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## Using WRF-Chem Volcano to model the in-plume halogen chemistry of Etna's 2018 eruption

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Volcanic eruptions emit halogen-containing species in varying quantities, with their emission ratio to tracer species such SO<sub>2</sub> varying between volcanoes, eruptions, and even phases of an eruptive event.

The bromine explosion is known to occur within volcanic plumes, converting bromine from HBr – the primary form in which it is emitted – to other forms, including the spectroscopically detectable BrO. Measurements of BrO have been made in the plumes of many volcanoes from both ground-based and satellite-based instruments. There also exist a small number of measurements of OCIO.

We present results from WRF-Chem Volcano (WCV), a modified version of the three-dimensional regional atmospheric chemistry and transport model WRF-Chem and associated utilities. We have simulated the Christmas 2018 eruptive event of Mount Etna using a nested implementation the model at maximum lateral resolution of 1km, as well as a weaker emission plume representing Etna's more common quiescent degassing state. The plume of this 2018 eruption was observed remotely by the TROPOMI instrument.

WCV is able to model the transport and dispersion of the plume. We compare these model outputs to the satellite observations and use this to estimate the volcanic emission column height.

In terms of chemistry, WCV is able to reproduce the bromine explosion and the major features of the satellite observation – including a cross-plume variation in the BrO/SO<sub>2</sub> column ratio. We find that variations in the BrO/SO<sub>2</sub> ratio are primarily caused by variations in the concentration of ozone. Ozone is consumed by bromine chemistry and is replenished by the mixing in of ozone-rich background air. This creates a zone of low ozone in the core of the plume which is consequently low in BrO and surrounded by a higher-ozone edge with a higher BrO/SO<sub>2</sub> ratio.

For the temporal evolution of the plume, we find that the bromine-chemistry of a concentrated emission plume can be divided into four phases, also governed by ozone availability. In the last phase ozone limitation is minimal and the proportion of bromine in the form of BrO (and the

BrO/SO<sub>2</sub> ratio) is approximately stable. We find this stable regime also with a simulation of a weaker emission plume. These results could facilitate the use of remote-sensing BrO measurements as a means of quantifying total bromine emissions from volcanoes.

Oxidized forms of chlorine are modelled to be formed within the plume due to the heterogenous reaction of HOBr with HCl, forming BrCl that photolyzes and produces Cl radicals. We also investigate the extent to which mercury could be oxidized by halogens within the plume.