

Evaluation of a reduced pressure chemical ion reactor utilizing adduct ionization for the detection of gaseous organic and inorganic species

Matthieu Riva^{1,2, †,*}, Veronika Pospisilova^{1,†}, Carla Frege¹, Sebastien Perrier², Priyanka Bansal¹, Spiro Jorga¹, Patrick Sturm¹, Joel A. Thornton³, Urs Rohner¹, Felipe Lopez-Hilfiker^{1,*}

¹ TOFWERK, 3645 Thun, Switzerland

² Université Claude Bernard Lyon 1 CNRS, IRCELYON 69626, Villeurbanne France

³ Department of Atmospheric Sciences, University of Washington, Seattle, Washington 98195, USA.

Correspondence to: matthieu.riva@tofwerk.com & lopez@tofwerk.com

[†] These authors contributed equally.

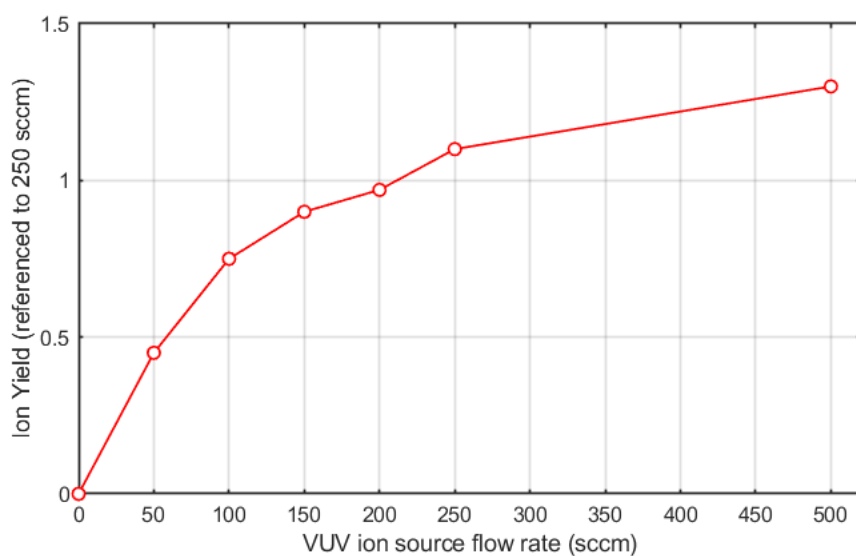


Figure S1. Ion yield as a function of flow rate within the VUV ion source using a mixture of methyl iodide and benzene. The reference corresponds to Vocus AIM normal operation conditions (i.e., 0.25 slpm at 50 mbar and 50°C).

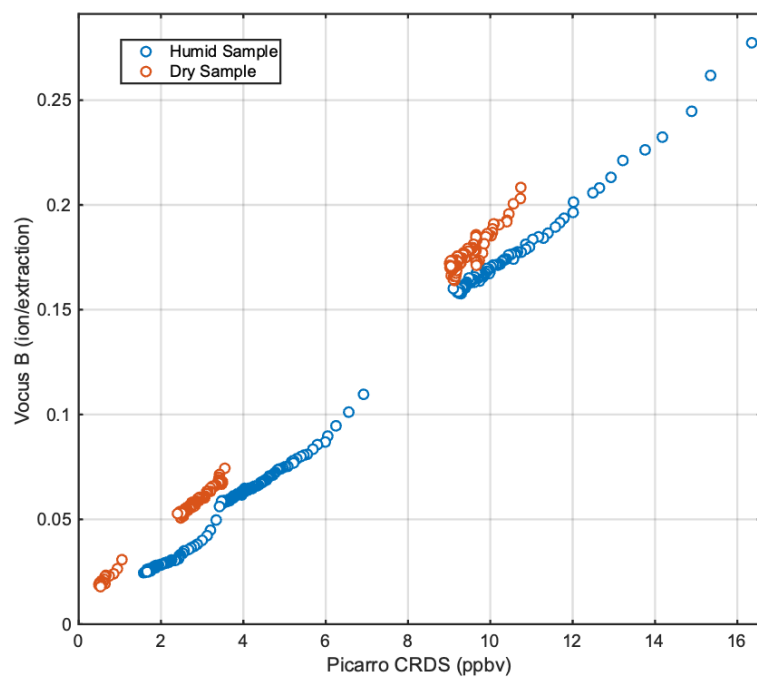


Figure S2. Comparison of the NH_3 concentration generated from the Vici permeation tube under dry and wet conditions and retrieved using the Vocus AIM operated in acetone mode and the Picarro.

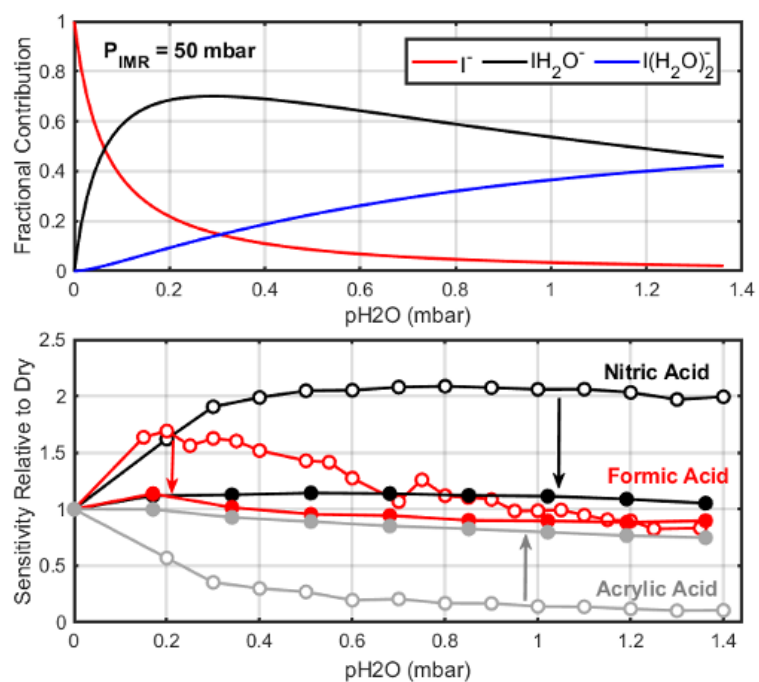


Figure S3. The top panel displays the reagent ion distribution as well as the water clusters as a function of the partial pressure of water within the AIM reactor. The bottom panel presents the variation of sensitivity as a function of relative humidity.

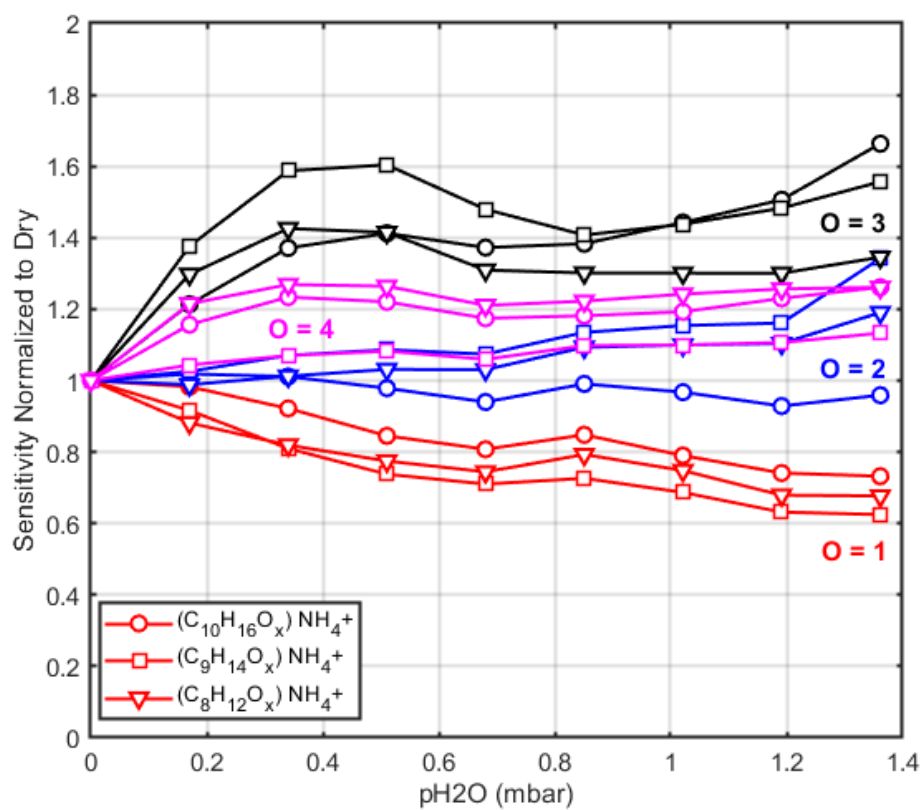


Figure S4. Impact of the relative humidity on the sensitivity of α -pinene oxidation products. The x-axis displays the partial pressure of water, corresponding to higher humidity levels within the reactor (0-100% humidity).

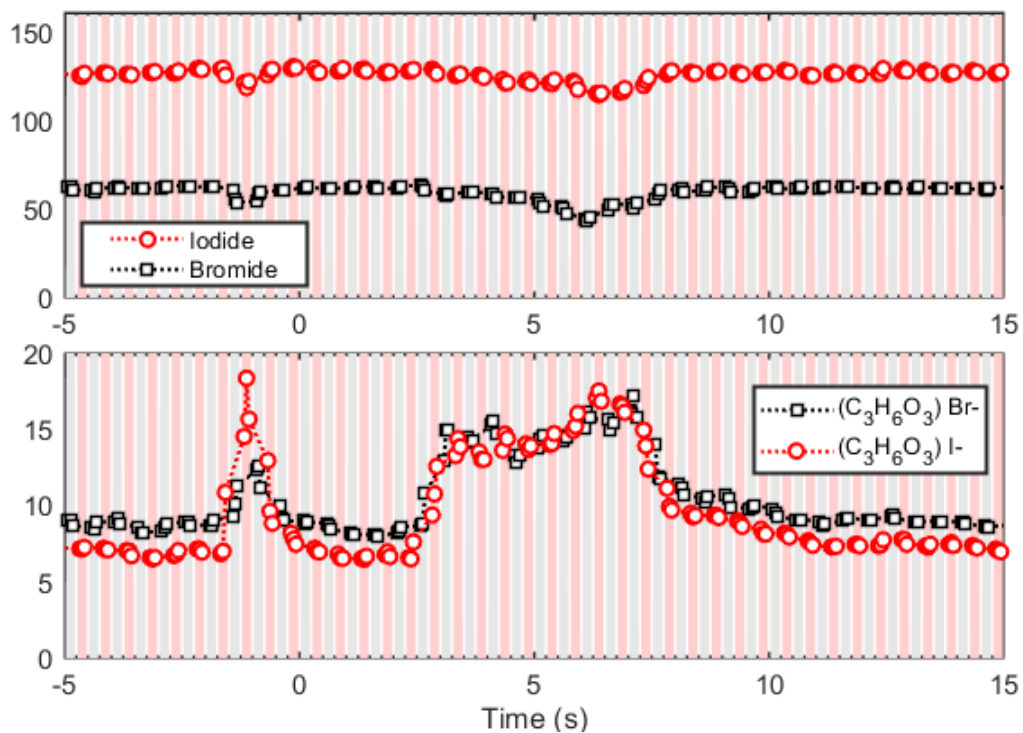


Figure S5. Fast reagent ion switching (i.e., 2 Hz) using the Vocus AIM reactor operated with two VUV sources using bromide and iodide ion chemistries. The total ion currents are reported on the top panel while the ion signal intensity of lactic acid ($C_3H_6O_3$) is displayed in the bottom panel.

Table S1. Multi-component calibration mixture (Apel Riemer Environmental, Inc) in nitrogen. Uncertainty is a conservative estimate of the combination of the uncertainties of the gravimetric preparation and analysis

Compound	CAS #	Concentration (ppb)	Uncertainty
acetaldehyde	75-07-0	1119	± 5%
methanol	67-56-1	1027	± 5%
acetonitrile	75-05-8	1011	± 5%
acetone	67-64-1	1031	± 5%
acrylonitrile	107-13-1	1005	± 5%
isoprene	78-79-5	1011	± 5%
methyl ethyl ketone	78-93-3	1022	± 5%
benzene	71-43-2	1009	± 5%
toluene	108-88-3	997	± 5%
m-xylene	108-38-3	982	± 5%
P	80-56-8	999	± 5%
1,2,4-trimethyl benzene	96-63-6	997	± 5%

Table S2. Relative contributions of VOC, IVOC, SVOC, LVOC, ELVOC, and ULVOC classes of compounds generated from the O₃/OH initiated oxidation of α -pinene and measured using different ion chemistry by the Vocus AIM reactor.

Percentual contributions	ULVOCs	ELVOCs	LVOCs	SVOCs	IVOCs	VOCs
Nitrate	4.3	16.9	62.4	12.6	3.5	0.4
Iodide	0.0	0.1	2.0	6.4	75.9	15.6
Ammonia	0.0	0.0	0.2	0.9	16.5	82.3
Chloride	0.0	0.1	1.3	3.7	30.1	64.8