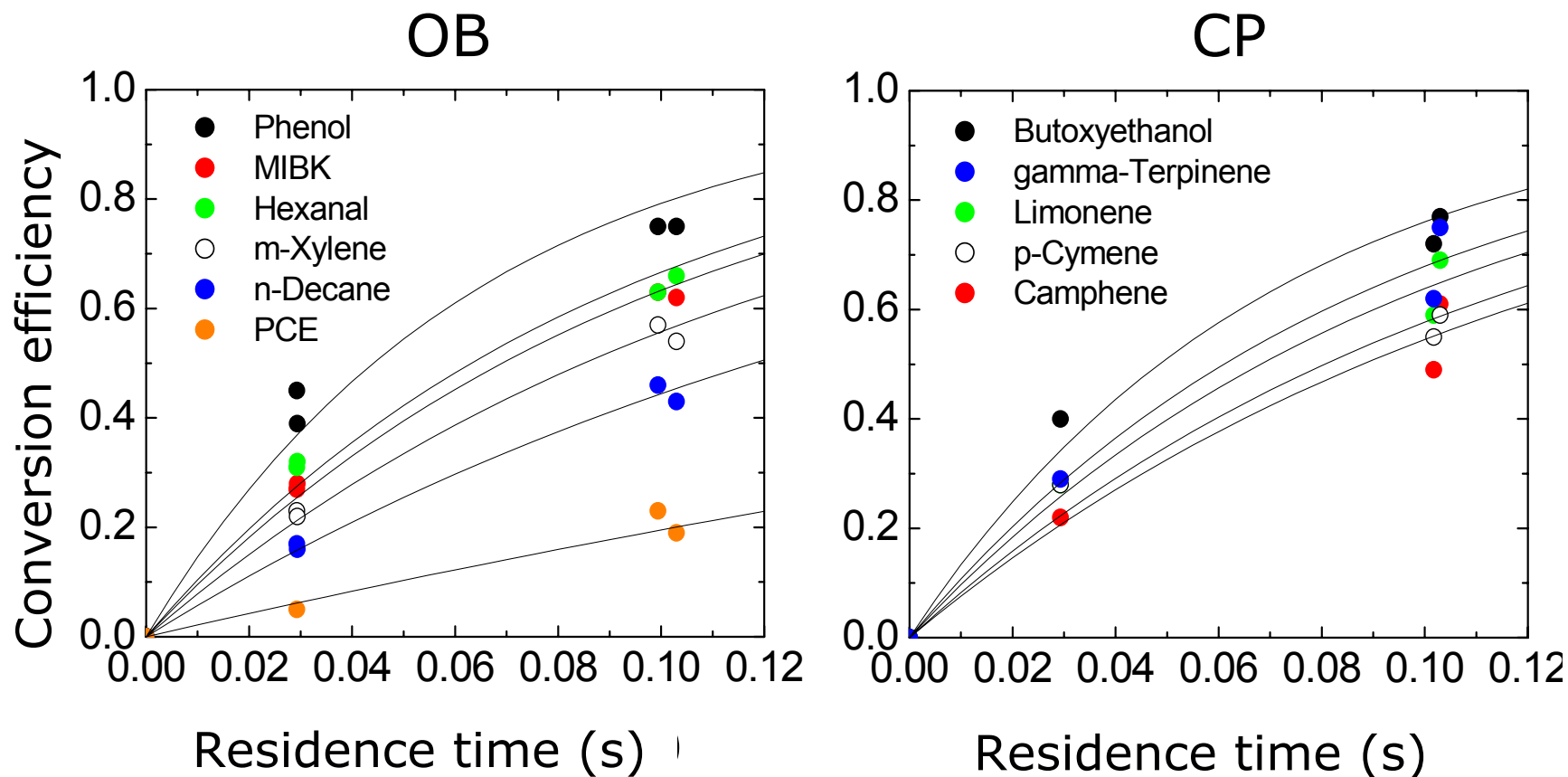
CP mixture: oxidation products





Influence of residence time on conversion efficiency

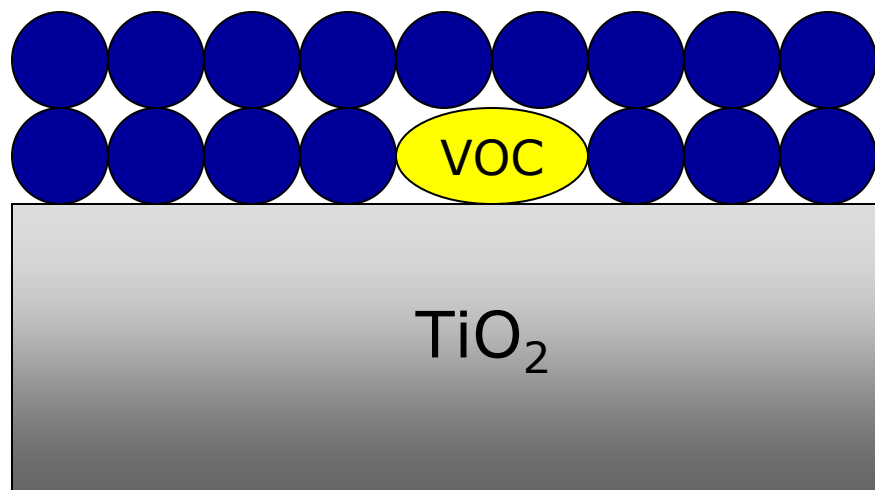
k_x : reaction rate of individual analyte x



$$CE_x = 1 - \exp(-k_x \tau)$$



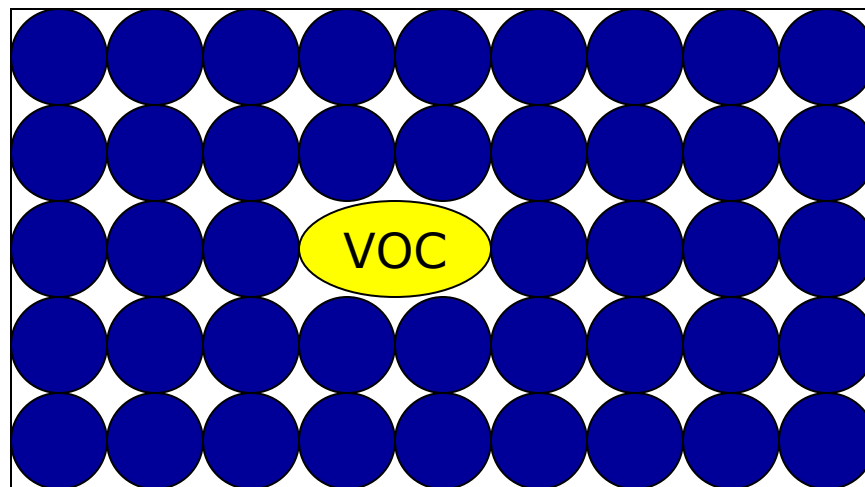
VOC



TiO₂ surface @ 40-60 % RH

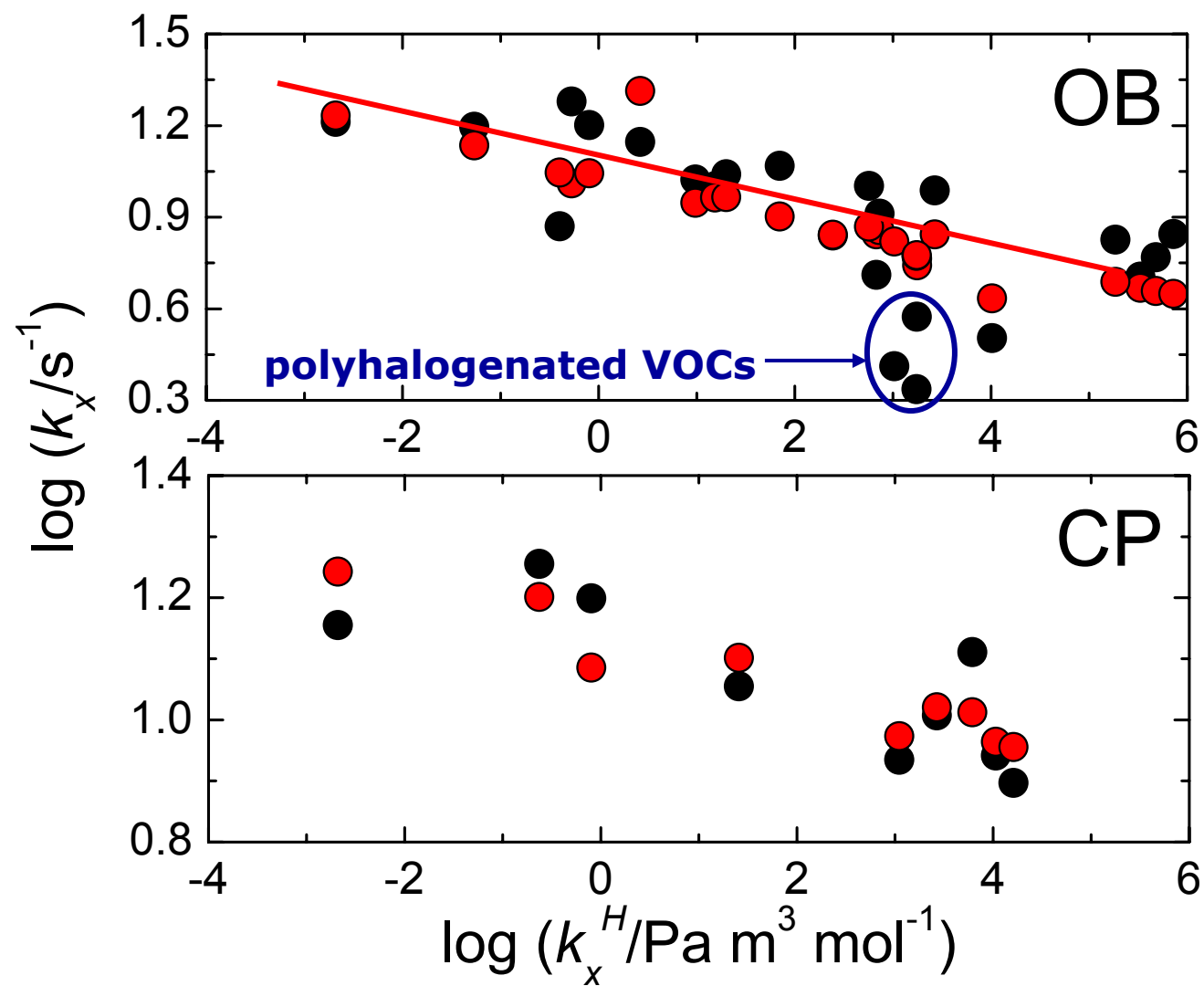
K_{ads}

VOC



bulk water

K_X^H



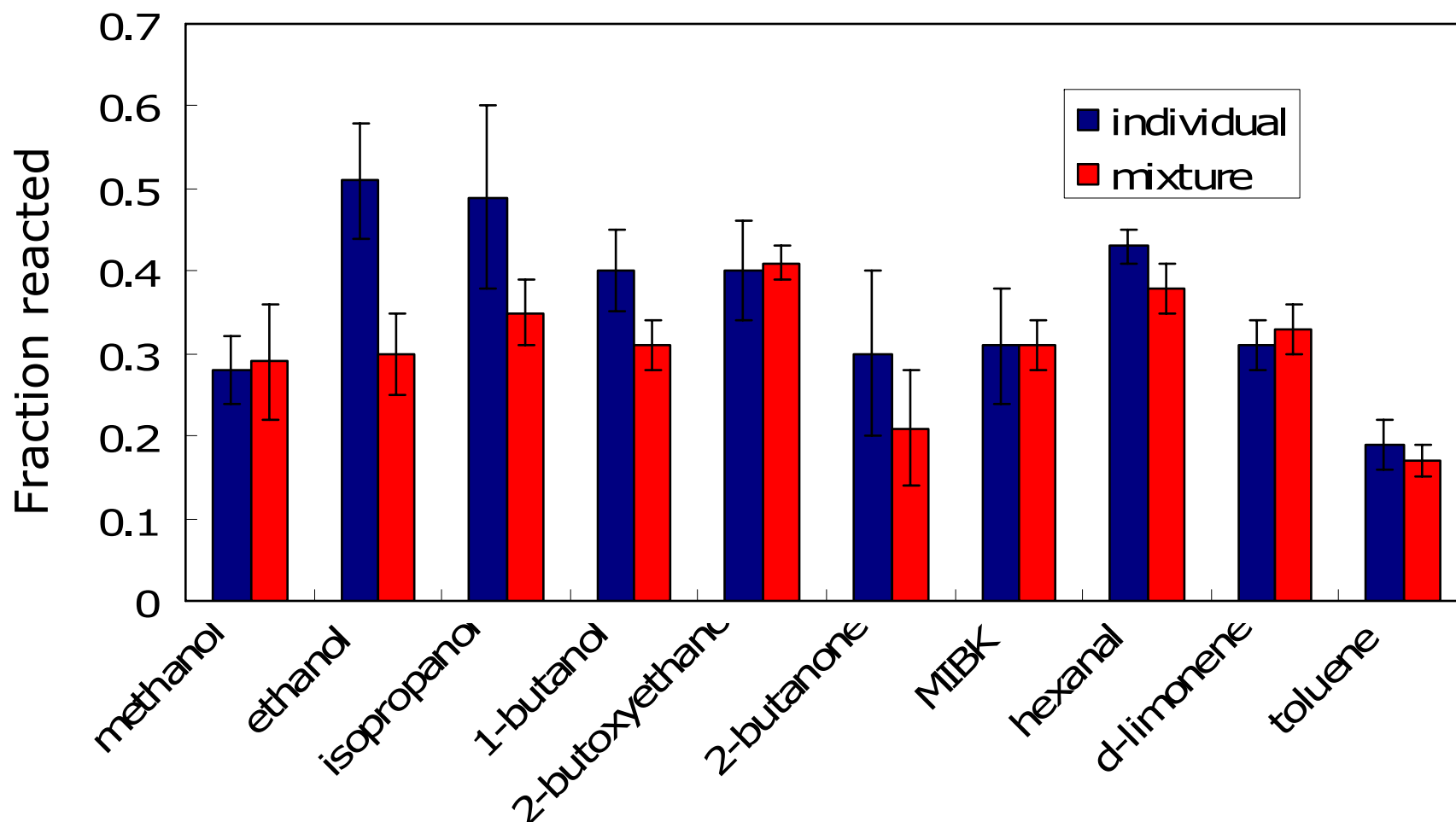
experimental

model

$$\log(k_x) = a + b \log(K_x^H) + c \log(k_x^{OH})$$

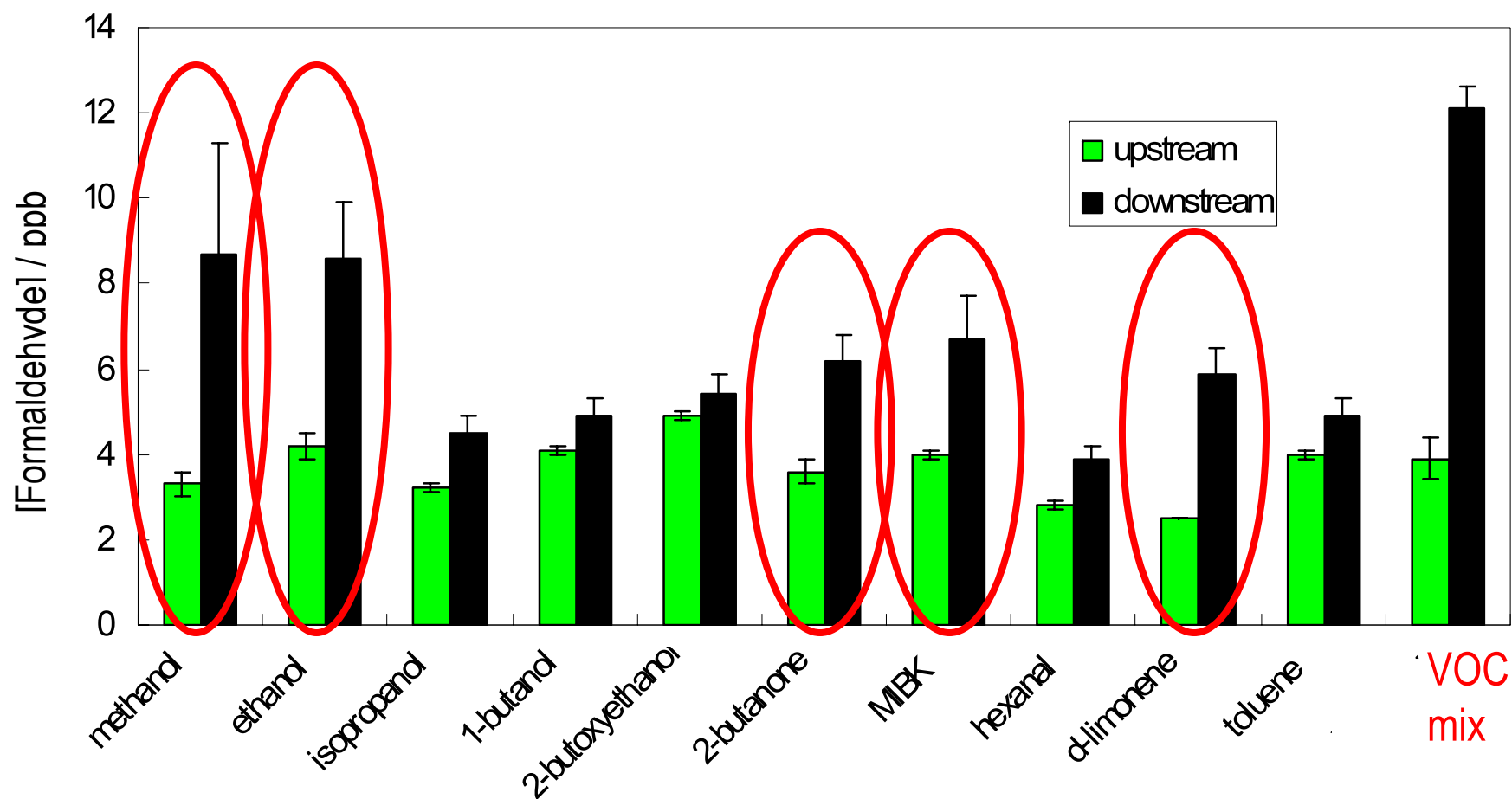


Is there competition between VOCs for TiO_2 active sites?





Byproduct formation: formaldehyde

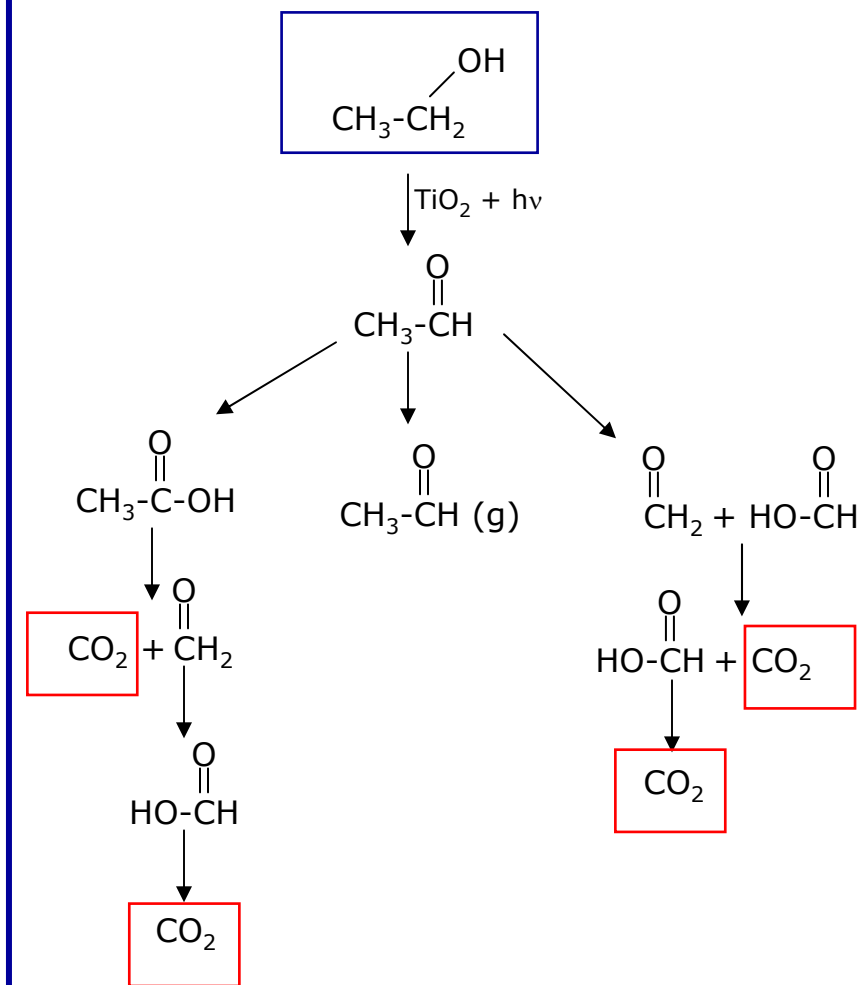




Performance of UVPCO

- Removal efficiency of target pollutants
- Formation of undesired oxidation byproducts
- Catalyst inactivation

Example: mineralization of ethanol





Summary

- Good single pass conversion efficiencies for nearly all VOCs > 20%; in some cases as high as 80%
- Formation of unwanted byproducts (aldehydes); can be fundamentally attributed to oxidation of certain alcohols, ketones and terpenes.
- Henry's law constant is good correlation parameter to predict reaction rate of individual pollutants
- At concentrations typical of buildings (low ppb range), there is no competition between VOCs for active TiO_2 sites

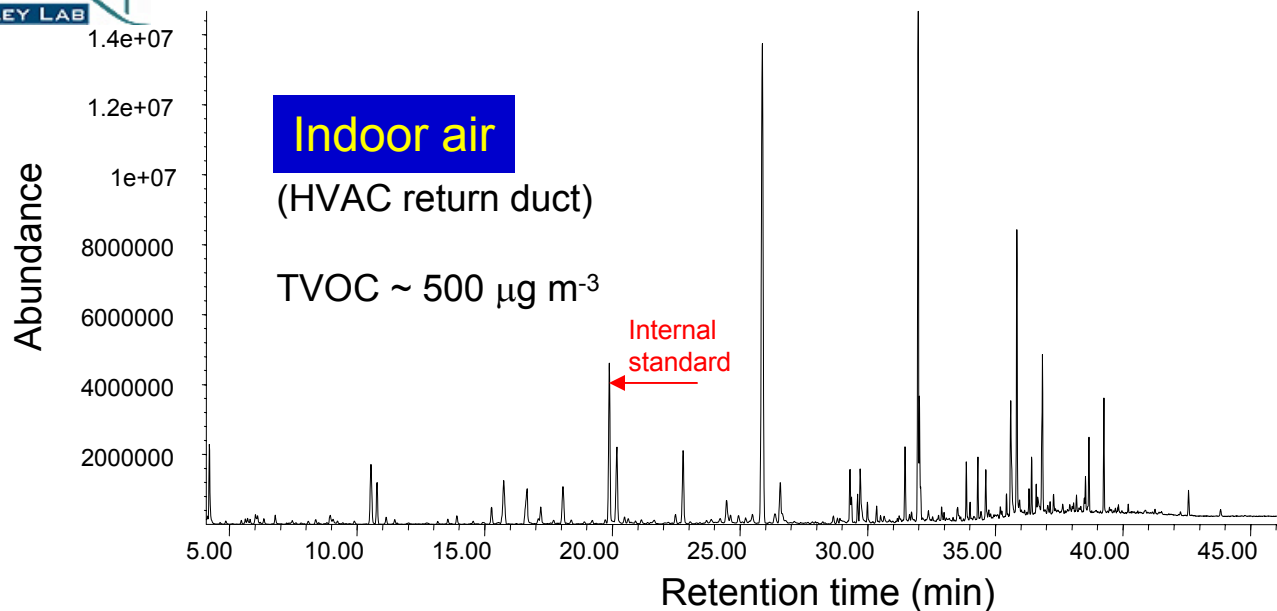


Questions for discussion: How to define and evaluate the performance of passive PCO ?

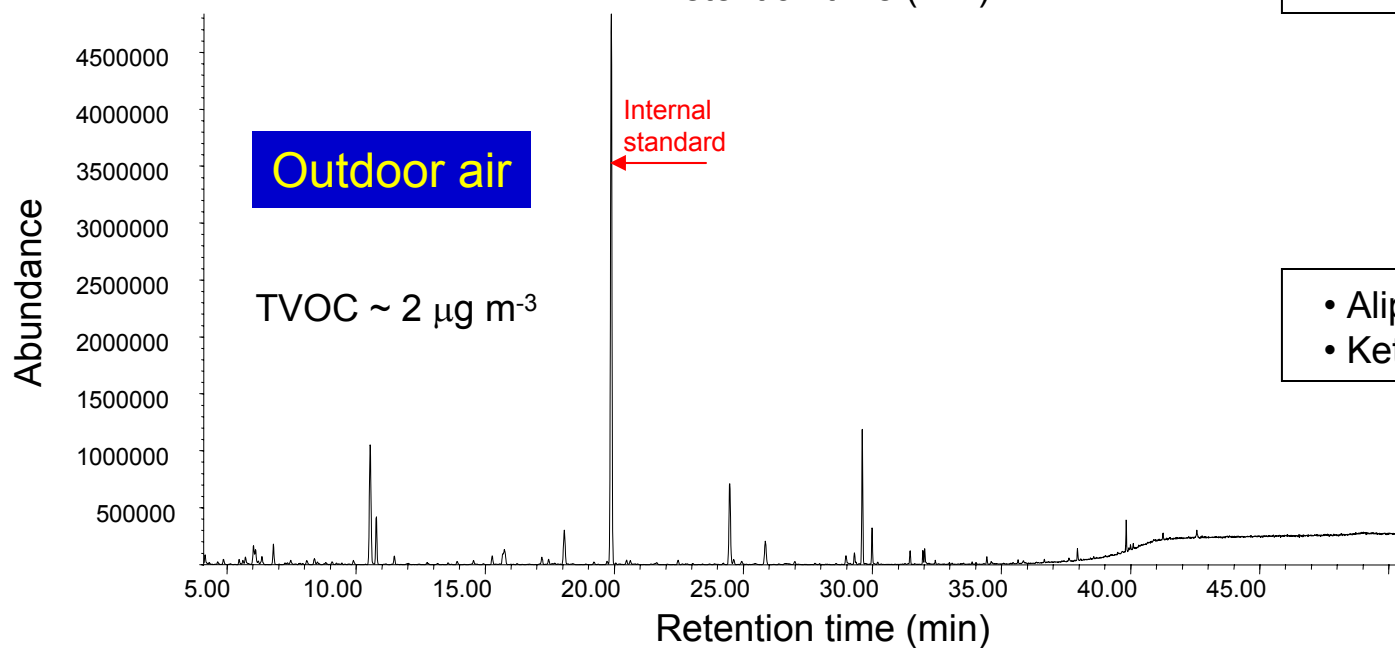
- Which are the most critical target pollutants?
- Is TiO_2 (anatase) the most appropriate photocatalyst for those target pollutants?
- Should we be concerned about secondary product formation?
- Evaluation of long-term inactivation of catalyst. Regeneration?
- Effect of relative humidity on catalyst performance
- Cost analysis



Raw data: office building in Los Angeles



- Alcohols
- Aliphatic hydrocarbons
- Aldehydes
- Ketones
- Aromatic hydrocarbons
- siloxanes
- Ethylene glycols
- Glycol ethers
- Light PAHs (naphthalenes)
- Terpenoids
- Phenols
- Phthalate esters
- ... (others)...

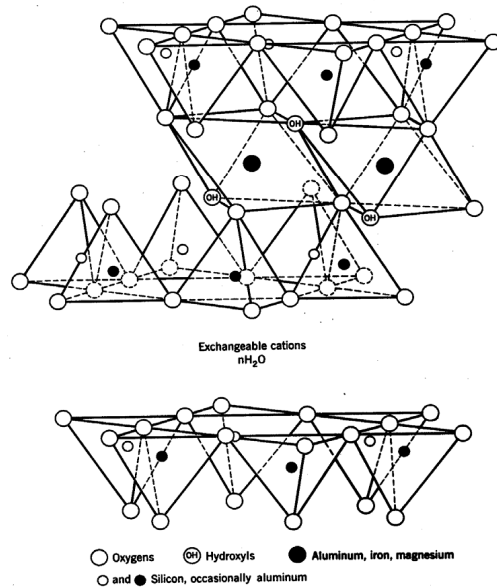


- Aliphatic hydrocarbons
- Ketones

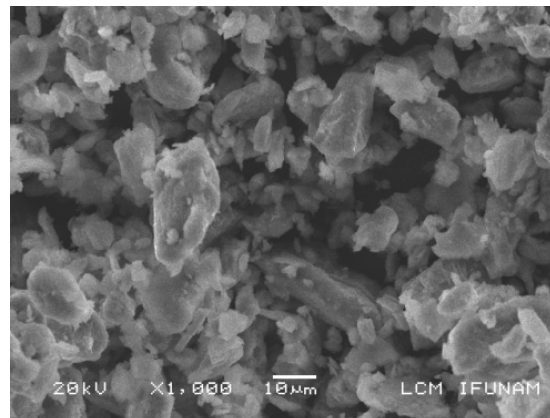


Composite photocatalysts materials

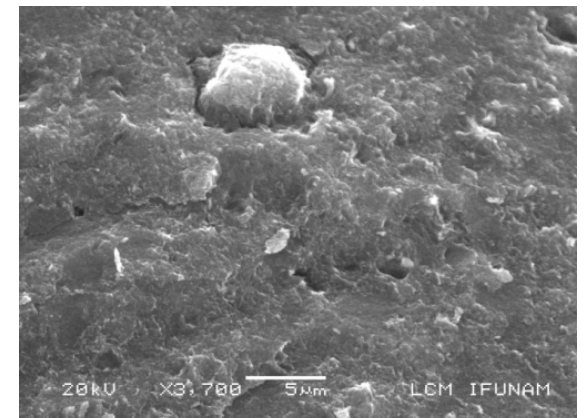
- PICADA project (Strini et al, 2005):
TiO₂-containing cementitious materials:
 - cement rendering (cement + lime + sand)
 - mineral paint
- TiO₂-pillared clays



Hectorite

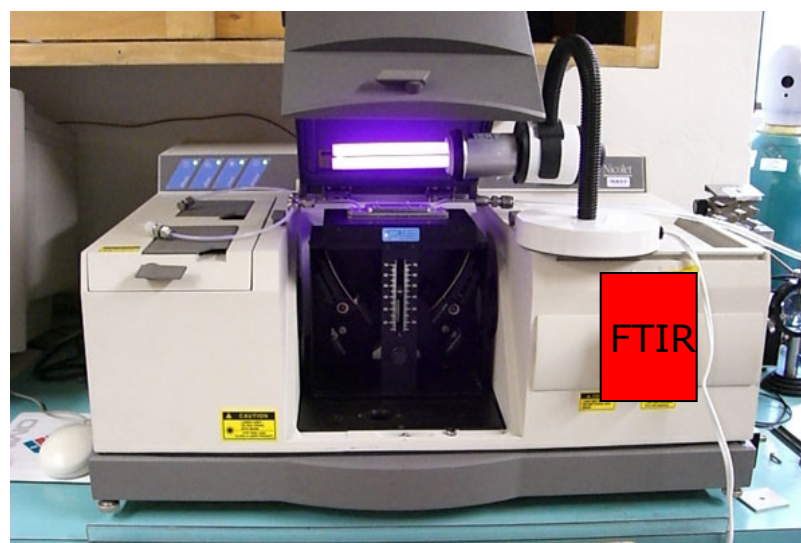
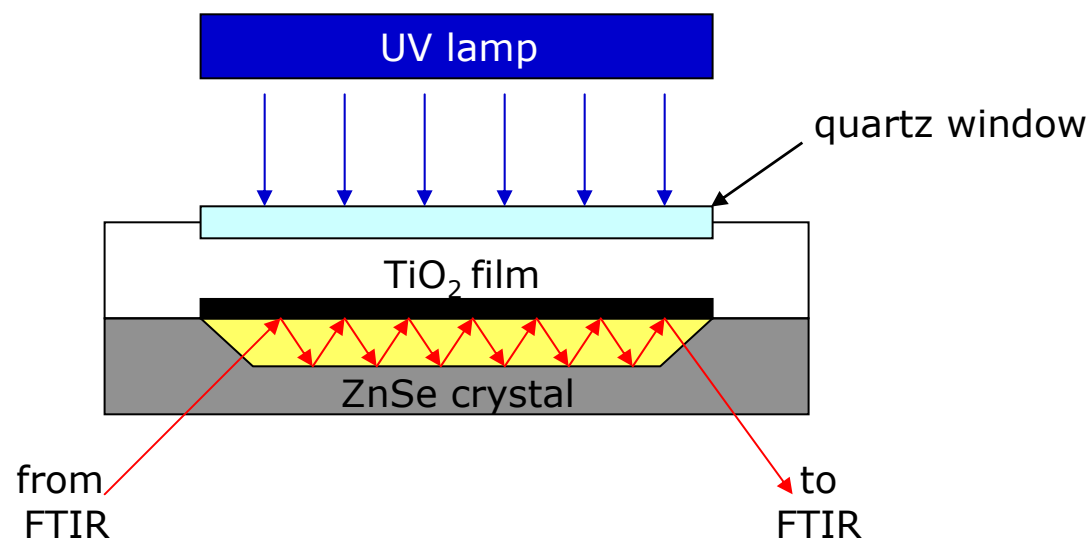


TiO₂ - Hectorite



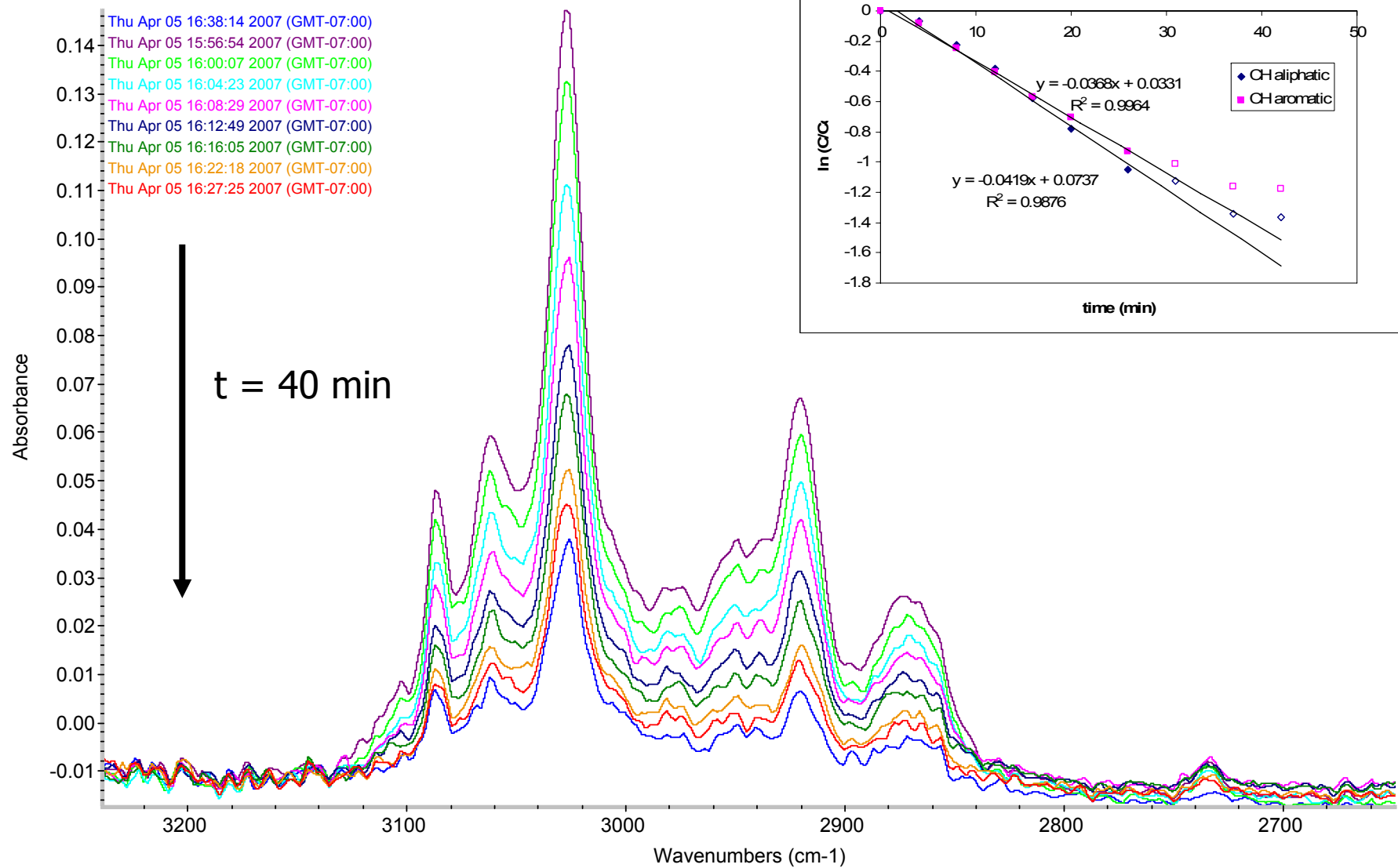


Attenuated total reflection-FTIR chamber





Attenuated total reflection-FTIR spectra





Acknowledgements

David Faulkner
Toshifumi Hotchi
Raymond Dod

Stephen O. Hay
Norberto Lemcoff

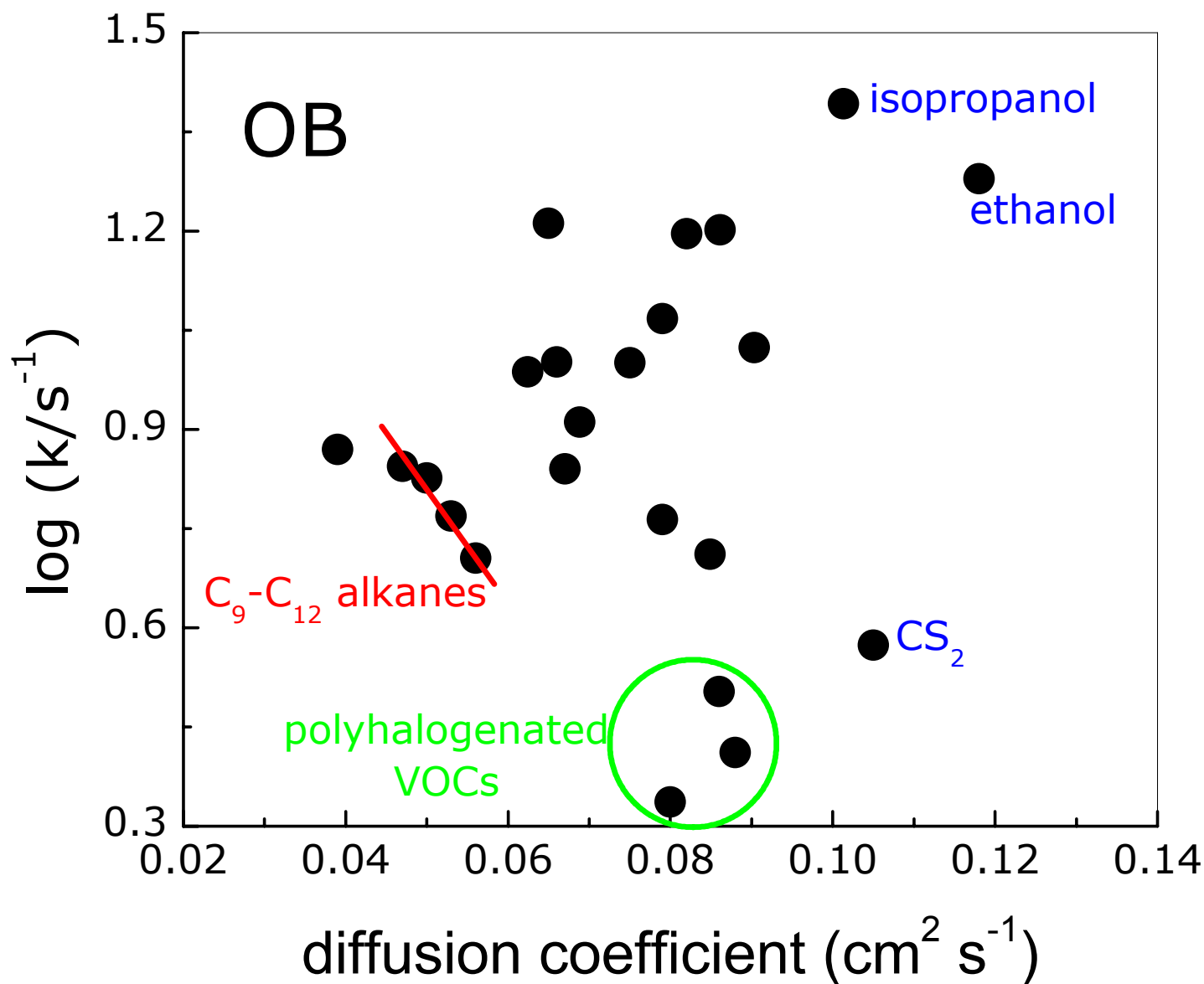
Javiera Cervini-Silva
Daria Kibanova

Funding: US Department of Energy (DOE)
Building Technologies Program
Terry Logee, Program Manager
Contract No. DE-AC02-05CH1123

Laboratory Directed Research and Development
(LDRD) program, LBNL.



Are kinetics controlled by mass-transfer?





Are kinetics controlled by the chemical step?

Langmuir - Hinshelwood

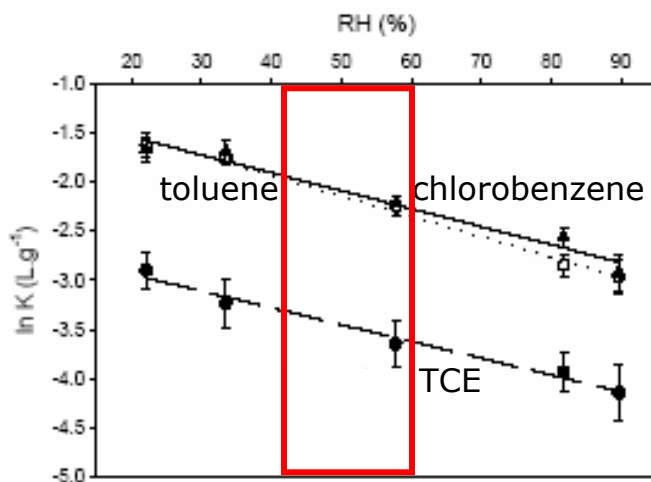
$$\frac{\partial[X]}{\partial t} \sim k \theta_X \theta_{O_2}$$

Parameters: k_x^{OH} ?

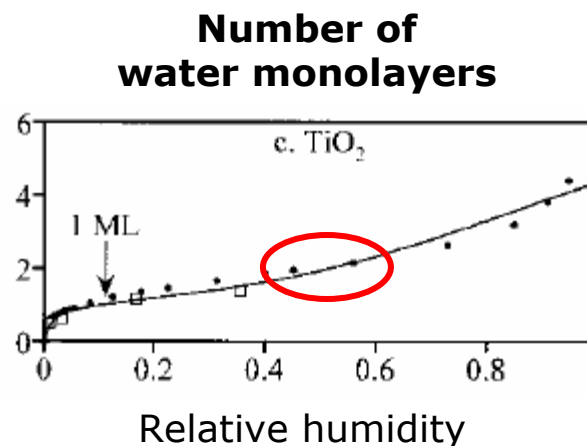
$$\theta_X = \frac{K_{ads}[X]}{(1 + K_{ads}[X])}$$

Apparent binding constant

K_{ads} depends on surface water



Demeestere et al. *Chem. Eng. Sci.* **2003**, 58, 2255-2267.



Goodman et al. *J. Phys. Chem. A* **2001**, 105, 6443-6457.



VOC removal efficiency

Fraction reacted

