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# SOA formation in the ozonolysis of biogenic VOC performed in a laminar flow reactor

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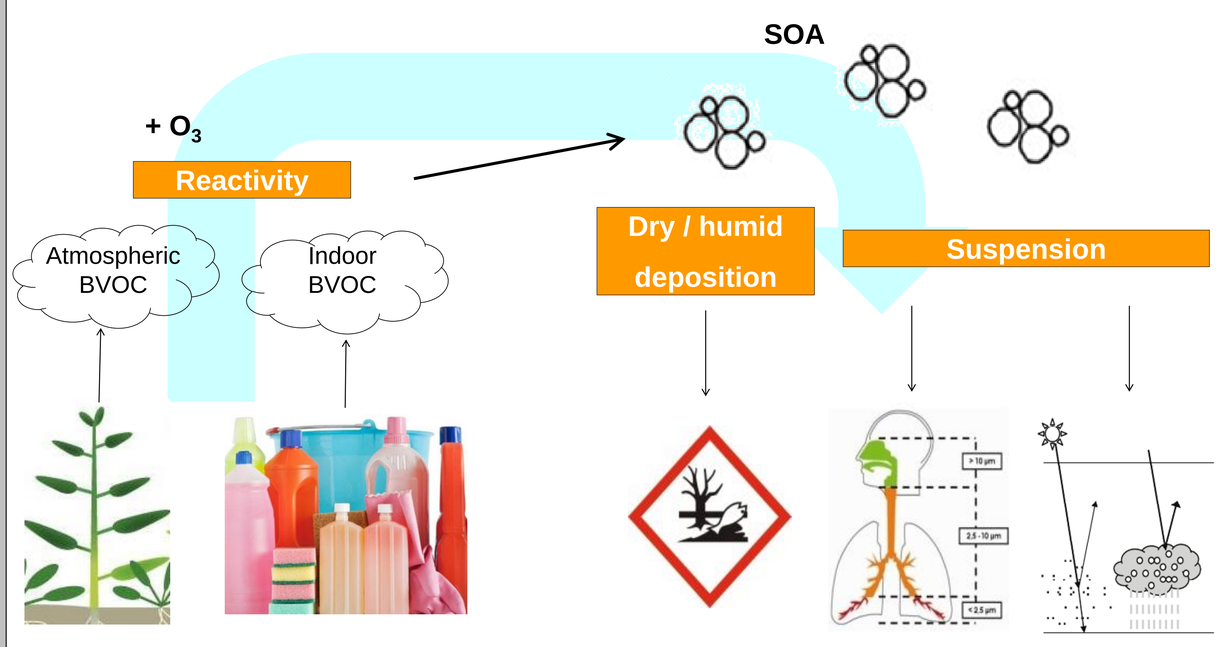
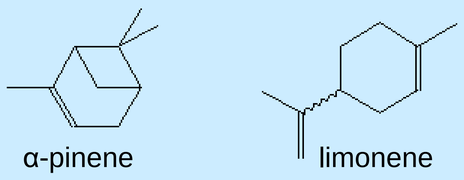
## Atmospheric background



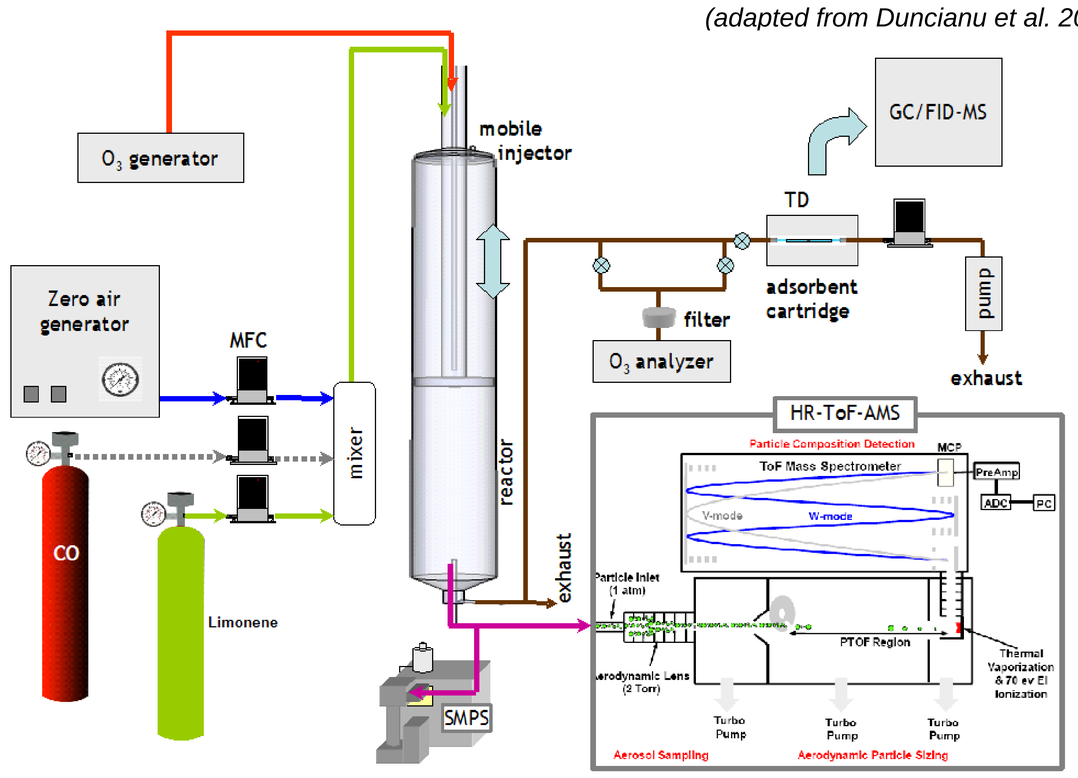

Aim of the study: to characterize the **reactions of 2 BVOCs with ozone** leading to the formation of SOA by the determination of:

- Rate coefficients
- Gas and particulate products
- Aerosol particle distributions and yields




## Experimental setup: Laminar flow reactor

*(adapted from Duncianu et al. 2012)*




- On-line measurement of [VOC] by thermodesorption and GC-FID-MS analysis
- Measurement of $[O_3]$ = f (reaction time) by ozone analyser (UV absorption at 254 nm)

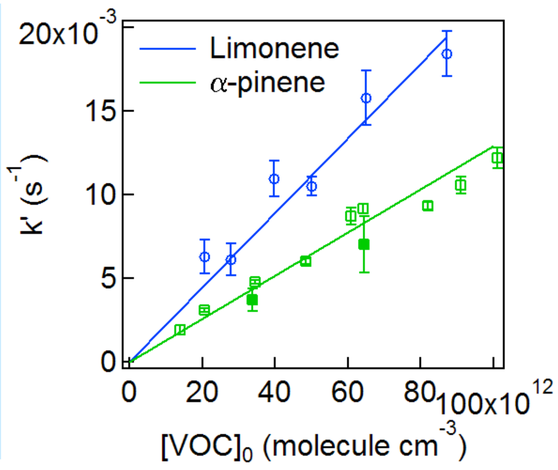
→ Work in a controlled environment:
temperature, concentrations of reactants ($O_3$, VOC), flow conditions

➔ 1st reaction steps: **short reaction times** from 38 s up to 4 min

## Results: kinetics

**limonene + $O_3$ → products**
**α-pinene + $O_3$ → products**

- Pseudo first order conditions: $[VOC]_0 \geq 10 \times [O_3]_0$
- Kinetic law: $\frac{d\ln[O_3]}{dt} = k'_{VOC} \times [O_3]_t$ with $k'_{VOC} = k_{VOC} \times [VOC]_0$
- Measurement of $[O_3]_t$ = f (reaction time) for ≠ [VOC]
- Calculation of the pseudo-first order coefficient k' : $\ln([O_3]_0/[O_3]_t) = k'_{VOC} \times t$ for ≠ [VOC]
- Determination of the rate coefficient for the ozonolysis reaction k : $k'_{VOC} = k_{VOC} \times [VOC]_0$




| Alkene | T (K) | $k_{VOC} \times 10^{16}$ (cm$^3$ molecule$^{-1}$ s$^{-1}$) | Setup | Reference |
|---|---|---|---|---|
| Limonene | 296 | 2.23 ± 0.08 | FR | This work |
| | 297 | 3.8 ± 0.3 | FR | *Bernard et al. 2012* |
| | 304 | 2.0 ± 0.4 | SC | *Bernard et al. 2012* |
| | 295 | 2.5 ± 0.3 | FR | *Witter et al. 2002* |
| | 298 | 2.13 ± 0.15 | SC | *Khamaganov et Hites 2001* |
| | 298 | 2.0 ± 0.5 | Review | *Calvert et al. 2000* |
| α-pinene | 297 | 1.29 ± 0.16 | FR | This work (*Duncianu et al. 2012*) |
| | 295 | 1.1 ± 02 | FR | *Witter et al. 2002* |
| | 298 | 0.84 ± 0.07 | SC | *Khamaganov et Hites 2001* |
| | 298 | 0.90 | Review | IUPAC data |

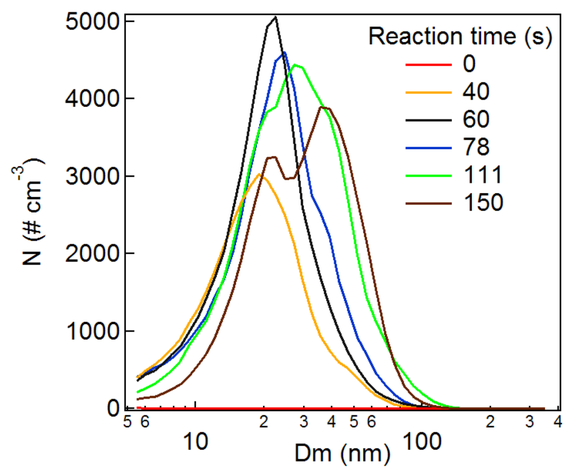
FR: flow reactor; SC: smog chamber

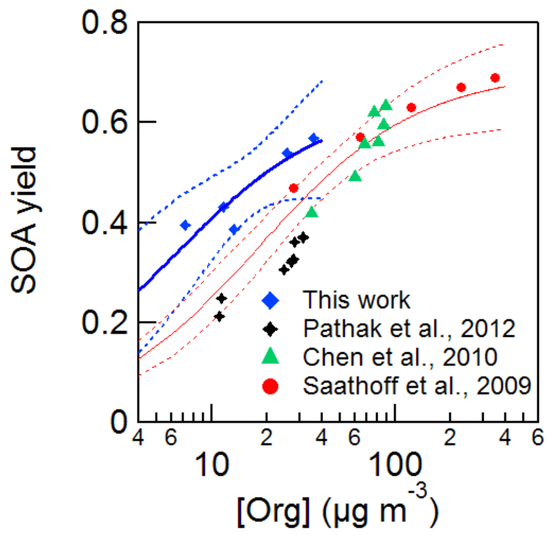
## Results: aerosol particle distribution and yield

**Example of the reaction limonene + $O_3$ → products**

Particle size distribution given by SMPS data :
- first mode centered on 20 nm
- enlargement of the particles with reaction time and appearance of a double mode at 20 and 40 nm

➔ Ozonolysis of unsatured gas products?




$$Y = \frac{M_0}{\Delta[LIM]}$$ with $M_0$ = [Org] (µg m$^{-3}$) (from AMS data)

$$Y_i = M_0\left(\frac{\alpha_i K_{om,i}}{1 + K_{om,i} M_0}\right)$$ *Odum et al. 1996*

Comparison with literature results obtained whether in simulation chambers (Chen et al., 2010; Saathoff et al., 2009) or in a flow reactor (Pathak et al., 2012)

## Conclusions and perspectives

➢ Conclusions

- Determination of $k_{LIM+O3}$ = (2.23 ± 0.08) × $10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and $k_{\alpha\text{-PIN}+O3}$ = (1.29 ± 0.16) × $10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ in agreement with literature
- Determination of SOA yield for the reaction limonene + $O_3$ → products
  - Relative agreement with *Chen et al., 2010* and *Saathoff et al., 2009*
  - Two times higher than *Pathak et al., 2012*

➢ Perspectives

- Analysis of gas products for both reactions
- Further characterization of particulate products and additional experiments at lower reaction extent

## References

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