INDOOR CHEMISTRY OF BUILDING MATERIALS

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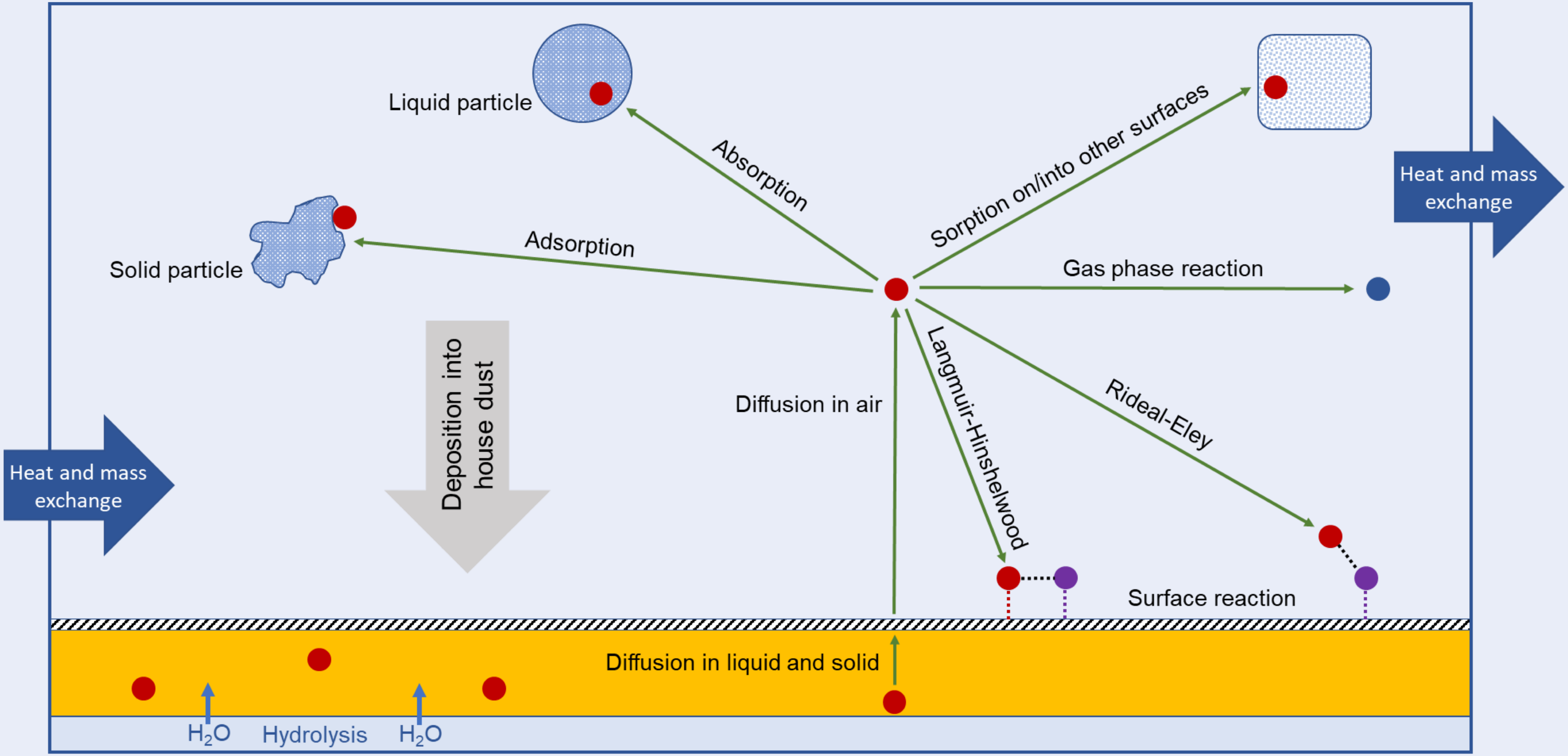
Dynamics and reactions of organic compounds in the indoor environment



Salthammer and Morrison (2021) to be published (© Figure: T. Salthammer)

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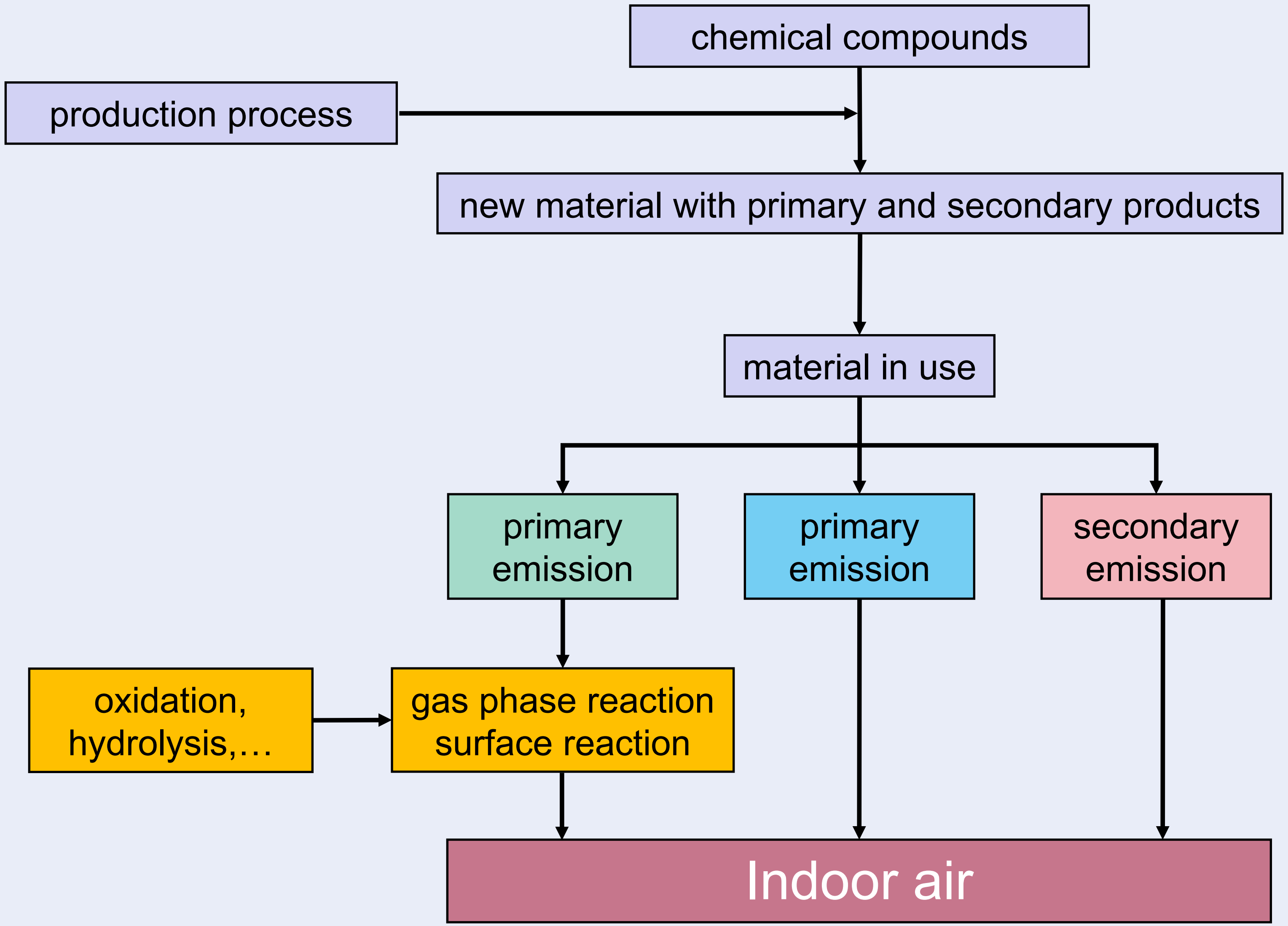
Formation of primary and secondary emissions from chemical constituents of building materials



Possible reaction products in indoor air with potential emission sources and reactants

	Reactants	Products	Possible source
Ozone chemistry	α-pinene	Pinene oxide, pinonaldehyde	Wood, wood-based products
	Limonene	Limonene oxide, carvone, formaldehyde	Wood, coating systems
Thermal degradation	Oleic acid	Heptanal, octanal, nonanal, decanal, 2-decenal	Linoleum, eco-lacquers, nitrocellulose-lacquers, alkyd resins
	Linolenic acid	2-pentenal, 2-hexenal, 3-hexenal, 2-heptenal, 2,4-heptedienal, 1-penten-3-one	
	Linoleic acid	Hexanal, heptanal, 2-heptenal, octanal, 2-octenal, 2-nonenal, 2-decenal, 2,4-nonadienal, 2,4-decadienal	
Thermal degradation	Hemicelluloses	Furfural, acetic acid	Cork
Photochemistry	PHMP	Benzaldehyde, acetone, benzil	UV-cured coatings
	HCPK	Benzaldehyde, cyclohexanone, benzil	UV-cured coatings
Hydrolysis	2-ethyl-hexyl acetate	Acetic acid, 2-ethyl-1-hexanol	Solvent
	Zn-2-ethylhexanoate	2-ethyl-1-hexanoic acid	Stabilizers
	n-butylacrylate	*n*-butanol	Acrylate coatings
	DEHP	2-ethyl-1-hexanol	Plasticiser
	DBP	*n*-butanol	Plasticiser
	DIBP	2-butanol	Plasticiser
Thermal degradation	TCPP	1-chloro-2-propanol, 2-chloro-1-propanol	Flame retardant
	TDCPP	1,2-dichloropropane, 1,2-dichloropropanol	Flame retardant
	TCEP	2-chloro-ethanol	Flame retardant
	TBPP	1-bromo-2-propanol, 2-bromo-1-propanol	Flame retardant
	TDBPP	2,3-dibromo-1-propanol	Flame retardant
Diels-Alder reaction	Styrene + cis-1,3-butadiene	4-phenyl-cyclohexene (4-PCH)	SBR
	Cis-1,3-butadiene + trans-1,3-butadiene	4-vinyl-cyclohexene (4-VCH)	SBR
	2-chloro-1,3-butadiene	1-chloro-4-(1-chlorovinyl)-cyclohexene 1-chloro-5-(1-chlorovinyl)-cyclohexene	Rubber
Thermal degradation	Zn-diethyldithiocarbamate	CS_2, diethylamine	Vulcanization accelerator
	Azodicarbonamide	Semicarbazide	Foaming agent
	Adipinic acid + 1,4-butanediol	1,6-dioxa-cyclododecane-7,12-dione	Adhesive
	Dimethylaminoethanol + formic acid	Dimethylformamide	"Green" paint
Metabolism	l-tryptophane	*o*-aminoacetophenone	Casein products
	2,3,4,6-tetrachlorophenol	2,3,4,6-tetrachloroanisole	Application of PCP
	T4MDD	MIBK, 3,5-dimethyl-1-hexyne-3-ol	Water-based paint
Thermal degradation	AIBN	Tetramethyl succinonitrile	Flexible PU foam

Uhde and Salthammer (2007) Atmos. Environ.

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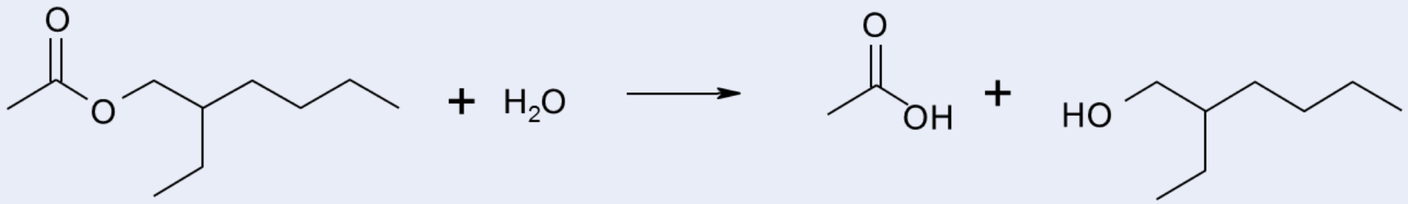
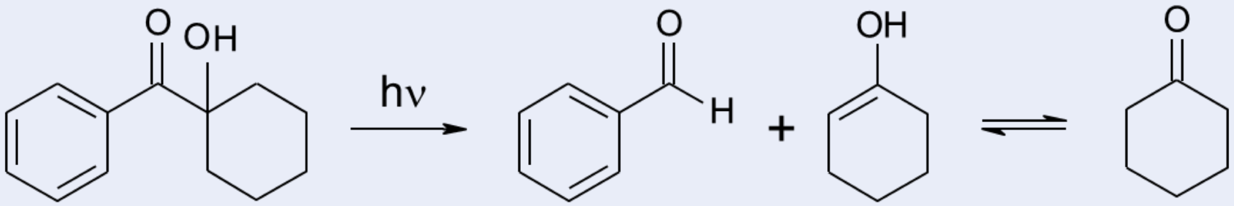
Release of VOCs – examples of indoor chemistry

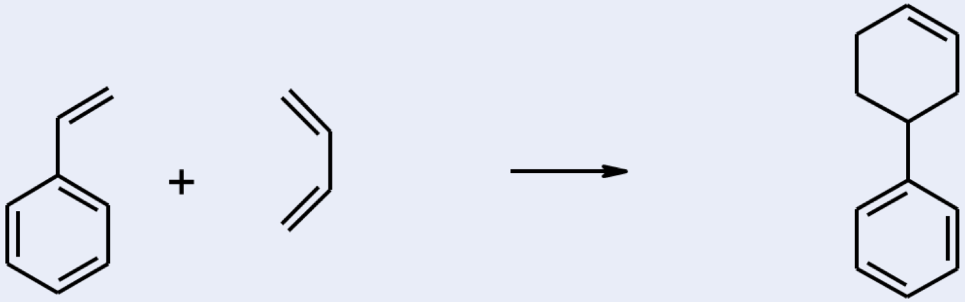
Hydrolysis in floorings
(degradation of esters)



Photochemisty in lacquers
(degradation of photoinitiators)

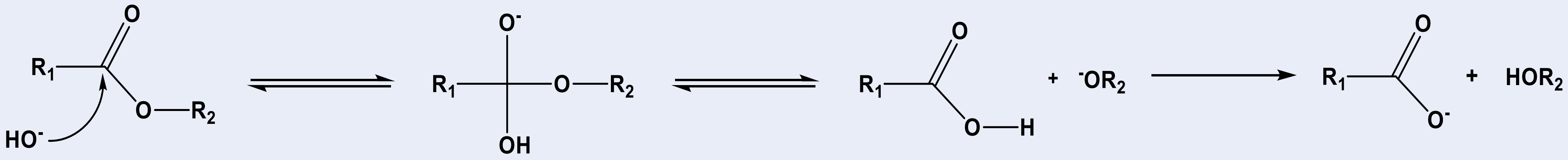


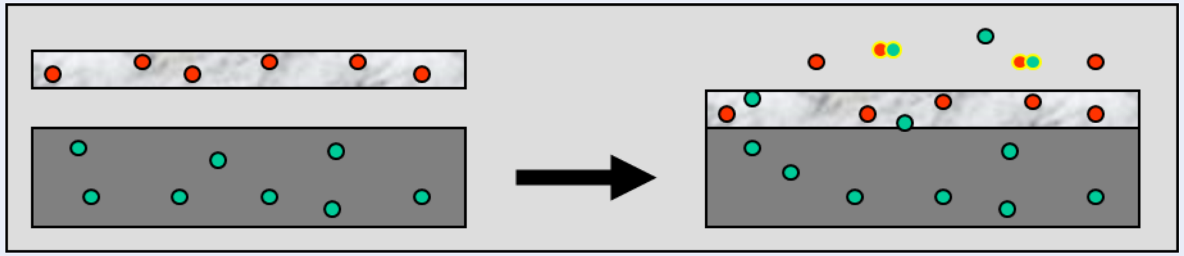
Diels-Alder reaction in SBR
(Styrene-Butadiene-Rubber)

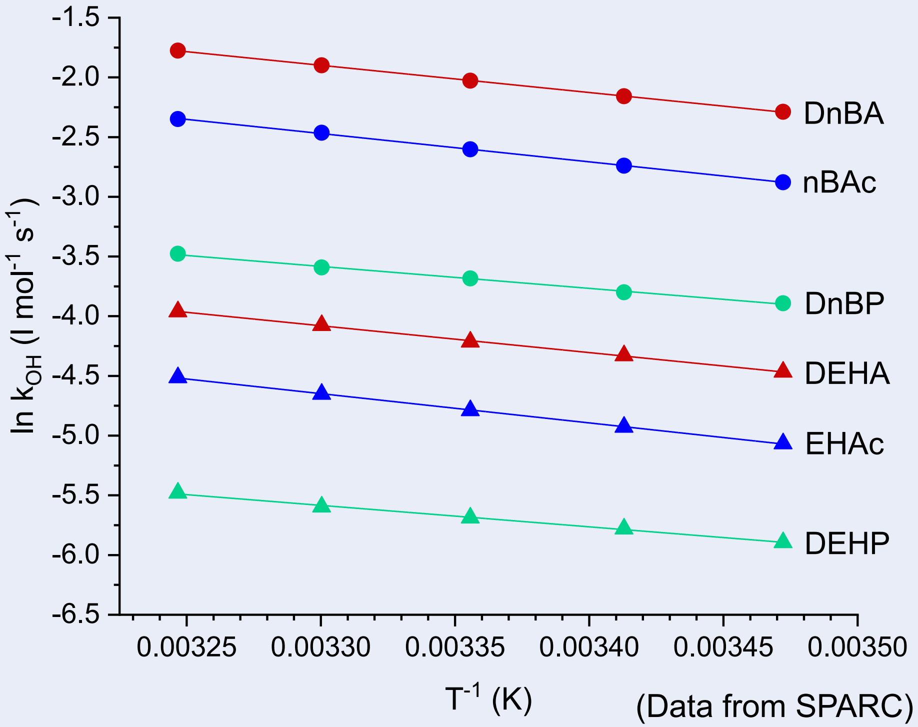


Uhde and Salthammer (2007) Atmos. Environ.

Ester hydrolysis in alkaline media: the classical reaction of indoor chemistry

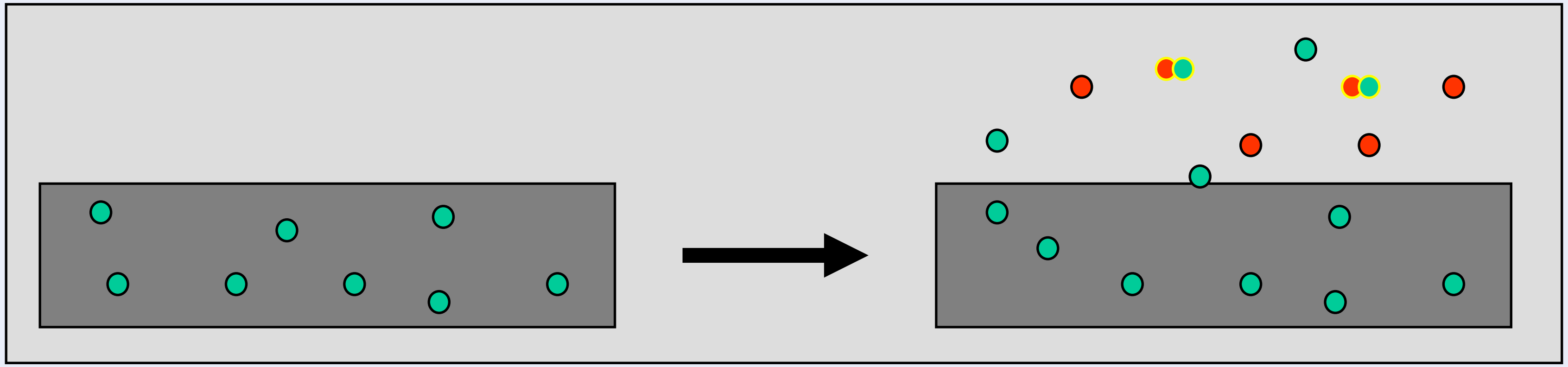


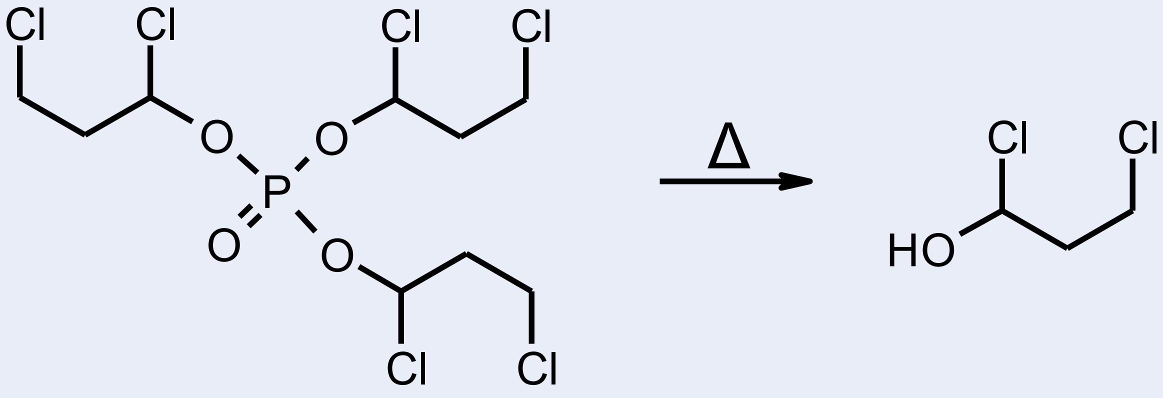




(Data from SPARC)

The thermal degradation of flame retardants in polyurethane foam



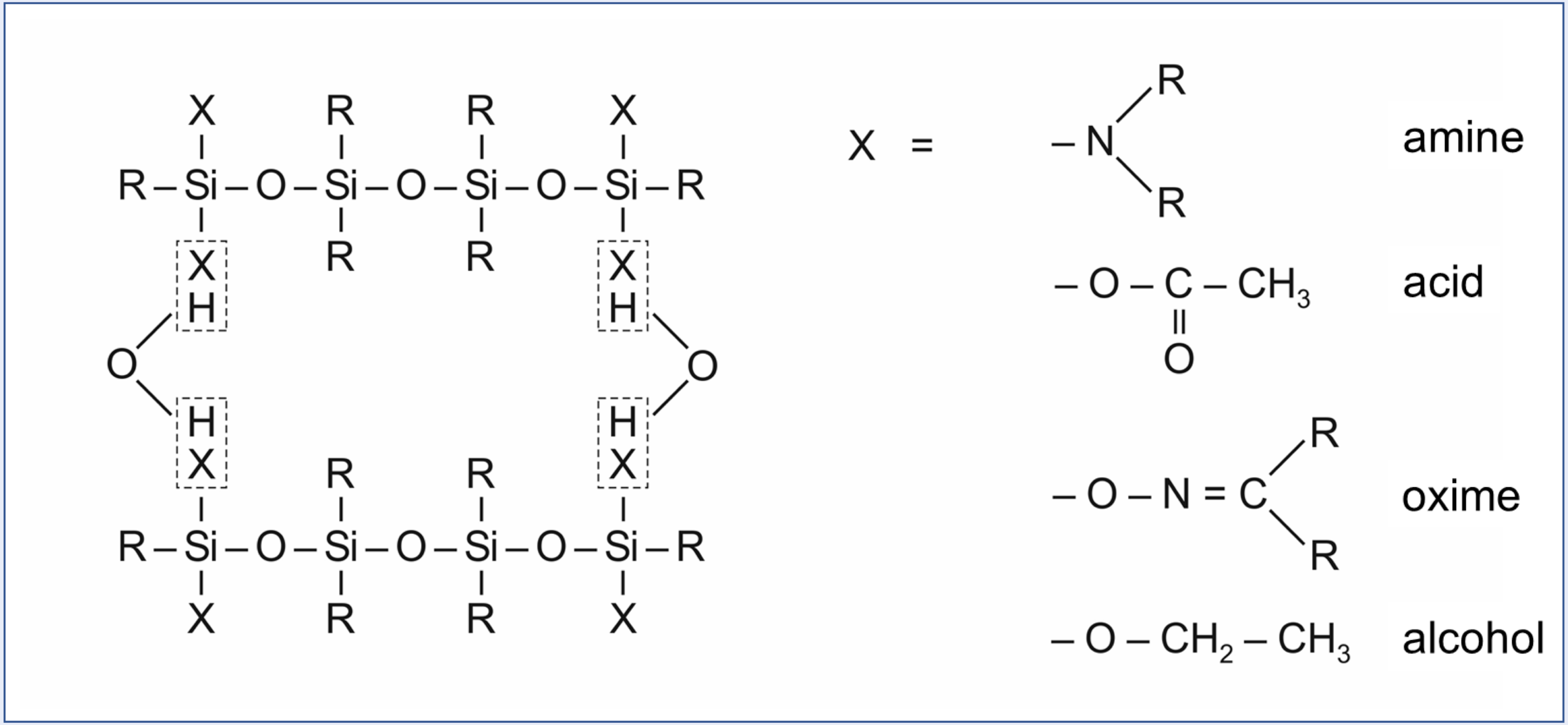


TDCPP

1,3-Dichloro-propanol

Salthammer et al. (2003) Indoor Air

Reaction products from condensation: the curing of silicone



Floor coverings: 1 m³ chamber test of UV coated cork parquet applied on concrete

Cork parquet (UV coated) + adhesive on concrete	24 h	168 h	576 h	Source
Compound	$\mu g\ (h\ m^{-2})$			
CS_2	3	< 1	< 1	Degradation of additive (adhesive)
Acetic acid	640	189	67	Degradation of hemicellulose
Furfural	203	43	31	Degradation of hemicellulose
Styrene	3	2	< 1	Monomer
Benzaldehyde	5	3	2	Degradation of photoinitiator
Cyclohexanone	4	3	7	Degradation of photoinitiator
Phenol	2044	729	276	Cork binder
Methylbenzoate	8	2	< 1	Degradation of photoinitiator
4-Phenylcyclohexene	13	2	1	Diels–Alder product
Benzophenone	136	219	189	Photoinitiator
Sum of other VOCs	216	42	28	

Test parameters: $T = 23\,°C$, r.h. $= 45\%$, $n = 1.0\,h^{-1}$, $L = 1.0\,m^2\,m^{-3}$.

Uhde and Salthammer (2007) Atmos. Environ.

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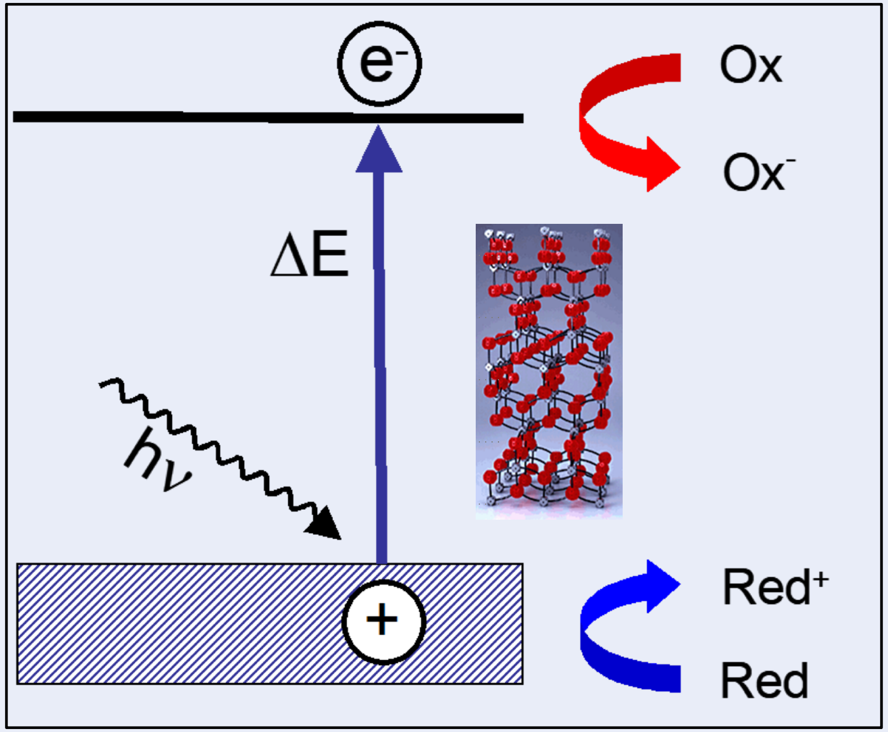
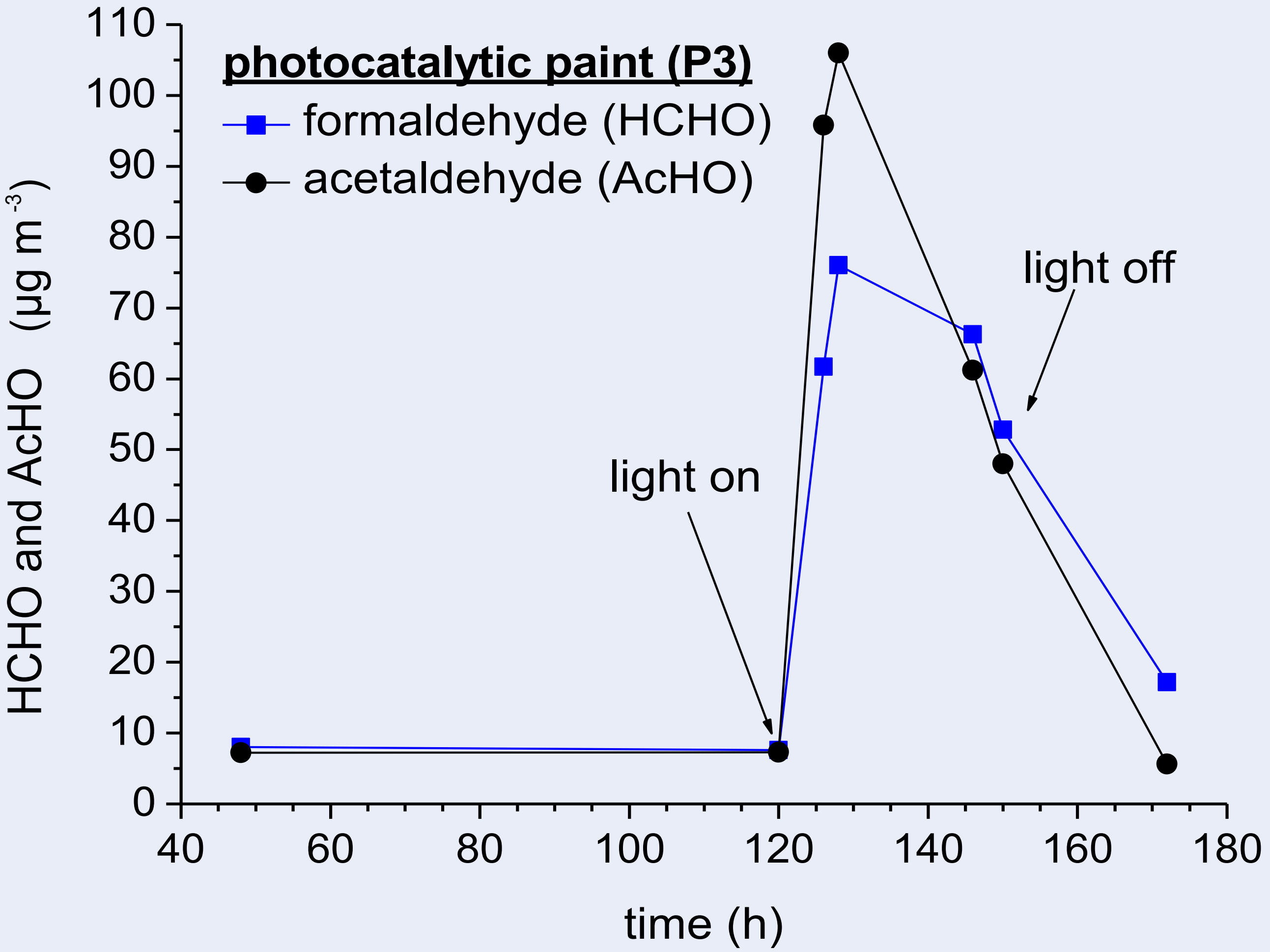
Formation of pollutants from a photocatalytic wall paint (chamber experiment)





Salthammer and Fuhrmann (2007) ES&T

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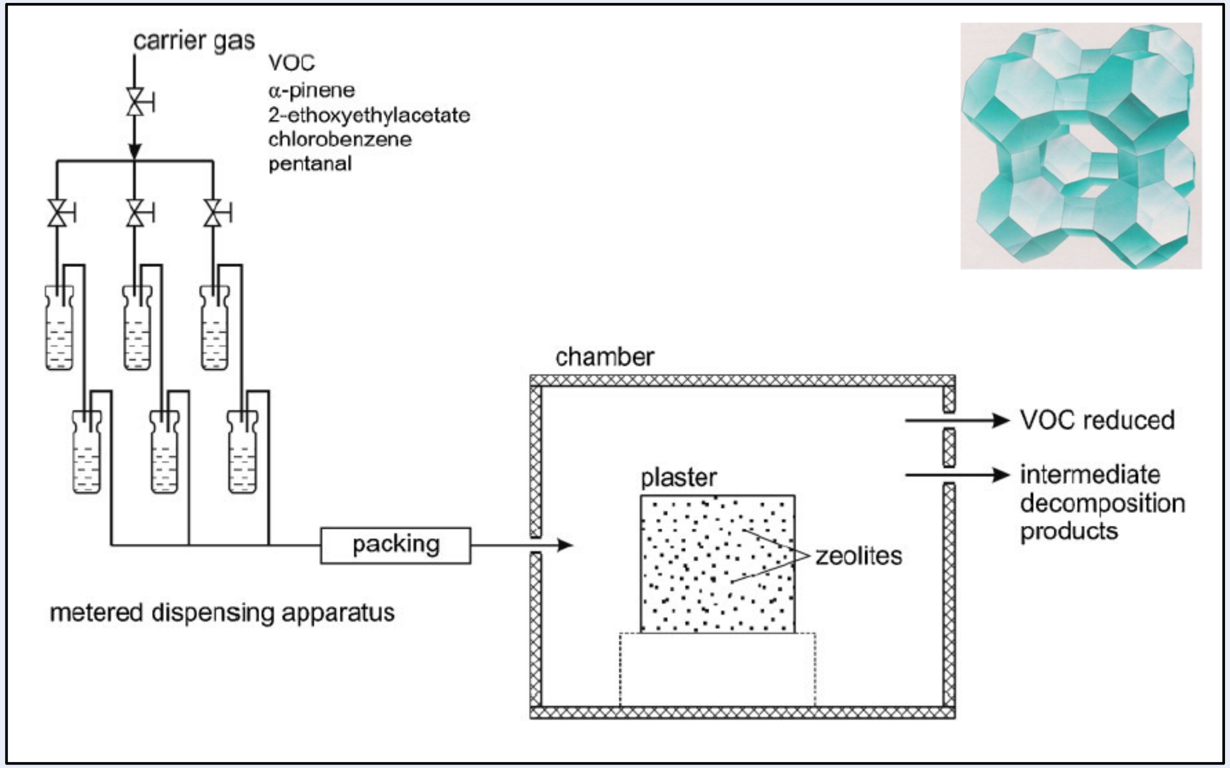
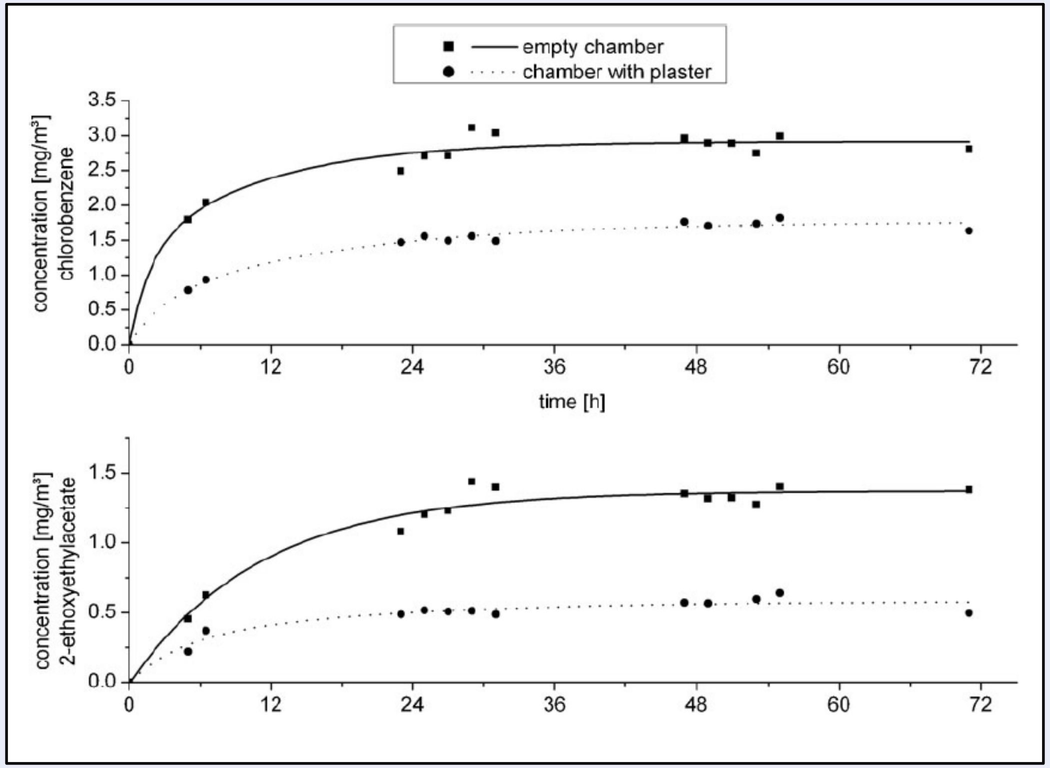
Catalyzed reactions on mineral plaster materials

Chamber experiment



Sorption effect



Gunschera et al. (2013) CLEAN – Soil, Air, Water

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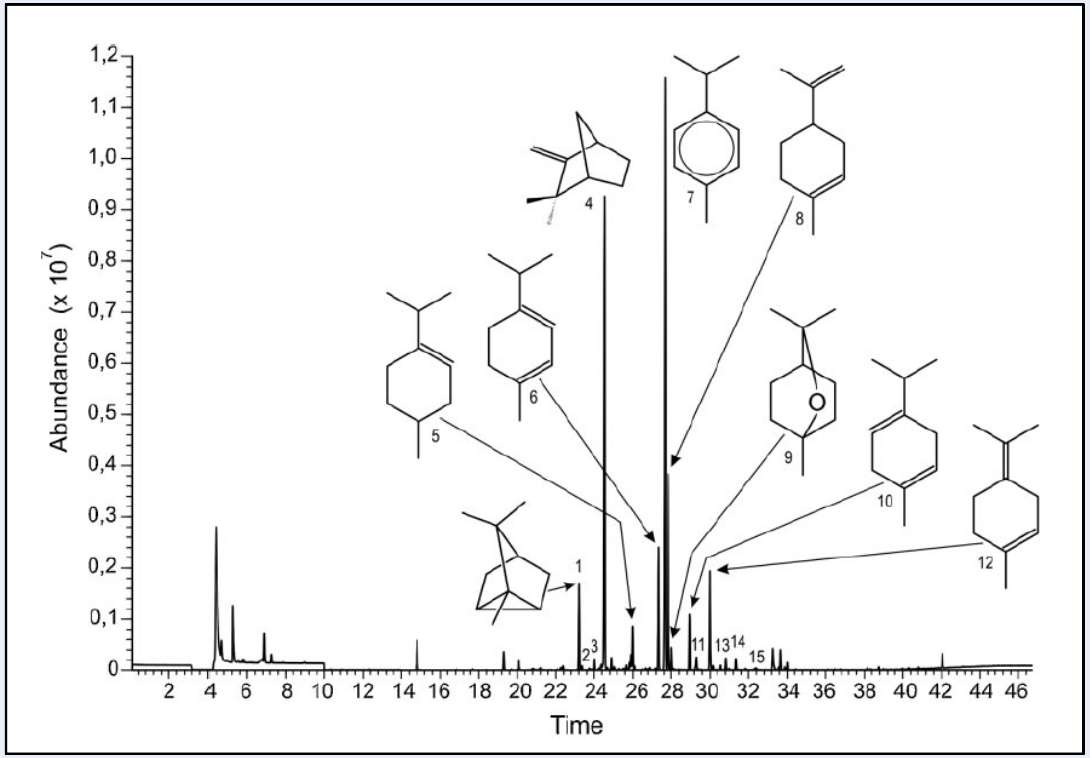
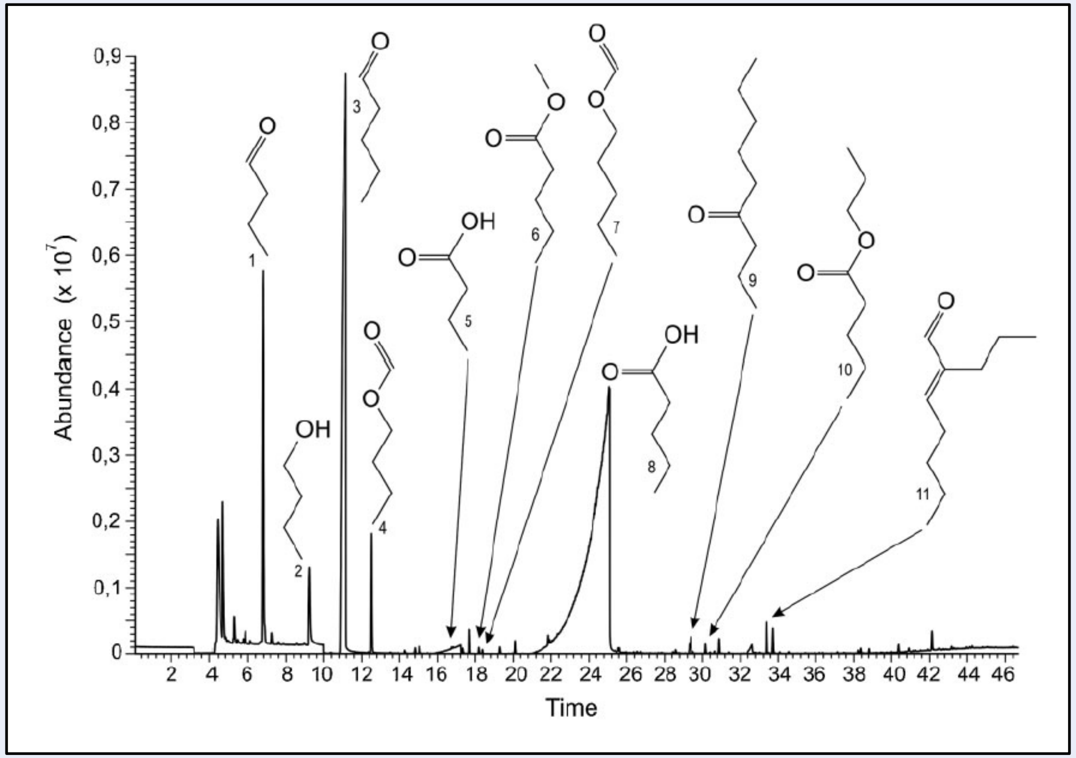
Catalyzed reactions on mineral plaster materials – degradation products

Zeoflair® with α-pinene added – thermal desorption



Zeolite with pentanal added – thermal desorption



Gunschera et al. (2013) CLEAN – Soil, Air, Water

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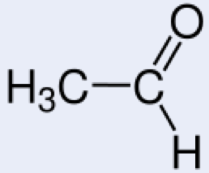
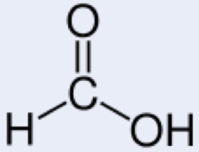
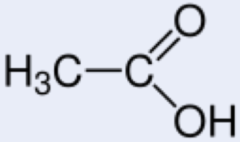
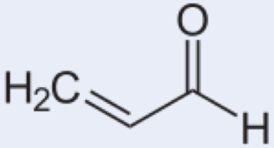
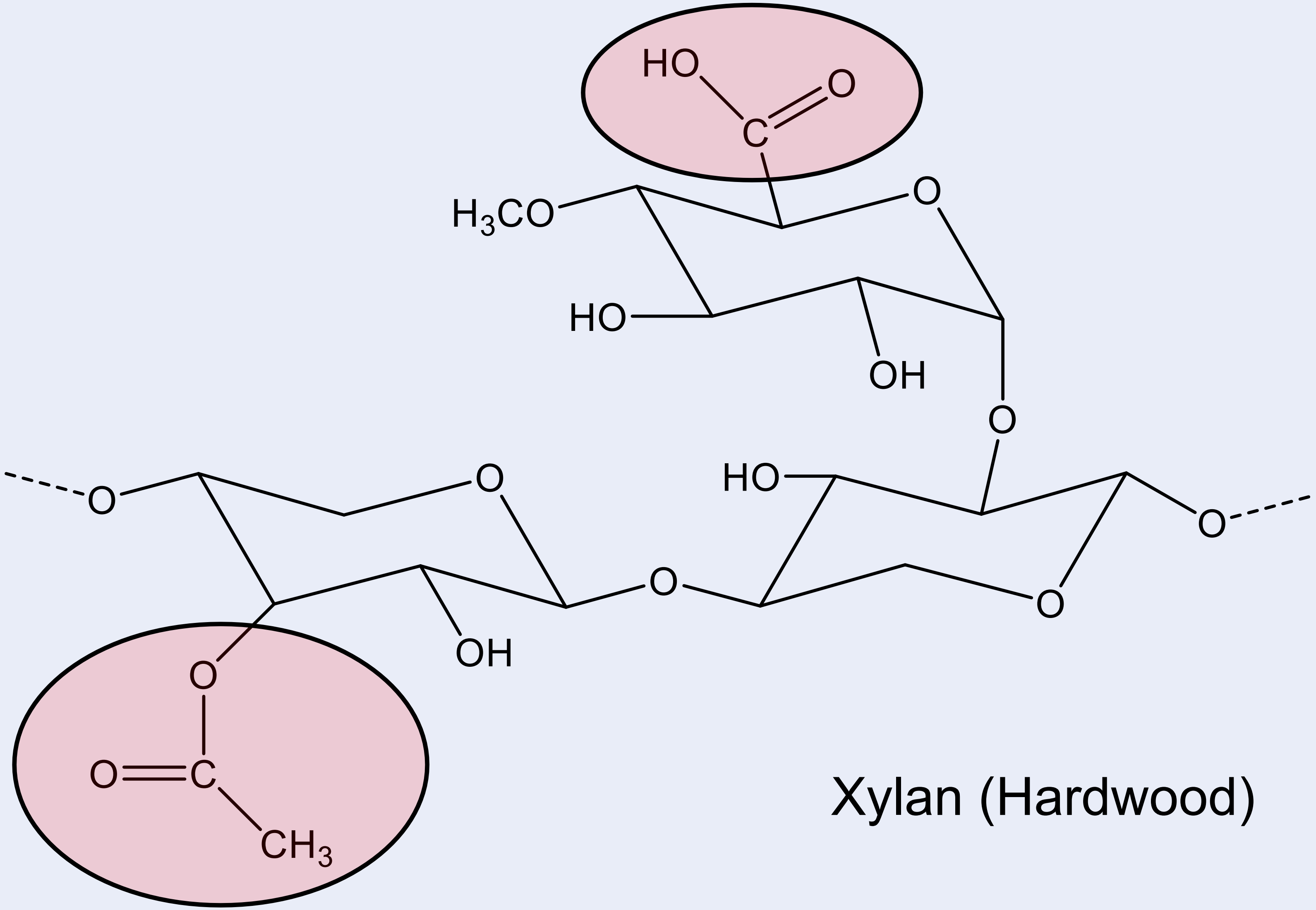
Emerging indoor air pollutants

Acetaldehyde [1]	75-07-0		GV I = 0.10 mg/m³ [2] GV II = 1.0 mg/m³ [2]
Formic acid	64-18-6		GV I = 1 mg/m³ [3] GV II = 0.3 mg/m³ [3]
Acetic acid	64-19-7		
Acrolein	107-02-8		

1) Classified as recognized carcinogen by ECHA
2) Guide value (GV) published by Ad hoc AG (2013) Bundesgesundheitsblatt
3) Preliminary guide value (GV) for the sum of C1-C8 alcanoic acids, German Committee on Indoor Guide Values

Salthammer (2020) Int. J. Hyg. Environ. Health

Wood releases organic compounds - this is a natural process



Xylan (Hardwood)

Pibiri et al. (2020) Build. Environ.

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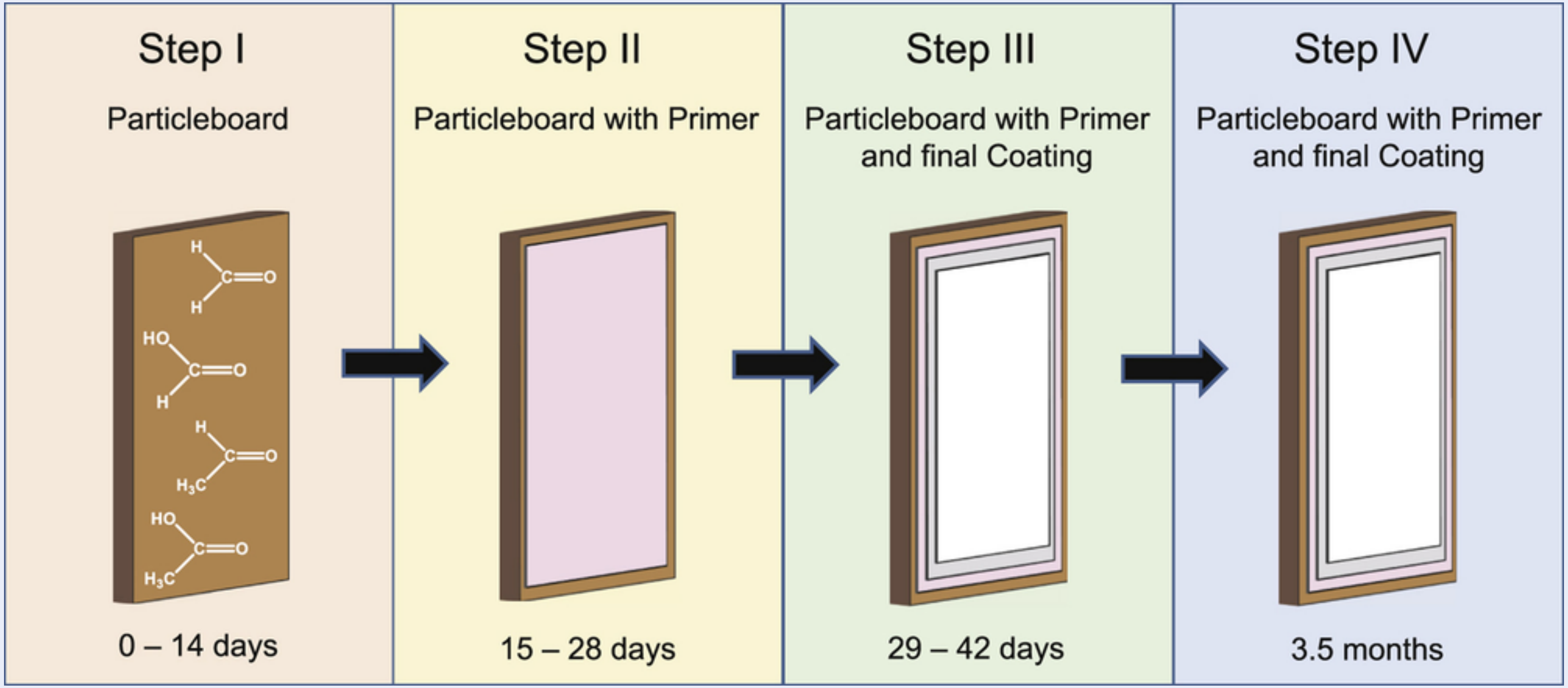
Covering effect of surface coatings: experimental setup



Test conditions: $1m^3$ stainless steel chambers; T = 23 °C; RH = 50%, AER = 0,5 h^{-1}

Pibiri et al. (2020) Build. Environ.

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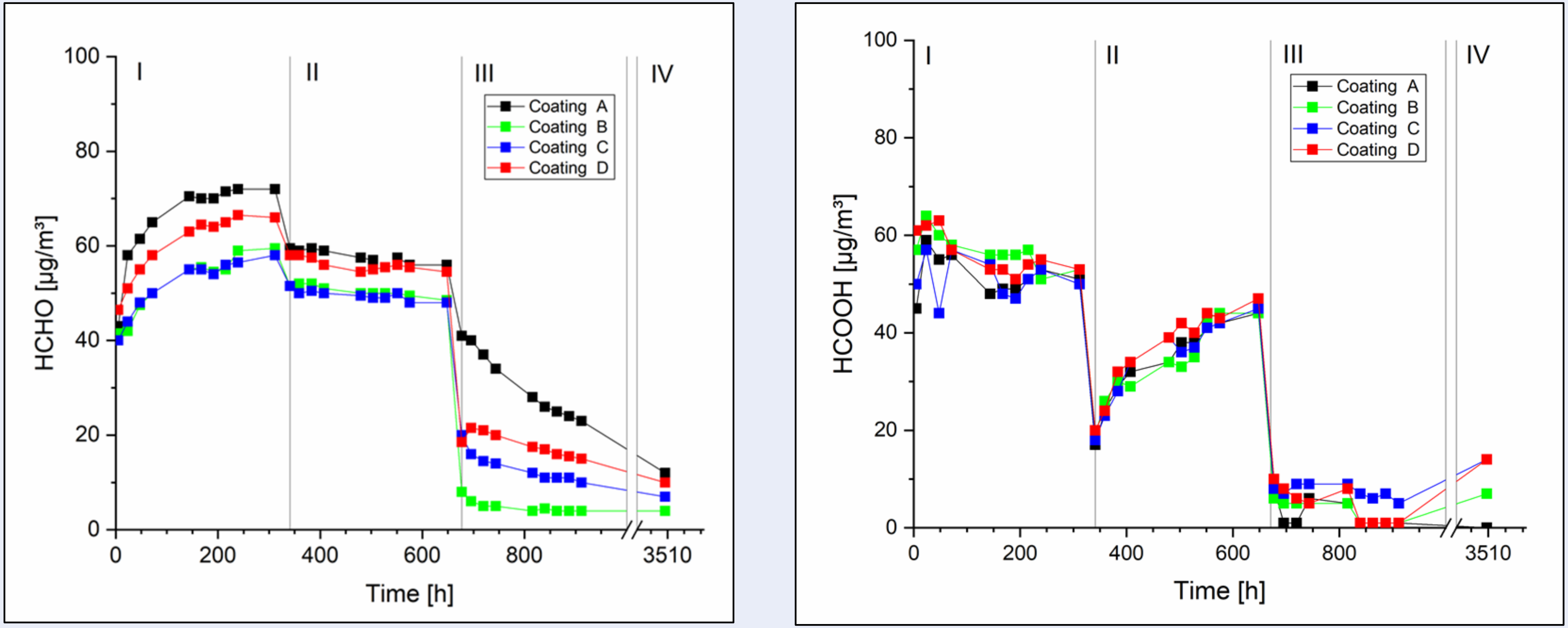
Results: formaldehyd and formic acid

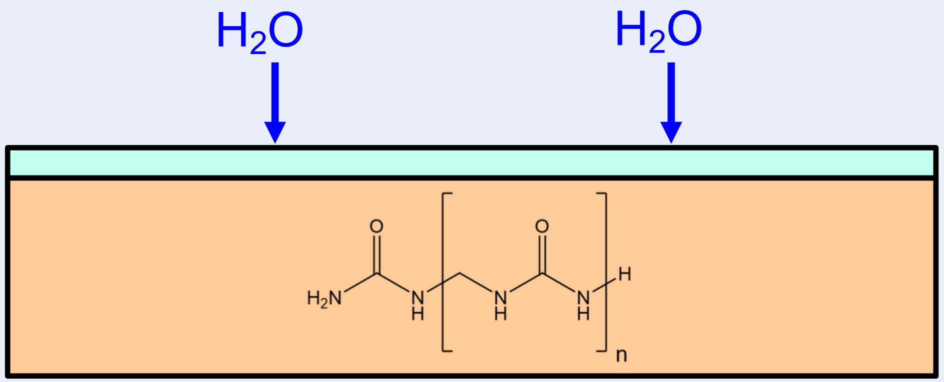


A: Primer + Ingrain wallpaper + Dispersion paint
C: Primer + Vinyl wall covering

B: Primer + Ingrain wallpaper + Latex paint
D: Primer + Plaster

Reduction of VVOC/VOC emissions from wood-based materials by surface oatings

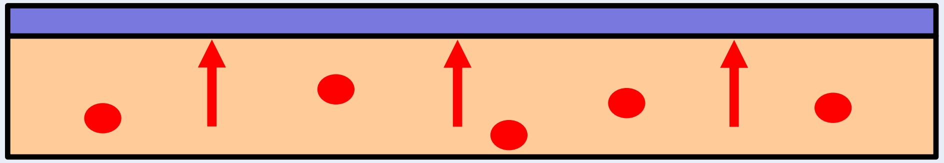
Hydrophobic effet (primer, formaldehyde)



Buffer (carbonate, formic acid)

$$CaCO_3 + 2\ HCOOH \rightarrow Ca(HCOO)_2 + H_2CO_3$$

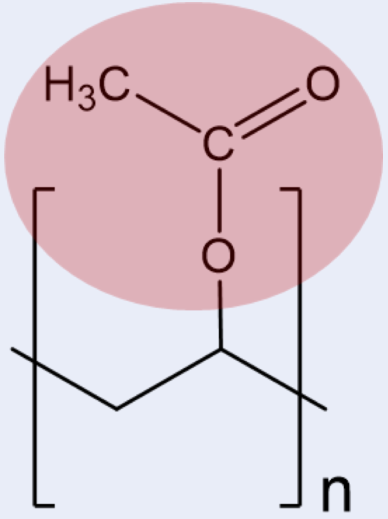
Diffusion hinderance (final coatings)



Pibiri et al. (2020) Build. Environ.

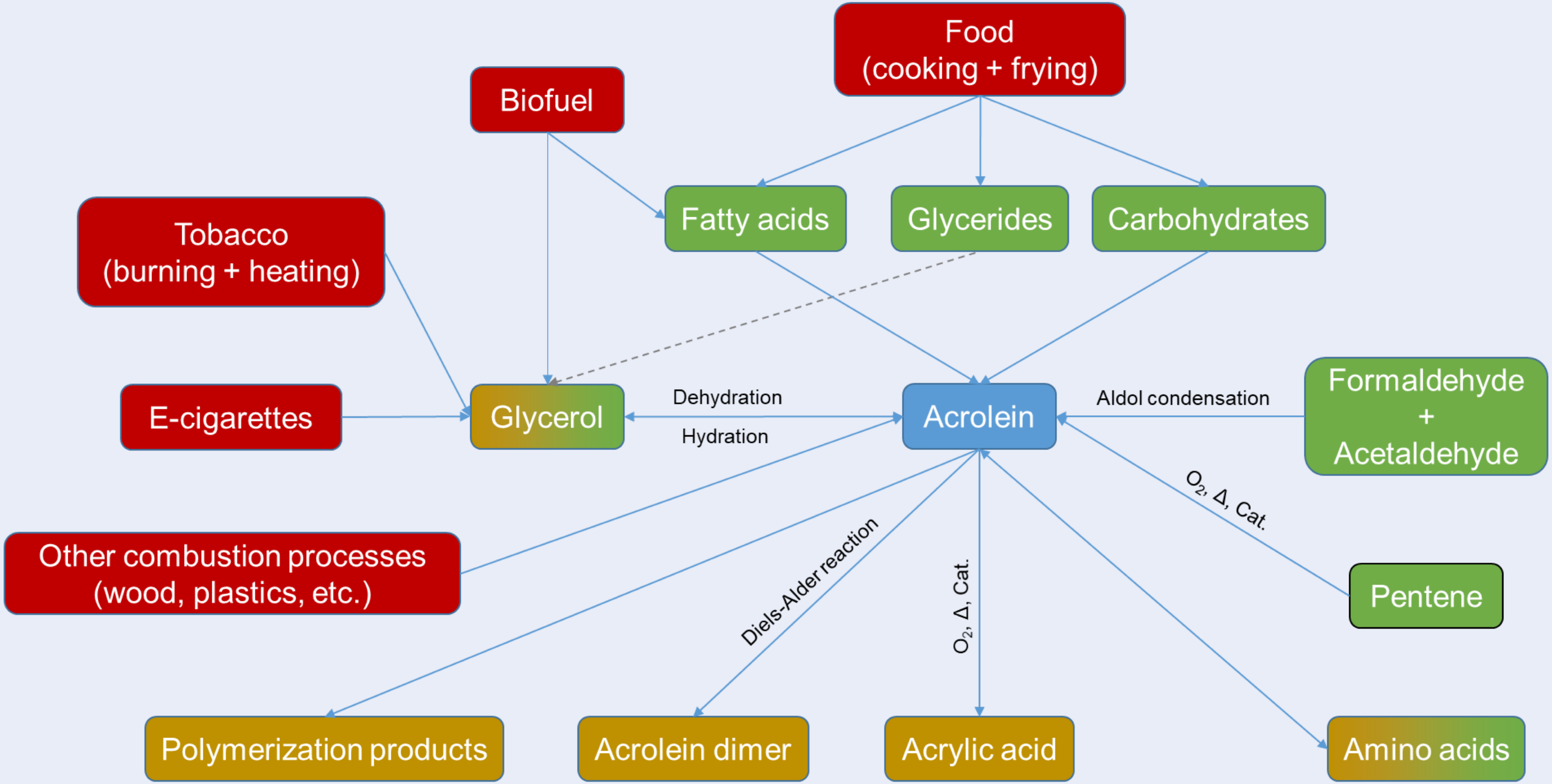
Emissions from surface coatings

Material	Chamber concentration after 72 h (µg/m³)			
	HCHO	CH_3CHO	HCOOH	CH_3COOH
Primer	<6	<8	5	26
Wallpaper adhesive	16	<8	11	28
Latex paint	<6	<8	<5	432
Dispersion paint	<6	<8	<5	<5
Plaster	<6	<8	10	44
Vinyl wallcovering	<6	<8	5	42
Ingrain wallpaper	<6	<8	<5	40



The cause of the release of acetic acid is polyvinyl acetate

Acrolein is coming into the focus: formation pathways and reactions



Schieweck et al. (2021) submitted for publication (© Figure: T. Salthammer)

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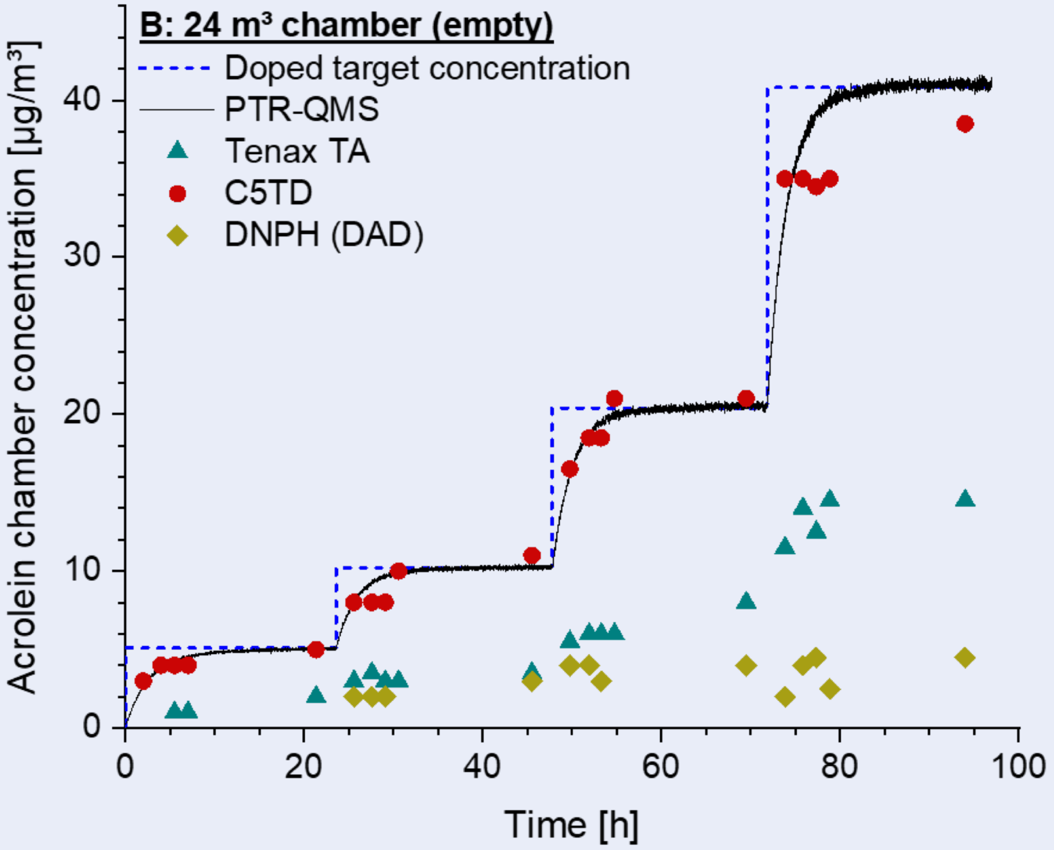
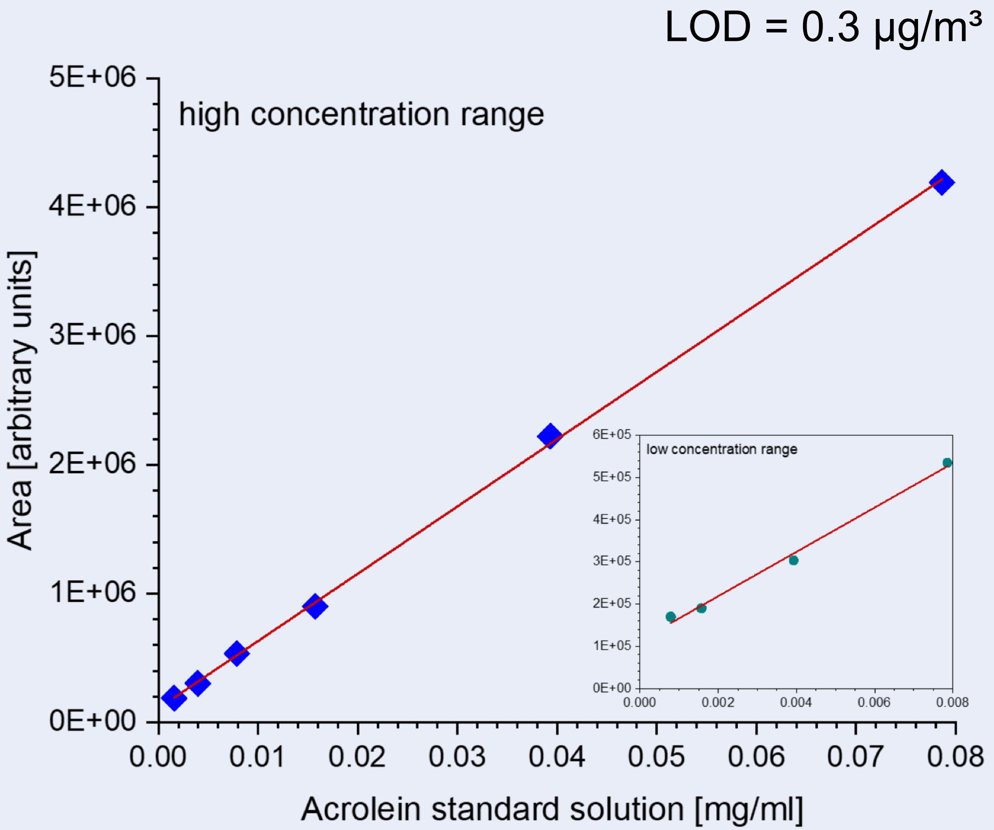
Determination of acrolein in air is an analytical challenge





Schieweck et al. (2021) submitted for publication (© Figure: T. Salthammer)

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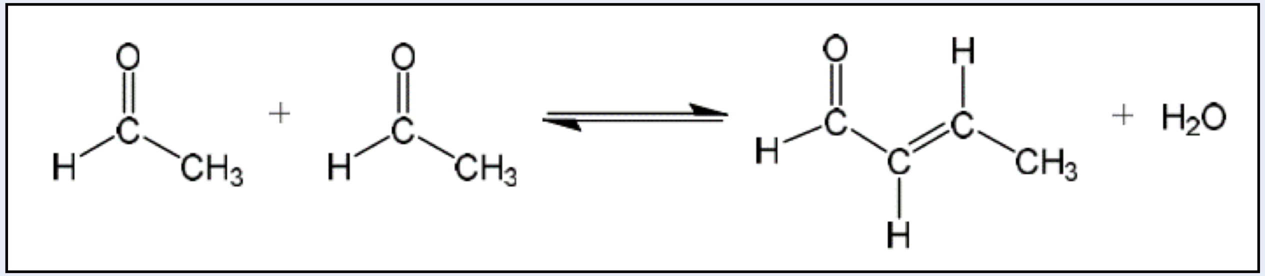
Challenges in VVOC and VOC analysis – reaction products on sorbents and in standards

2-Butenal (croton aldehyde)

aldol condensation reaction of two acetaldehyde molecules

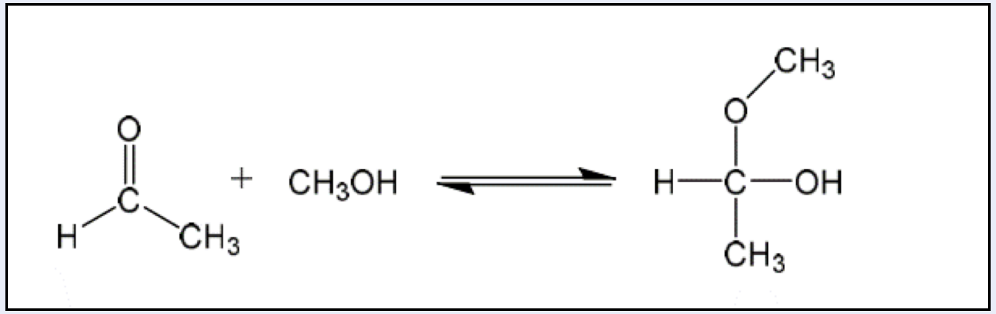
after thermal desorption from Tenax TA®, GCBs, CMS



1-Methoxyethanol

hemiacetal from acetaldehyde and methanol

(the acetal 1,1-dimethoxyethane could not be identified as conditions were not acidic after thermal desorption from CMS)



Schieweck et al. (2018) Anal. Bioanal. Chem.

Challenges in VVOC and VOC analysis – reaction products on sorbents and in standards

Methyl acetate

Esterification? Acetic acid as an impurity of CMS-blank values

4-Vinylcyclohexene (4-VCH)

Dimerization of 1,3-butadiene

(Dettmer and Engewald (2002) Anal. Bioanal. Chem. 373, 490-500)

1,1-Dimethoxycyclohexane

Formation of acetal from cyclohexanone in methanolic solution

(Uhde and Salthammer (2007) Atmos. Environ. 41, 3111-3128)

Decomposition of α-pinene and sabinene

Incomplete thermal desorption due to strong adsorption on CMS surface?

(Coeur et al. (1997) J. Chrom. A 786, 185-187)

Schieweck et al. (2018) Anal. Bioanal. Chem.

Acknowledgement

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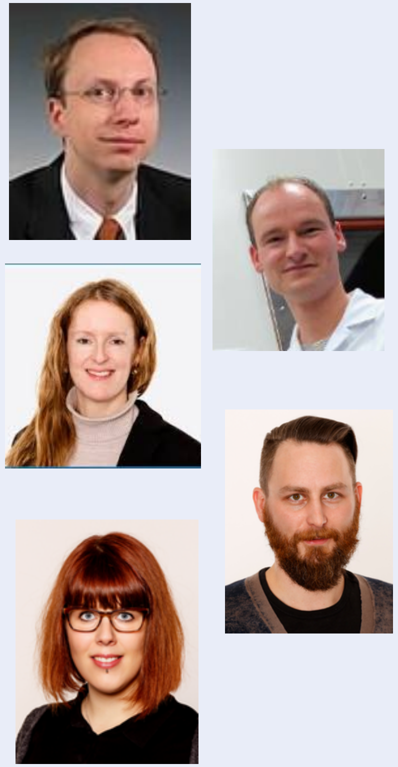
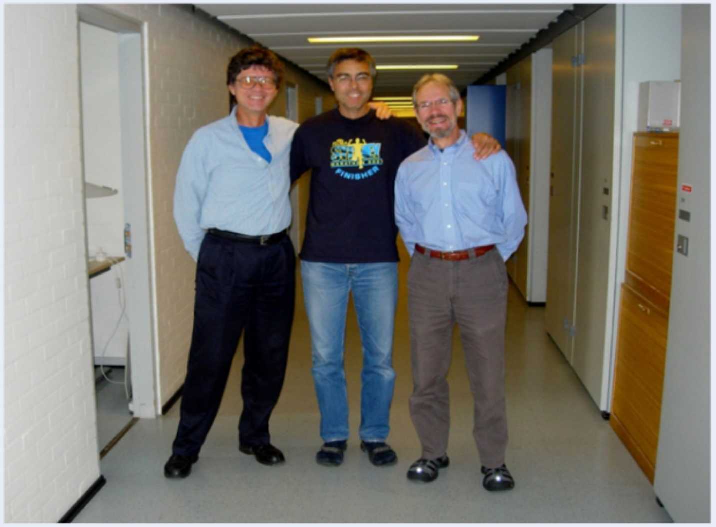
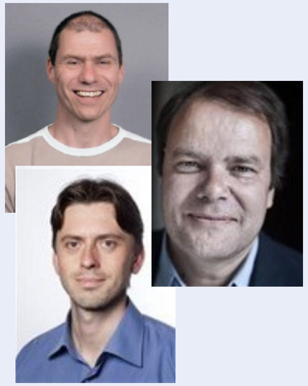


Three Amigo's Talk Chemistry



DANVAK – Seminar, DTU, 21.9.2006, 14:00 – 16:00

DTU Danmarks Tekniske Universitet



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