# Characterization of a Novel Laminar-Flow Oxidation Reactor for Simulating Atmospheric Multiple-Day Oxidation

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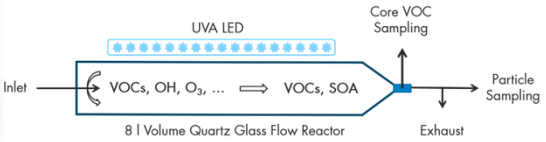
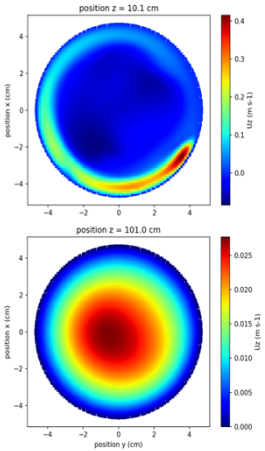
## IONICON Laminar-Flow Oxidation Reactor – ILOx


The automatable IONICON Laminar-flow Oxidation Reactor (ILOx) consists of a 110 cm long Quartz glass tube with a total internal volume of 8 l. Typical residence times range from 2 to 16 min. All materials are optimized for purest experiments possible (Quartz glass, Teflon and passivated surfaces only).
The flow reactor is surrounded with a powerful 300 W UVA LED lamp (365 nm) for direct irradiation over 80 cm of the reactor. To maintain stable temperatures inside the ILOx reactor active cooling via a set of fans is fully sufficient.
To achieve a laminar flow condition inside the reactor, the carrier gas is injected by a circular motion, suppressing any formation of injection jets. Various oxidants can be supplied via multiple customizable inlet ports, e.g. ozone can be generated externally from $O_2$ by UVC irradiation.




## Flow Conditions

The geometries for optimal sample injection and extraction were optimized via 3D computational fluid dynamics (CFD) simulations using OpenFOAM (openfoam.org).

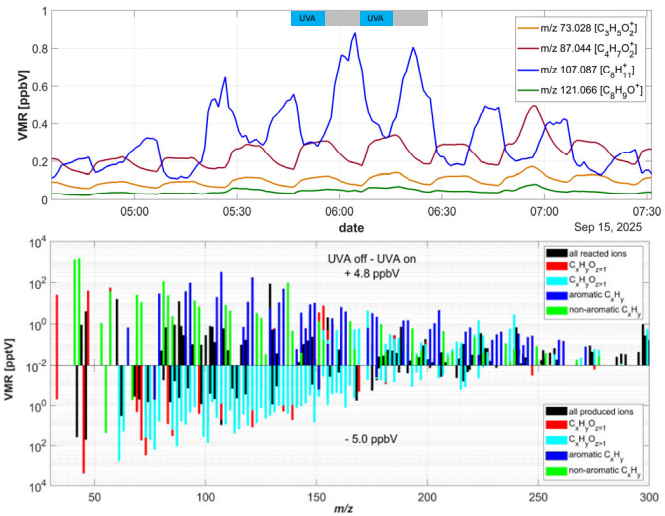



➢ *Inlet*
Our 3D CFD simulations resulted in a best initial mixing and following optimal laminar flow conditions via a dual radial injection of the buffer gas and the sample. A benefit of this radial injection is the prevention of a formation of a jet at the center of the reactor.

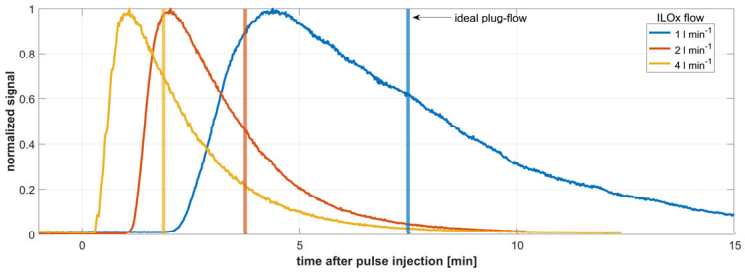
➢ *Reactor*
We have chosen a length-to-diameter ratio of > 10 for reaction conditions that resemble a traditional aerosol-flow-tube reactor. With the optimized inlet geometry optimal laminar flow conditions can be reached at various residence times.

➢ *Outlet*
A conical outlet is followed by a core sampling of VOCs to minimize the loss of low volatiles while simultaneously transmitting the particles at highest efficiencies.

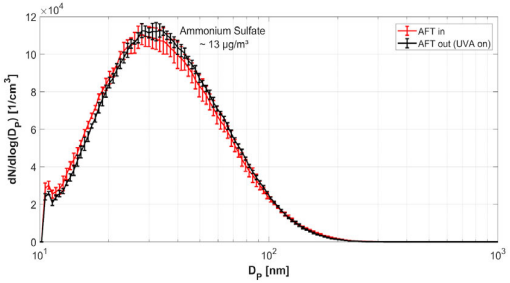
## Atmospheric Multiple-Day Oxidation




## Laminar-Flow Characterization



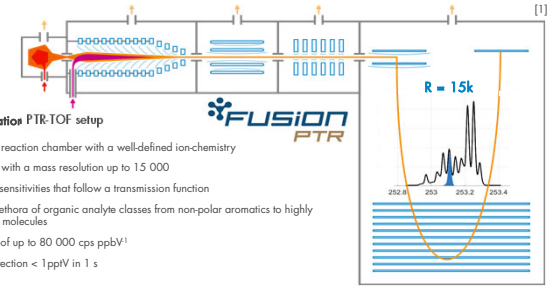

## Particle Transmission Efficiency




➢ Measurement of Ammonium Sulfate (AS) particles before and after ILOx.

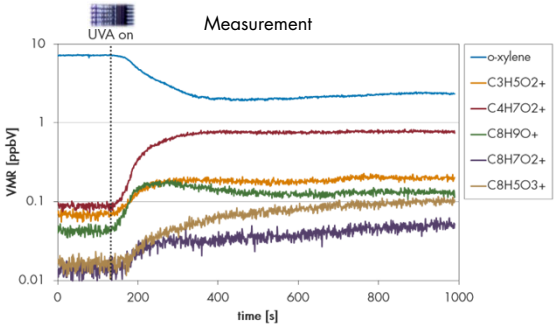
➢ Excellent transmission of AS particles almost independent of particle size.

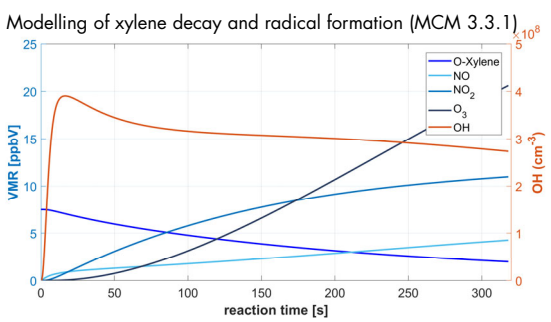
## FUSION PTR-TOF 10



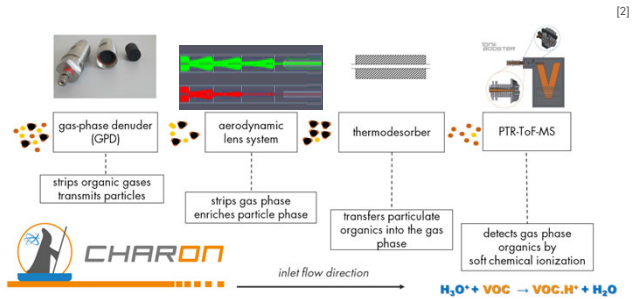

## Rapid Oxidation of Xylene

- 8 ppbV of o-xylene were injected to study the rapid oxidation potential of the ILOx reactor.
- IPN was added as a OH precursor. With active UVA irradiation IPN is photolyzed to produce OH radicals and acetone.
- This allows for a rapid oxidation of xylene resembling an atmospheric oxidation of approximately two days.
- MCM 3.3.1 simulations of this experiment result in average OH concentrations of 3x10⁸ $cm^{-3}$, which equals to an OH exposure $OH_{exp}$ of $10^{11}$ $cm^{-3}s$.




## CHARON Particle Inlet




**References**
[1] Tobias Reinecke, Markus Leiminger, Alfons Jordan, Armin Wisthaler, and Markus Müller, 2023, Ultrahigh Sensitivity PTR-MS Instrument with a Well-Defined Ion Chemistry, Anal. Chem., 95, 32, 11879–11884, https://doi.org/10.1021/acs.analchem.3c02669
[2] Tobias Reinecke, Markus Leiminger, Andreas Klinger, and Markus Müller, Direct detection of condensed particulate polycyclic aromatic hydrocarbons on a molecular composition level at low pg m-3 mass concentrations via proton-transfer-reaction mass-spectrometry, Aerosol Research, 2, 225–233, 2024.