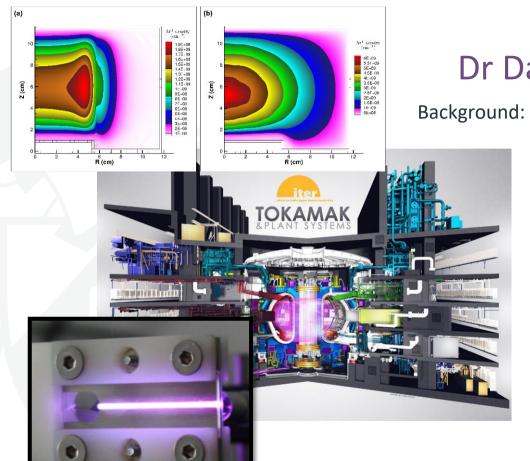


Indoor air chemistry

David Shaw - 04/05/2020





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ckground: BSc Physics with Astrophysics

MSc Fusion Energy PhD Plasma Physics







Funded by the Horizon 2020 Framework Programme of the European Union







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Why study indoor air?









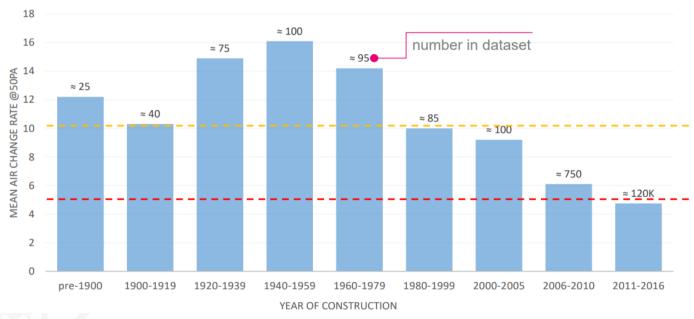




Why now?



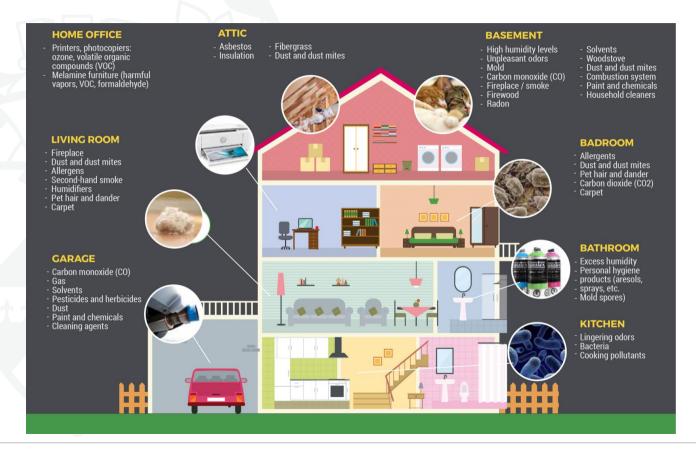
Air permeability trends: house age



https://www.property-care.org/wp-content/uploads/2017/05/lan-Mawditt-presentation-PCA-Conference-4th-May-2017.pdf

Indoor sources?







The indoor atmosphere Formaldehyde ppm - 0.018 -0.016 -- 0.014 -- 0.012 -- 0.010 -- 0.008 -Indoor air Outdoor air - 0.006 -- 0.004 -- 0.002 Formaldehyde 1,4-dichlorobenzene Tetrachloroethylene





Hexaldehyde

Acetaldehyde

n-Undecane

m/p-Xylene

n-Decane

Toluene

1,2,4-trimethylbenzene

1-methoxy-2-propanol

2-butoxyethanol

o-Xylene

Ethylbenzene

Benzene

Acroleine

Styrene

Trichloroethylene

2-butoxy-ethylacetate

1-methoxy-2-propylacetate

Cooking



Particle numbers per cm³

Frying vegetables (500 g) – gas stove	1.4×10^5
Frying bacon (4 racers) — gas stove	5.9×10^{5}
Frying vegetables (500 g) — electric stove	0.11×10^{5}
Frying bacon (4 racers) — electric stove	1.6×10^{5}
Bake cake – gas oven	0.9×10^{5}
Bake cake — electric oven	0.3×10^{5}
Roast meat and potatoes — gas oven	1.2×10^5
Roast meat and potatoes — electric oven	0.2×10^5
Toast – gas grill	1.4×10^5
Toast — electric grill	1.4×10^5

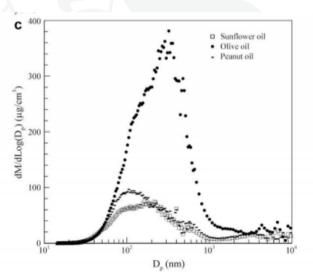


- Cooking with gas generally leads to higher emissions than cooking with electric
- Cooking meat generally gives higher emissions than cooking vegetables

Cooking

Frying 50 g of chips in a gas stove at maximum power with:

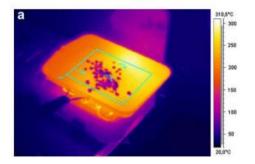
Olive oil Peanut Oil Sunflower Oil



Concentration μg/m³

118 68 60





- Olive oil > Peanut oil > Sunflower oil
- Note that these concentrations are very much higher (x2-10) than those you would measure outdoors in most urban environments

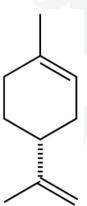
ALFRED P. SLOAN FOUNDATION

Abdullahi et al., Atmospheric Environment 71 (2013) 260-294

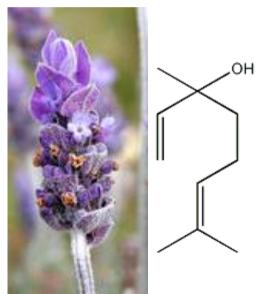
Cleaning - Terpenes



Limonene



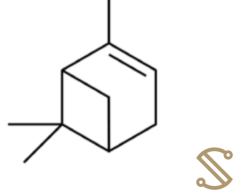
Linalool

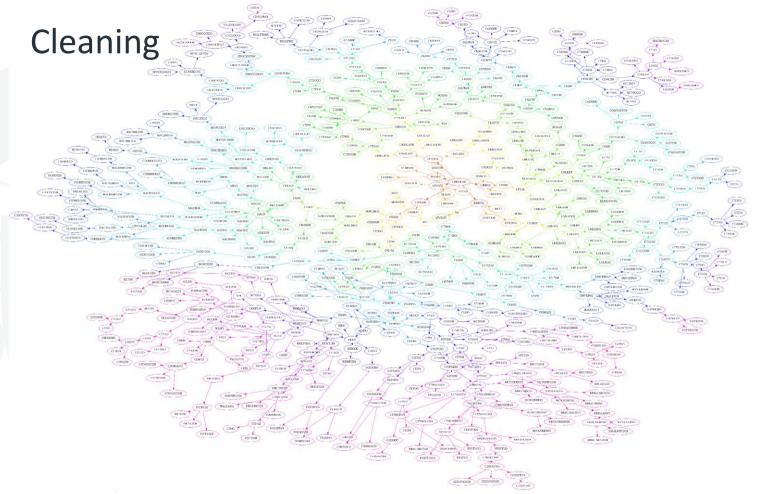






Pinene







Limonene reaction pathways to oxidation end product, CO₂ and Water

713 species in 1241 reactions



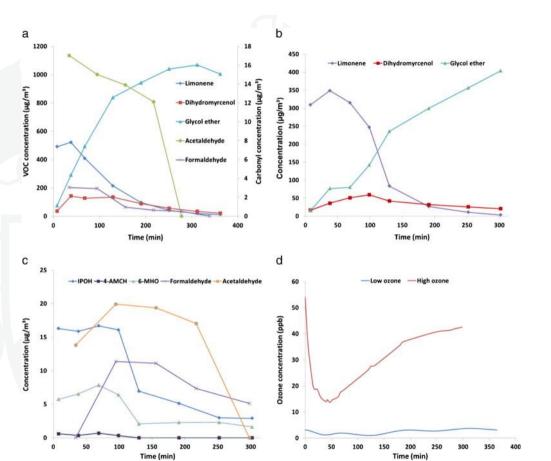




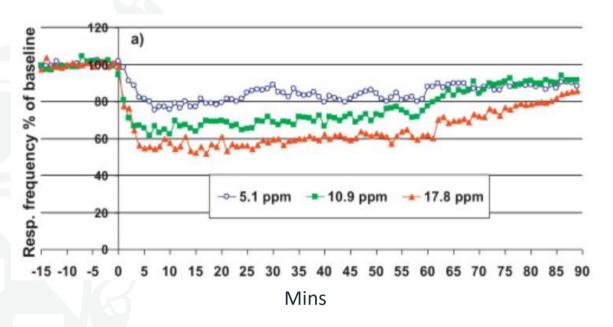
Fig. 1. Gas-phase concentrations of selected VOCs emitted from a kitchen cleaning agent and ozone-initiated reaction products.

- a) Low ozone test concentration (< 5 ppb).
- b) High ozone test concentration (55 ppb).
- c) Reaction products at high ozone test concentration.
- d) Ozone time profiles.



A.W. Nørgaard et al. / Environment International 68 (2014) 209-218





3-Isopropenyl-6-oxo-heptanal (IPOH) concentration versus decrease of the respiratory frequency curve.



Scented candles





Global candles market was valued at US\$ 7.5 Billion in 2016 and is expected to reach US\$ 11.7 Billion by 2025 (5-6% growth per year)!!



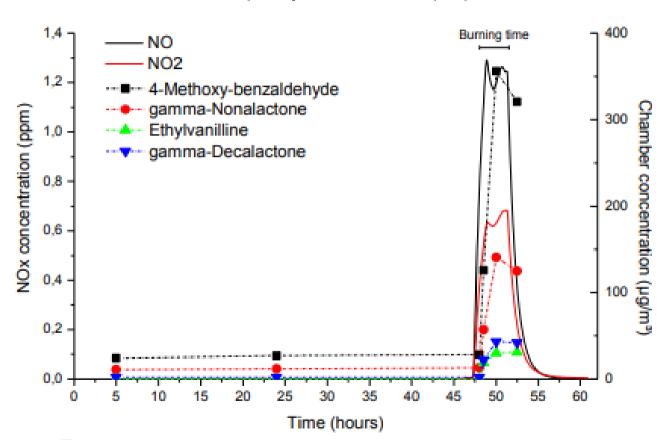


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https://www.businesswire.com/news/home/20170621005792/en/Global-Candles-Market-Reach-11.7-Billion-2025

FOUNDATION

E. Uhde, N. Schulz / Atmospheric Environment 106 (2015) 492-502

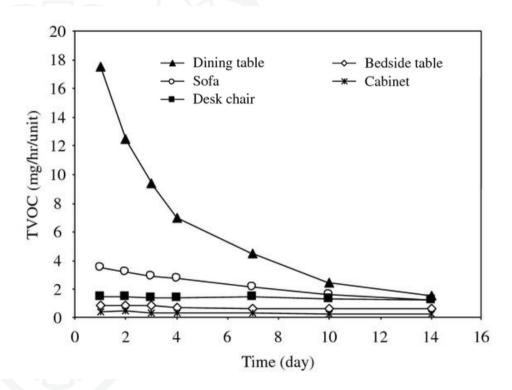




NO₂ levels similar to central London morning rush hour



Surface emissions













Human emissions

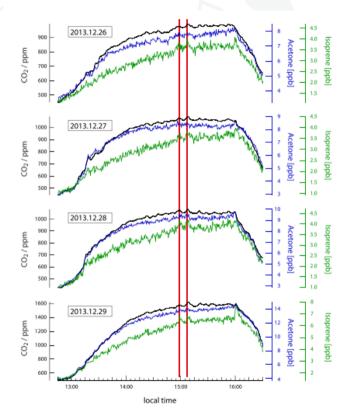


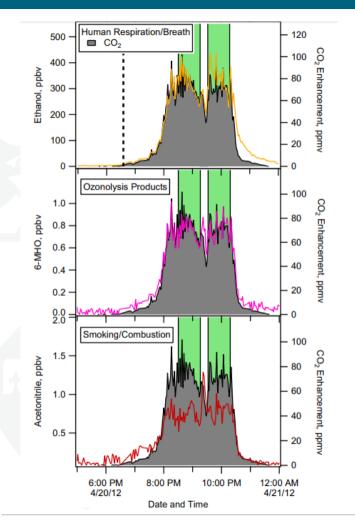
Figure 2. Measurements of ${\rm CO}_2$, isoprene and acetone taken during four separate screenings of "Hunger Games 2".





Nature Scientific Reports | 6:25464 | DOI: 10.1038/srep25464





Human emissions







Atmospheric Environment 77 (2013) 1052-1059

The Indoor Detailed Chemical Model (INDCM)



$$\frac{dC_i}{dt} = -V_d \left(\frac{A_i}{V_i}\right) C_i + \lambda_r f C_o - \lambda_r C_i + \frac{Q_i}{V_i} + \sum_{j=1}^n Rij$$

C_i = Concentration of species indoors

 V_d = Deposition velocity

 A_i = Surface area of the room

 V_i = Volume of the room

 λ_r = Indoor/outdoor exchange rate

f = Penetration factor

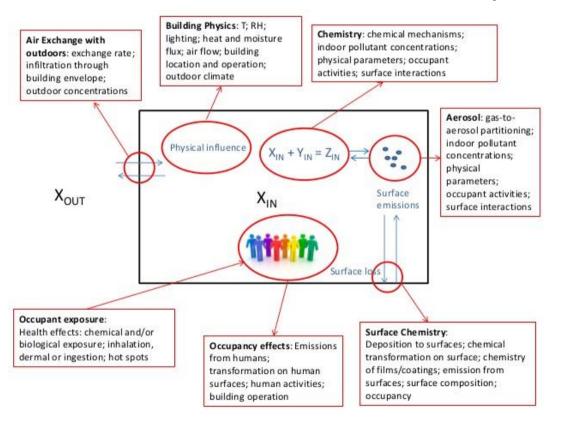
Q_i = Indoor emission rate

Rij = Gas phase reaction between species i and j



The Indoor Detailed Chemical Model (INDCM)

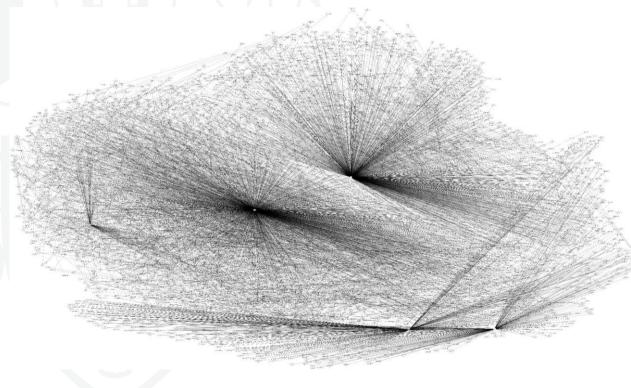






The Master Chemical Mechanism (MCM)





http://mcm.leeds.ac.uk/MCM

"The Master Chemical Mechanism (MCM) is a near-explicit chemical mechanism which describes the detailed gas-phase chemical processes involved in the tropospheric degradation of a series of primary emitted volatile organic compounds (VOCs). Currently, the degradation of methane and 142 non-methane VOCs is represented"



Assumptions

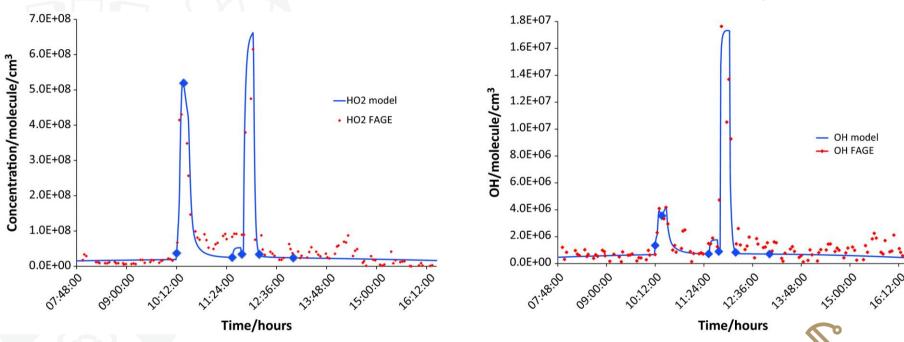


- A single well mixed environment (1d box model)
- Irreversible deposition on surfaces, consistent with measurements and 10-100 times lower than measured outdoors
- Surface production for some measured species. Most notably HONO
- Photolysis is dealt with in distinct UV and visible bands. Constants have been determined from data in the recent IUPAC recommendation. They are attenuated for windows and then summed for each species
- Outdoor concentrations are average profiles of specific locations



Results



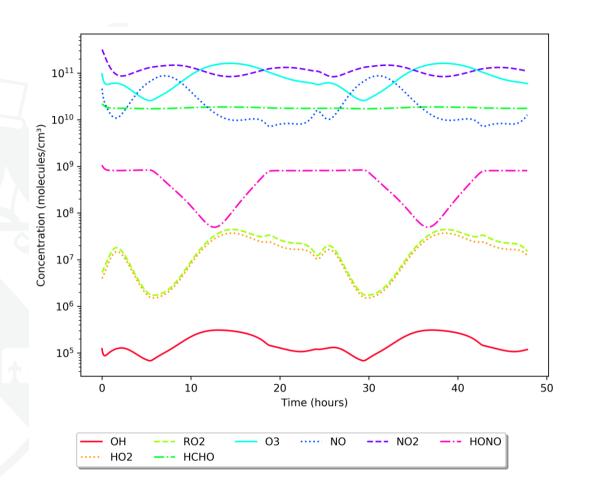


Fluorescence assay by gas expansion (FAGE) of cleaning followed by air cleaning device

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Carslaw et al. Indoor Air, 2017. https://doi.org/10.1111/ina.12394

Python Output

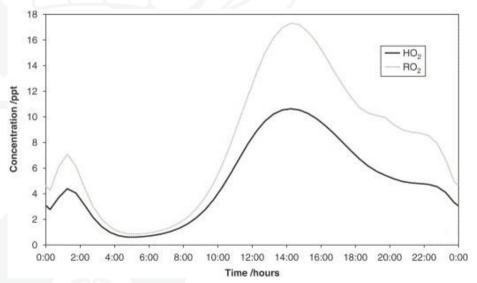


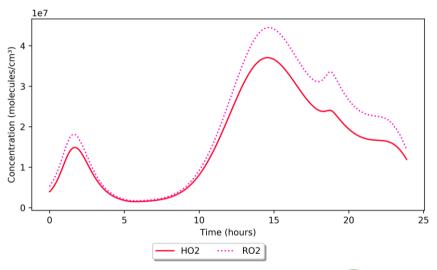




Comparison









Thank you, any questions?



