

Validation of a Newly Designed Simulation Chamber (ESCQ-UAIC) Using Gas Phase Investigations on Aromatic Compounds

Iustinian Bejan,^{1*} Sebastian Laurentiu Marin,² Marius Duncianu,^{1,3}
Cecilia Arsene,^{1,2} Romeo Iulian Olariu,^{1,2}

¹"Alexandru Ioan Cuza" University of Iasi, Integrated Center of Environmental Science Studies in the North Eastern Region - CERNESIM, 11 Carol I, 700506 Iasi, Romania

²"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, 11 Carol I, 700506 Iasi, Romania

³Ecole des Mines de Douai, Chimie et Environnement, Douai, France

Corresponding author: iustinian.bejan@uaic.ro

A new 760 l gas-phase simulation chamber, Environmental Simulation Chamber - Quartz - University "Alexandru Ioan Cuza" (ESCQ-UAIC), Iasi, Romania, has been developed to study relevant atmospheric reactions at ambient pressure and temperature. For validation purposes measurements of selected VOCs have been performed using long path absorption *insitu* FTIR spectroscopy (492±1.2 m) and *on-line* PTR-TOF mass spectrometry. Other state-of-the art instruments (e.g., GC-MS, HPLC, LC-MS, SMPS, AMS) are available for *on-* and *off-line* measurements.

Infrared (IR) cross section, kinetic and mechanistic investigations have been used as significant tools to check/validate the performance of the ESCQ-UAIC chamber. Mass measurement procedure has been used in order to determine the IR cross section for a selected aromatic hydrocarbons (AHs) series. Experimental data obtained for toluene, *p*-xylene and mesitylene are within 15% agreement range with those reported in literature [1]. IR cross sections for other AHs are reported for the first time.

The kinetic of mesitylene reaction with OH radicals has been investigated in the ESCQ-UAIC chamber. A rate constant of $5.61 \pm 0.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ has been obtained by a relative rate method using three reference compounds. The reported value is in very good agreement with the existing literature data [2].

For the last item in the ESCQ-UAIC validation process the reaction of *p*-xylene with OH radicals has been investigated in order to seek for the gas phase products. Ring retaining (*p*-tolualdehyde, 2,5-dimethylphenol) and ring opening (glyoxal, methylglyoxal, 3-hexene-2,5-dione and 2-methyl-butenedial) products have been measured by FTIR and PTR-TOF-MS. The product yields obtained in the present work are in good agreement with literature data.[2] The use of the PTR-TOF-MS technique for products analysis in the OH radical initiated oxidation of *p*-xylene is reported for the first time. Due to its increased sensitivity the PTR-TOF-MS revealed the existence of few other oxygenated compounds.

The entire set of experimental data generated by using the ESCQ-UAIC chamber strongly confirms the suitability of the chamber for further similar studies. Investigations are in progress both on relative rate kinetic and gas phase mechanistic investigations with relevance for atmospheric chemistry.

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