

A Novel Flow Tube Method for Measuring Gas-Phase Reactions Kinetics and Uptake on Solid Surfaces: Application to Organic Peroxy Radical

EGU General Assembly 2025

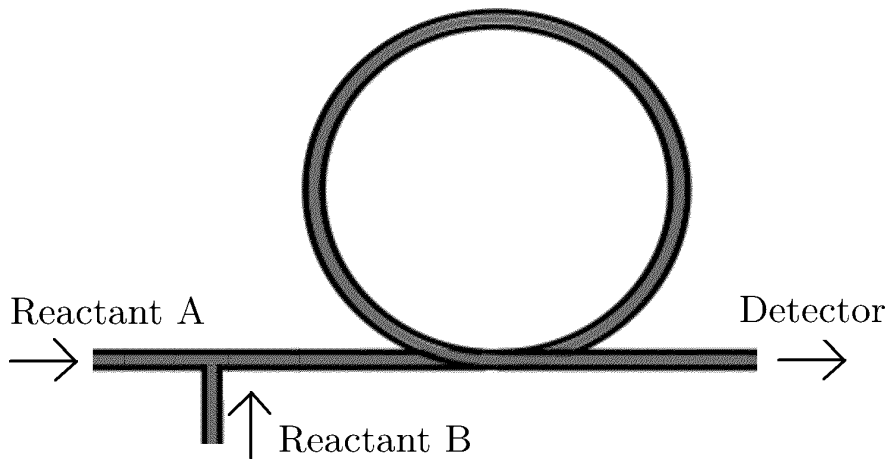
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Vienna, 27 April - 2 May 2025

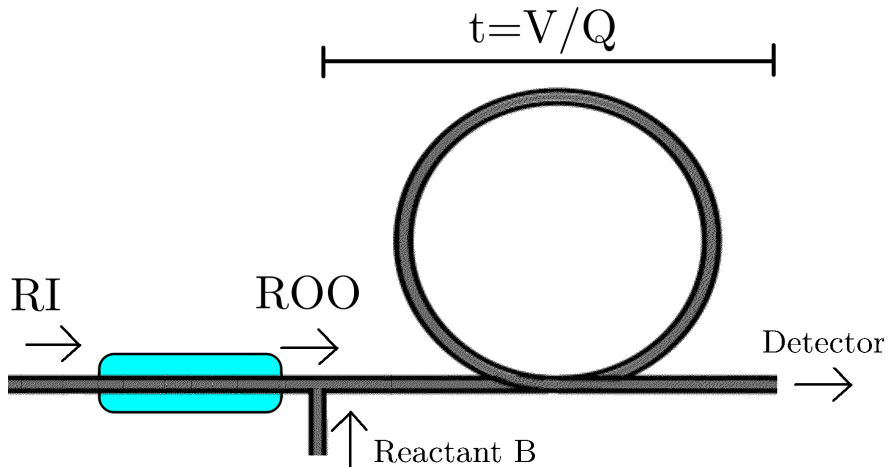


A Simple Flow Tube for Chemical Kinetics



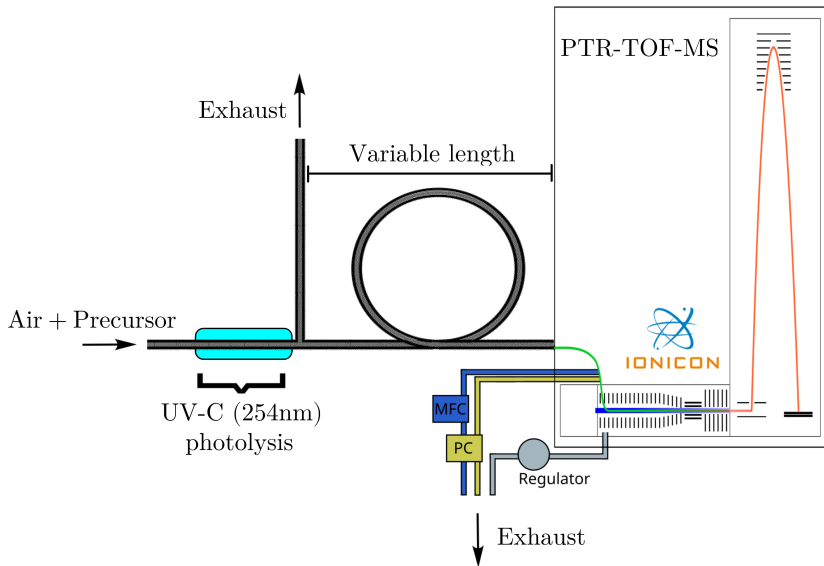
Simply what we need for chemical kinetics.

A Simple Flow Tube for Chemical Kinetics



Simply what we need for chemical kinetics of organic peroxy radicals.

The Coupling with a PTR-TOF-MS

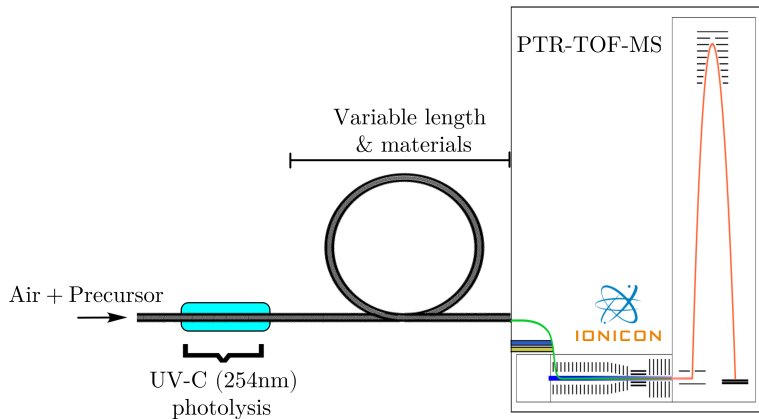


First question

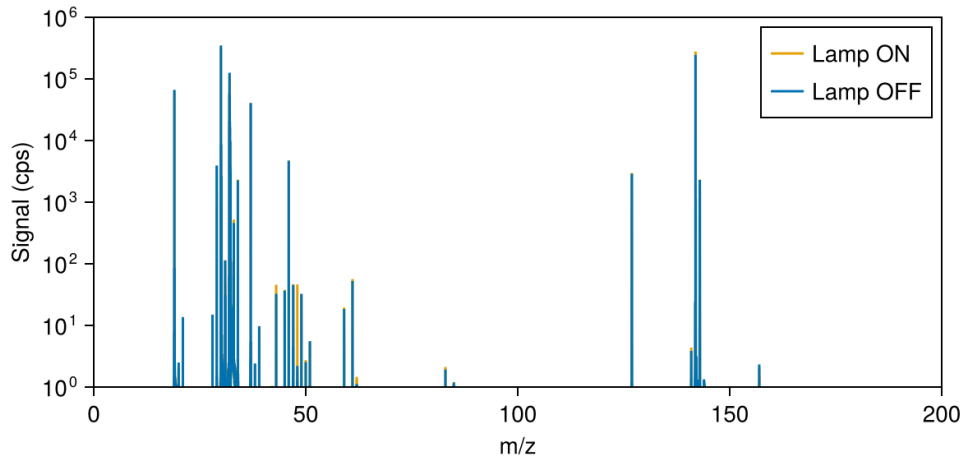
Which material to use for the flow tube reactor to study RO_2 ?

Uptake on walls

- PFA
- Glass
- Copper
- Brass
- Stainless Steel
- Aluminum

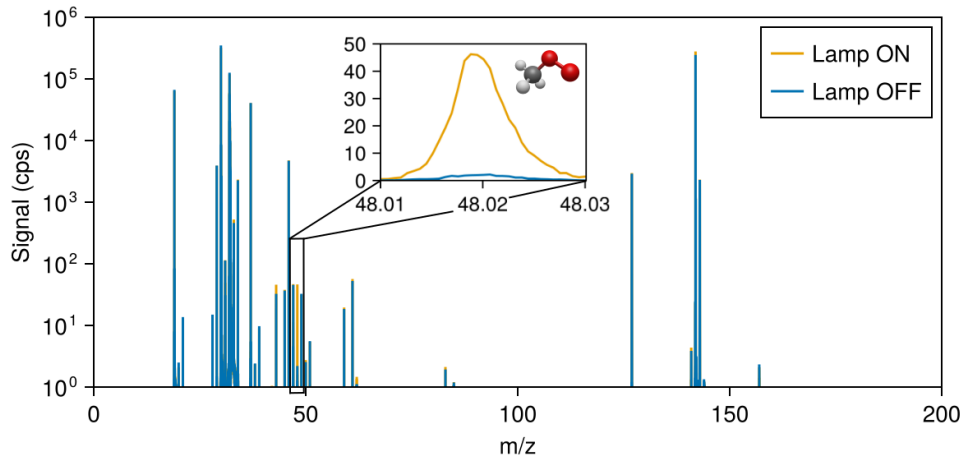


Uptake on walls



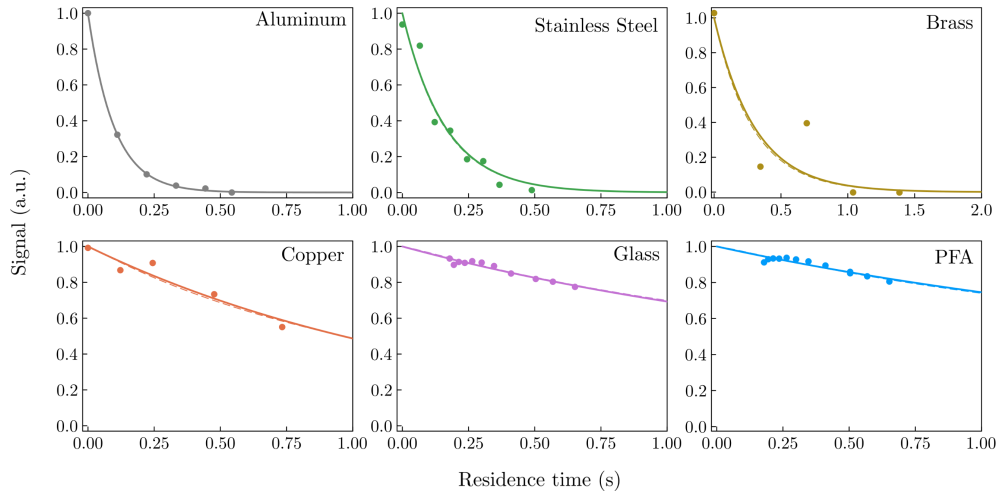
Typical mass spectrum recorded for one kinetic point.

Uptake on walls



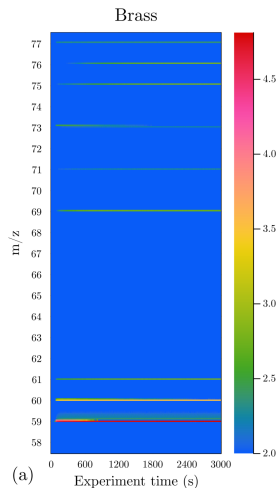
Direct detection of $\text{CH}_3\text{OO}\cdot$ at ppb sensitivity.

Uptake on walls



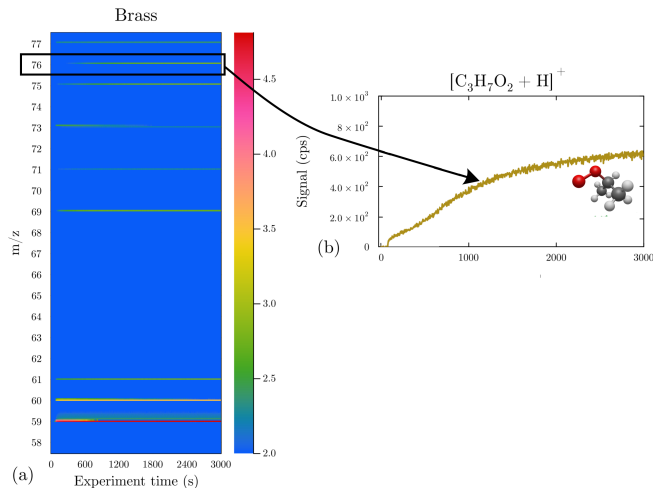
Kinetics measurements using different reactor materials.

Uptake on walls



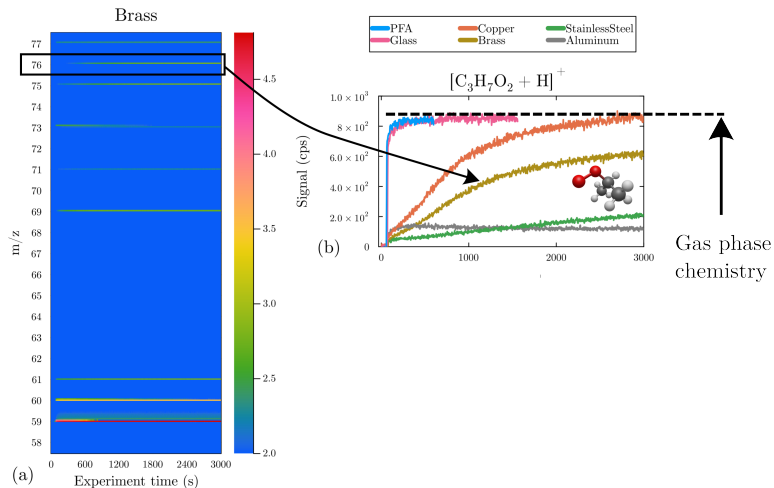
Durif et al, 2024 (JACS Au), DOI:10.1021/jacsau.4c00060
Dataset, DOI: 10.5281/zenodo.10790197

Uptake on walls



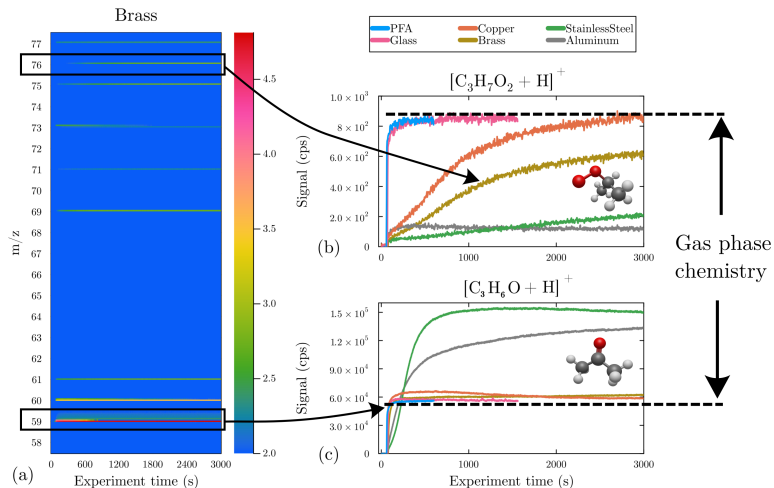
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First conclusion

- Strong ROO[•]-Metals interactions.
- PFA walls do not affect (at least not directly) RO₂ chemistry (!)

Use PFA, not metals, in experiments.

Recommended uptake: 0.

Second question

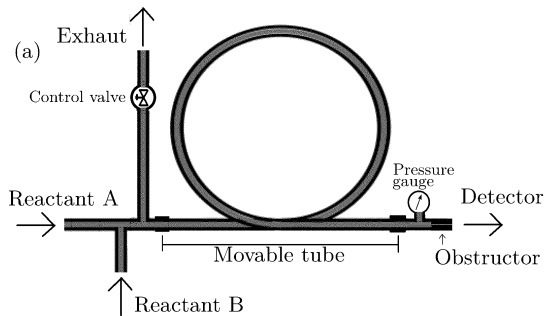
Can we also quantify uptake by atmospherically relevant materials?

Third question

How to proceed when the material is not a tube, but in its simplest state: a powder?

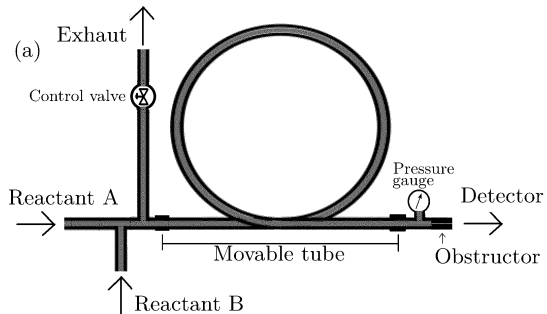
Flow tube variants

Varying the tube length

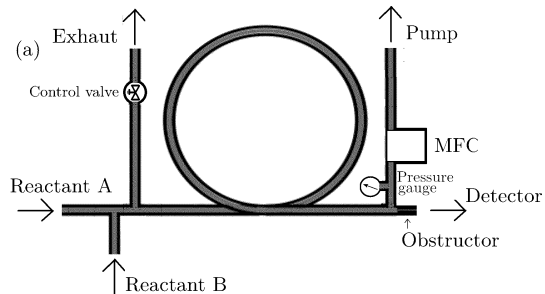


Flow tube variants

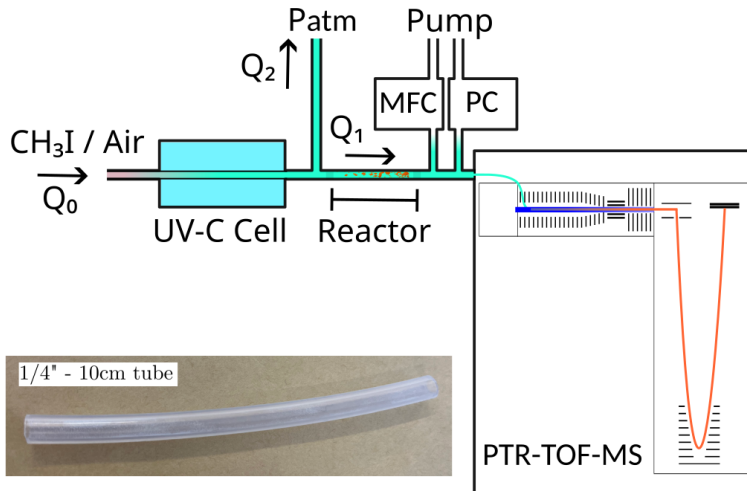
Varying the tube length



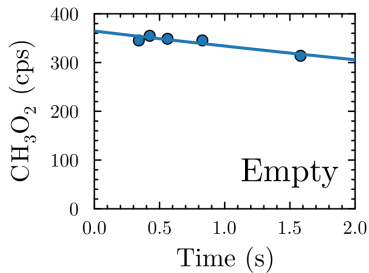
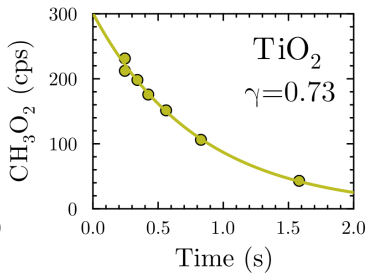
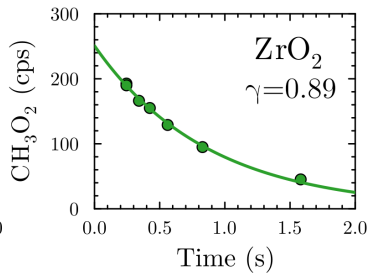
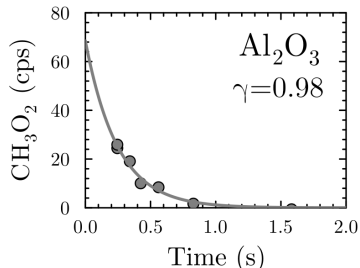
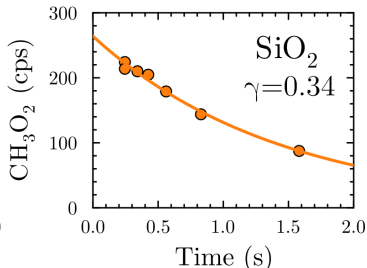
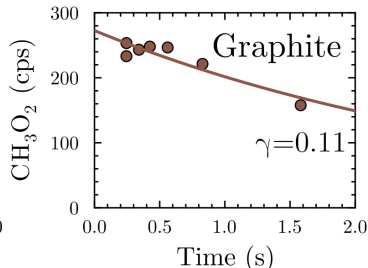
Varying the reactor flow (no mechanical parts)



Setup for measuring uptake on surfaces



Uptake on surfaces



Summary

- A Versatile Flow Tube Approach: applicable for gas-phase reaction but also gas-liquid and gas-surface uptake.
- Simple 1/4" tubing, no gas-mixing issues, easy-to-build, easy-to-use, robust, cost-less, precise.
- PFA, glass and dry salts are founds inert toward RO_2 .
- CH_3O_2 unambiguously detected at a ppb sensitivity.
- A complete framework for PTR-MS data processing and kinetics analysis: `MassSpec.jl`: <https://gitlab.com/odurif/MassSpec.jl>.

EPHEMERAL Project

Pr. Barbara Nozière

Principal Investigator

PhD Candidates & Post-docs:

- ▶ Lauren Cork
- ▶ Clara Strunz
- ▶ Juana Salas



Thank you