Characterisation of Ozone levels and associated NMVOC emissions in Spain: a preliminary assessment

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I. EXTENDED ABSTRACT

In Europe, for the last decades, multiple efforts have been made to regulate and reduce air pollution. Despite the overall reduction trends in emissions, air quality remains poor in many areas, where 99% of the urban population is exposed to tropospheric ozone (referred to as O_3 from here on) concentrations above the World Health Organization Air Quality Guideline value [1].

O_3 is a secondary atmospheric pollutant with complex mechanisms of formation and reaction processes, transport, and deposition. The nonlinear nature of its production is one of the main challenges in controlling ozone levels [2].

Spain shows several areas with O_3 problems. Regarding the target value of O_3 for health protection, out of the 127 areas where it was evaluated in 2019, 34 of them show values above the target value, 81 values between the target value and the long-term target value, and the remaining 12 are below the long-term objective. These results have not substantially improved since 2011 and are constant since 2016 [3].

The Spanish Ministry is currently designing a strategy to tackle the O_3 problem in Spain. In this context, air quality modelling systems become an important complementary tool on which to quantify and evaluate the impact of such air quality plans.

Two major directly emitted precursors drive O_3 formation: nitrogen oxides (NOx) (which includes both nitrogen monoxide, NO, and nitrogen dioxide, NO_2) and non-methane volatile organic compounds (NMVOC), so in order to assess O_3, a correct characterization of its precursors is required.

This work focuses on producing a speciated NMVOC inventory for anthropogenic emissions in Spain to support more effective control strategies. The type of NMVOCs emitted varies widely from one source to another, differing substantially by, e.g. fuel, technology, and others. The significant differences between NMVOC species lead to differences in atmospheric chemical reactivity and result in differences in their influence on the formation of ozone. Therefore, speciated NMVOCs emissions and the estimation of ozone formation potential (OFP) are essential to the reactivity-based control approach.

A. Methodology

In this study, in order to develop a speciated inventory for NMVOC, we select all SNAPs (Selected Nomenclature for reporting of Air Pollutants) related to anthropogenic emissions (i.e. SNAPS 1 to 10). For Spain, for the year 2019, we worked with 158 SNAP sectors. The speciated profiles are crucial to a correct characterization of the inventory. Different profile sources were used, where more recent and/or well-defined profiles were chosen. We used 105 profiles, where the majority come from the SPECIATE database [4], followed by EMEP/EEA guidelines. Specific profiles from state of the art were used when available. Resulting in a total of over 800 species.

The emission of an individual NMVOCs species was calculated as:

$$E_i = \sum_j E_j \times R_{ij} \tag{1}$$

where i is a specific NMVOCs species, j is the emission source, is the total emission of the species i, is the total emission of the source j, and is the ratio of species i to source j.

Then the OFP of an individual NMVOCs species for all sources was calculated as:

$$OFP_i = \sum_j E_{ij} \times MIR_i \tag{2}$$

where OFP_i is the total ozone formation potential of species i, E_{ij} is the emission of the species i for source j, and MIR_i is the maximum increment reactivity of species i. The updated MIR values from [5] were adopted in this work.

B. Results

Figure 1 shows the percentage contribution of each SNAP group for the total emissions and for the total OFP. Despite the slight reduction (<3%) in the contribution of SNAP 6 (solvent use), it's still the major contributor for OFP with around 45%, followed by SNAP 10 (livestock) with 12%, and SNAP 8 (Other mobile sources and machinery) with 11%. The latter has a similar emission contribution as SNAP 2 but gains importance when looking at OFP.

The top 10 major SNAP subgroup sectors contributing to the total of OFP show the majority belonging to the SNAPS

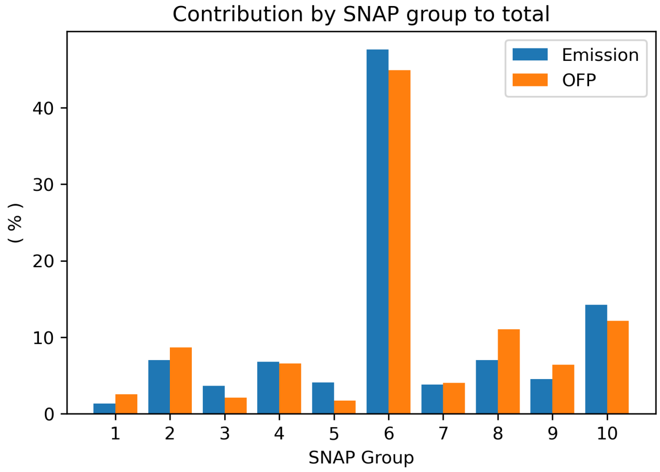

Fig. 1. Contribution, in percentage, of each SNAP sector group to the total of emissions and OFP.

previously identified as major contributors, but other subgroups appear as important as, e.g. residential combustion (0202), burning of agricultural waste (0907), and industry (0405/06).

Figure 2 shows the composition of species emissions for each SNAP where sectors such as the distribution of oil products (SNAP 5) and combustion in the manufacturing industry (SNAP 3) are mainly emitting alkanes (low reactivity). While farm-level agricultural operations (SNAP 10) and production processes (SNAP 4) show a majority of OVOCs.

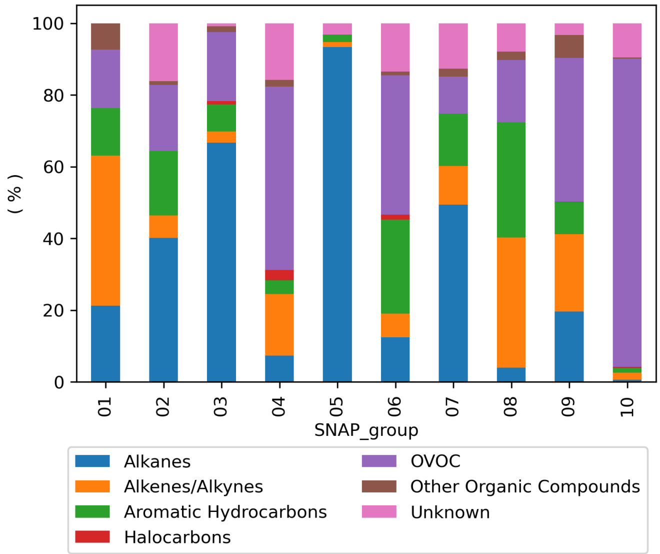

Fig. 2. Composition by grouped species of each SNAP group emissions.

C. Conclusion

When focusing on O_3 problems, this methodology allows prioritising sectors based on their importance to ozone formation, proving to be helpful in terms of control strategies.

The main challenges of adequate characterization of the real world NMVOC emissions are mainly related to the lack of continuous measurements of NMVOCs compounds, limited emission inventories reporting by compound, and lack of recent and more specific speciated profiles for different technologies/fuels. Further complicating this issue is a lack of understanding of the relative importance as to whether total NMVOC emissions or NMVOC speciation is more, less, or equally important, including the relative importance of the changes in speciation and total emissions over time.

Future works will include performing a spatial and temporal analysis of the distribution of NMVOC speciated emissions across Spain. The spatial analysis will allow to determine the importance of acting toward different sectors depending on the area of Spain. While the temporal analysis (i.e. monthly) will deliver information on how to tackle specific sectors based on their activity profile throughout the year. For that, we will make use of the in-house emission model system HERMESv3 [6], which is capable of computing emissions at high spatial (up to 1kmx1km) and temporal resolution (1 hour). To investigate the impact of using more refined NMVOC speciated emissions on the modelling of O_3 levels using the MONARCH atmospheric modelling system [7], which has also been developed at BSC.

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Kevin Oliveira received his MSc degree in Environmental Engineering from the University of Aveiro (UA), Portugal in 2018. In the same year, he started working at the research group on emissions, modelling and climate change (GEMAC) from the Department of Environment and Planning of the UA. In 2021, he joined the Atmospheric Composition group of Barcelona Supercomputing Center (BSC) as well as a PhD student of the Universitat Politècnica de Catalunya (UPC), Spain.