TNA User Report

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Project title	Mechanisms and secondary organic aerosol formation from the atmospheric oxidation of 2,5-dimethylfuran and gamma-valerolactone
Name of the accessed chamber	IASC
Number of users in the project	2 (1 PI and 1 visitor)
Project objectives (max 100 words)	The scientific objectives of this work were: 1. To identify gas- and particle phase organic compounds produced by the OH-initiated oxidation of 2,5-dimethylfuran and gamma-valerolactone. 2. To propose reaction mechanisms for the formation of the oxidation products. 3. To assess the secondary organic aerosol formation potential of the compounds under different reaction conditions.
Description of work (max 100 words):	A series of simulation chamber experiments was performed to characterise the products from the photooxidation of 2,5-dimethylfuran and gamma-valerolactone under different experimental conditions. Nitrous acid and hydrogen peroxide were used as radical precursors to study reactions at high NOx and low NOx respectively. Seed aerosols were also used in some experiments. An Aerodyne FIGAERO time-of-flight chemical ionisation mass spectrometer (ToF-CIMS) was used to identify oxidation products and follow their evolution during the reaction process. Aerosol formation was monitored using a scanning mobility particle sizer, while NOx and ozone were measured continuously by automated gas analysers.

Principal Investigator's and group's information	
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New user	Yes

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[1] *PLEASE CHOOSE ONLY ONE DOMAIN* Physics; Chemistry; Earth Sciences & Environment; Engineering & Technology; Mathematics; Information & Communication Technologies; Material Sciences; Energy; Social sciences; Humanities.

[2] UNI= University and Other Higher Education Organisation;
RES= Public Research Organisation (including international research organisations and private research organisations controlled by public authority);
SME= Small and Medium Enterprise;
PRV= Other Industrial and/or Profit Private Organisation;
OTH= Other type of organization.

[3] UND= Undergraduate; PGR= Post graduate; PDOC= Post-doctoral researcher; RES= Researcher ENG= Engineer; ACA= Academic; TEC= Technician.

[4] Reproduce the table for each user who accessed the infrastructure

Trans-National Access (TNA) Scientific Report

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Name of the PI: Alfonso Aranda
Chamber name and location: IASC, Cork, Ireland
Campaign name and period: Mechanisms and secondary organic aerosol formation from the atmospheric oxidation of 2,5-dimethylfuran and gamma-valerolactone, 04/06/2019 – 31/07/2019

• Introduction and motivation

2,5-Dimethylfuran and gamma-valerolactone (Figure 1) are breakdown products of cellulose, with great potential for use as biofuels [ref]. These oxygenated VOCs are also emitted directly into the atmosphere as a result of biomass burning [ref] where they can be transformed further by atmospheric oxidation processes, i.e. gas-phase reaction with OH radicals, NO_3 radicals, ozone and Cl atoms to produce ozone and secondary organic aerosol (SOA). Detailed investigations of the atmospheric chemistry of these VOCs is thus required in order to understand their potential impact on air quality and climate.

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Figure 1. Chemical structures of 2,5-dimethylfuran and gamma-valerolactone.

• Scientific objectives

The scientific objectives of this work were:

1. To identify gas- and particle phase organic compounds produced by the OH-initiated oxidation of 2,5-dimethylfuran and gamma-valerolactone.
2. To propose reaction mechanisms for the formation of the oxidation products.
3. To assess the secondary organic aerosol formation potential of the compounds under different reaction conditions.

• Reason for choosing the simulation chamber

The IASC chamber has been selected for this activity for two main reasons. Firstly, it is equipped with the FIGAERO ToF-CIMS instrument, which will enable connections between the gas and particle phase organic composition to be established and also provide valuable insights into SOA formation processes. This technique will complement our offline analytical techniques in University of Castilla La Mancha (UCLM). Secondly, the host research group is very well known for its simulation chamber studies of SOA formation and also has considerable expertise in the atmospheric chemistry of oxygenated VOCs like those involved in this study.

• Method and experimental set-up

• Preliminary results and conclusions

• **Outcome and future studies**

To the best of our knowledge, this is the first study of SOA formation from the photo-oxidation of 2,5-dimethylfuran. Online mass spectrometry has provided valuable insights into the species and mechanisms influencing the SOA generation and growth. The results will therefore further our knowledge of SOA production from biomass burning emissions. The new information produced on the atmospheric impact of these two compounds will also be relevant and useful to the biofuels industry. The results of this work will contribute to the PhD thesis of Mercedes Tajuelo Diaz Pavon, will be published in peer-reviewed scientific journals and also presented at conferences.

Future studies will focus on the NO_3 initiated oxidation of 2,5-dimethylfuran, which is expected to be an important reaction pathway for this compounds during night-time.

• **References**

Please add