

Supplementary Information

Global sensitivity and uncertainty analysis of an atmospheric chemistry transport model: the FRAME model (v. 9.15.0) as a case study

Ksenia Aleksankina,^{1,2} Mathew R. Heal,¹ Anthony J. Dore,² Marcel Van Oijen,² Stefan Reis^{2,3}

¹ School of Chemistry, University of Edinburgh, Edinburgh, UK

² NERC Centre for Ecology & Hydrology, Penicuik, UK

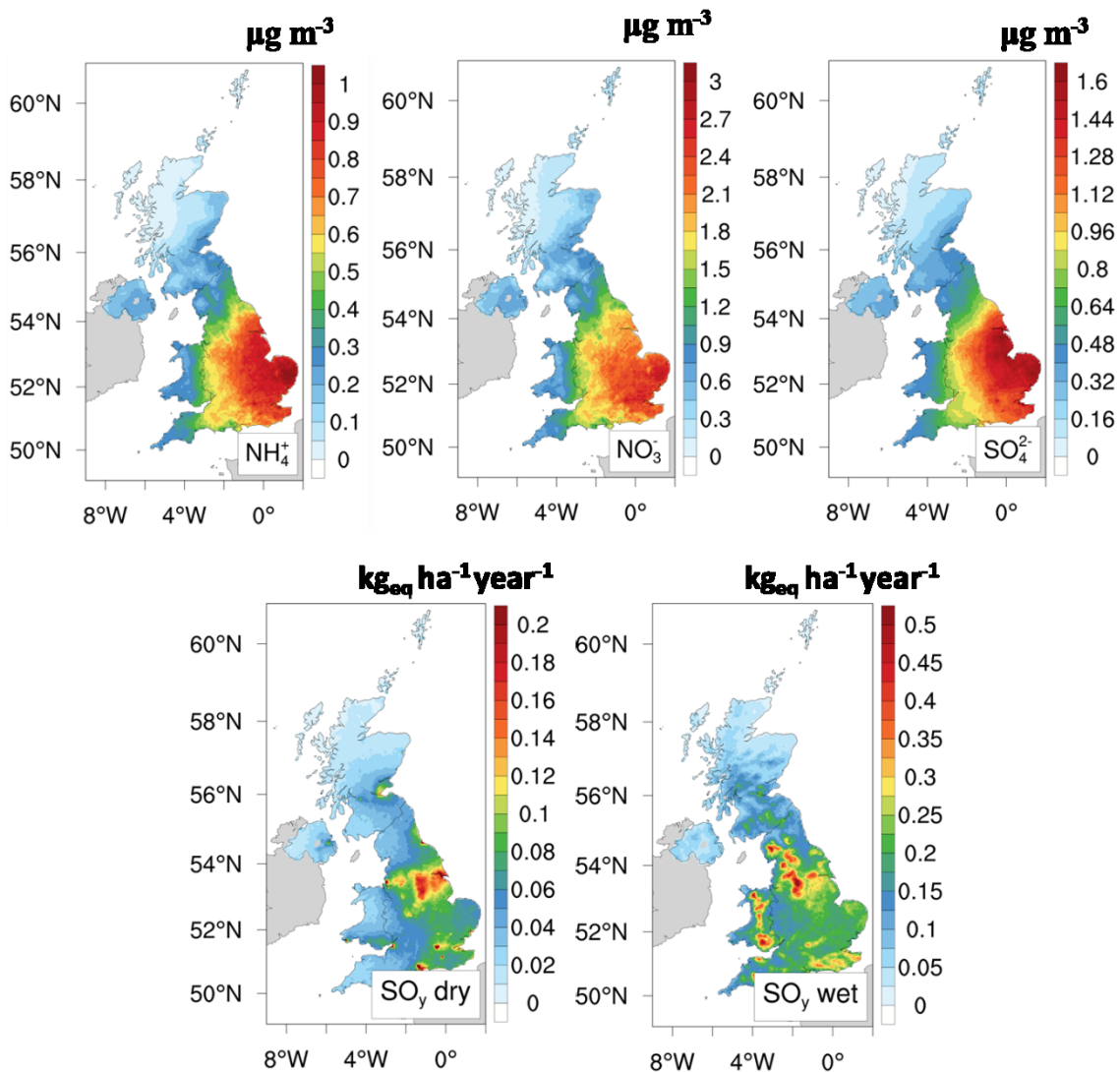
³ University of Exeter Medical School, European Centre for Environment and Health, Knowledge Spa, Truro, UK

Figure S1 shows annual average surface concentrations of particulate NH_4^+ , NO_3^- , SO_4^{2-} , and annual wet and dry deposition of SO_y calculated by the FRAME model with baseline emissions for the year 2012.

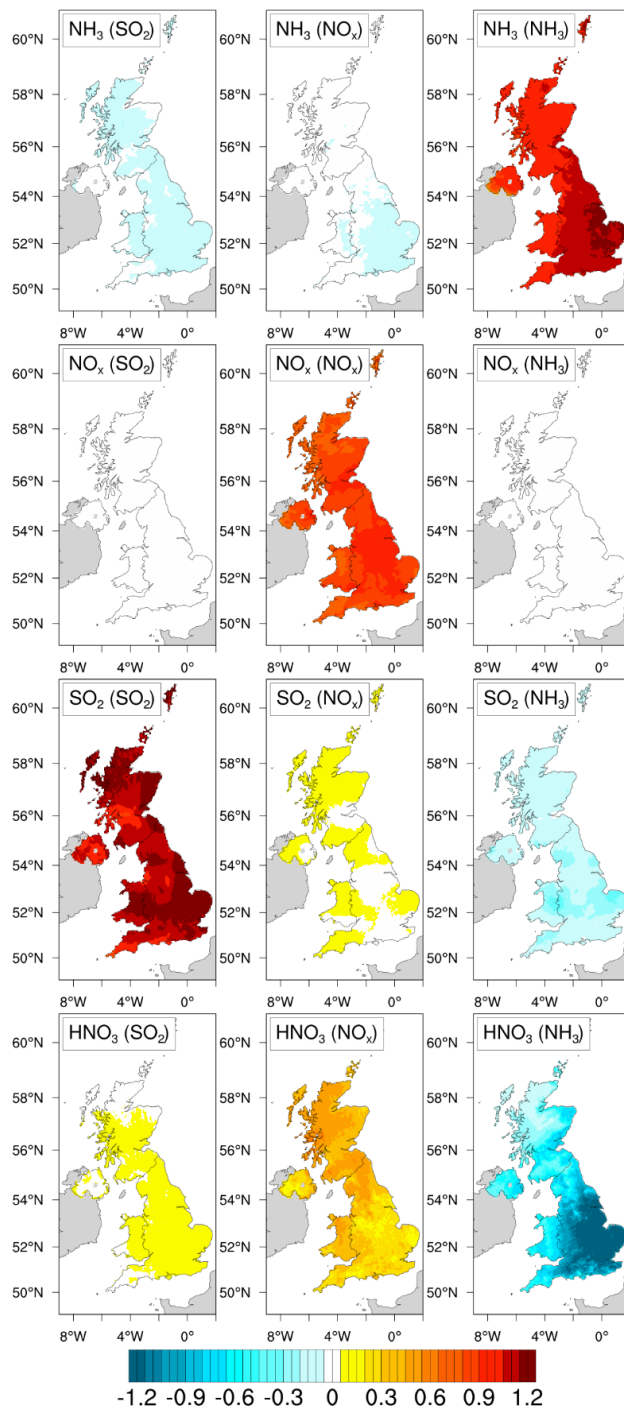
Figures S2 and S3 show spatial distributions of regression coefficients for NH_3 , NO_x , SO_2 , HNO_3 and wet and dry deposition of NH_x and NO_y with respect to input emissions of the pollutant in brackets.

Figure S4 shows spatial distributions of the relative uncertainties in surface concentrations of NH_3 , NO_x , SO_2 and HNO_3 and dry and wet deposition of NO_y and NH_x for uncertainties of $\pm 4\%$, $\pm 10\%$, and $\pm 20\%$ in emissions of SO_2 , NO_x and NH_3 respectively. The uncertainty values are represented as \pm range relative to the baseline value and with the full range represents the 95 % confidence interval.

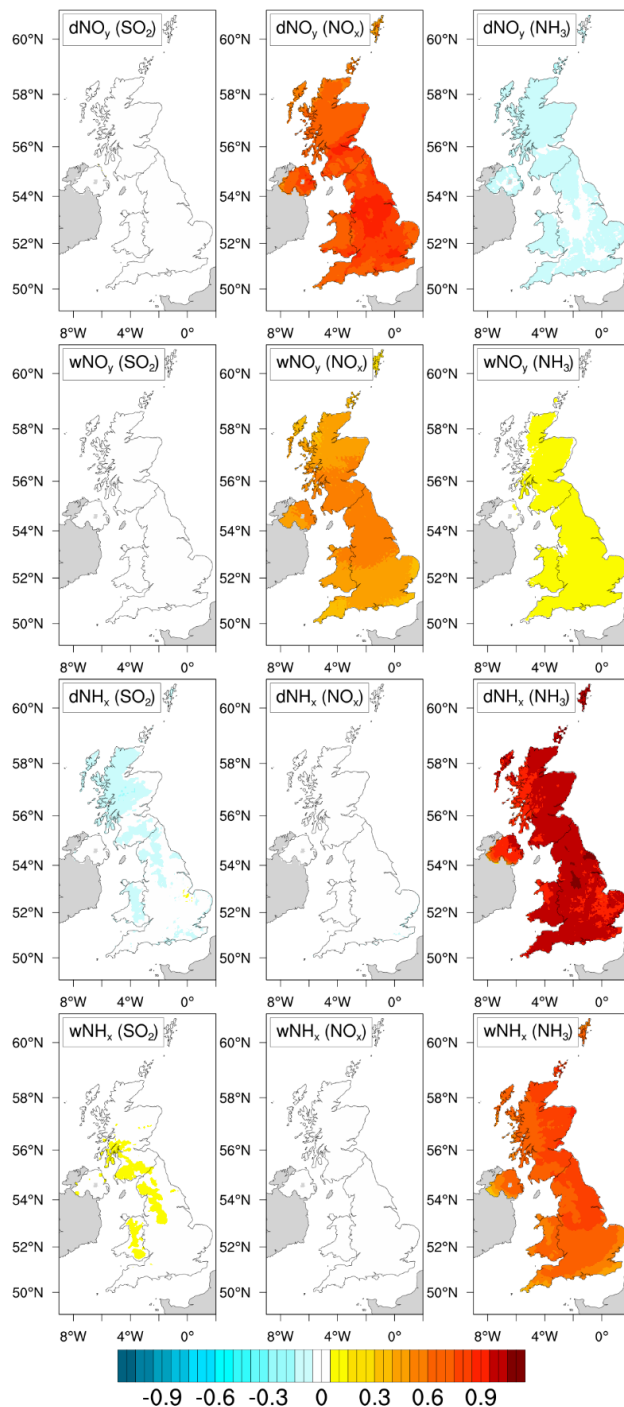
Figures S5 and S6 show spatial distributions of the squared SRC values which represent the fractional contribution of the uncertainty in the input emissions given in brackets to the overall uncertainty in NH_3 , NO_x , SO_2 , HNO_3 and dry and wet deposition of NO_y and NH_x .



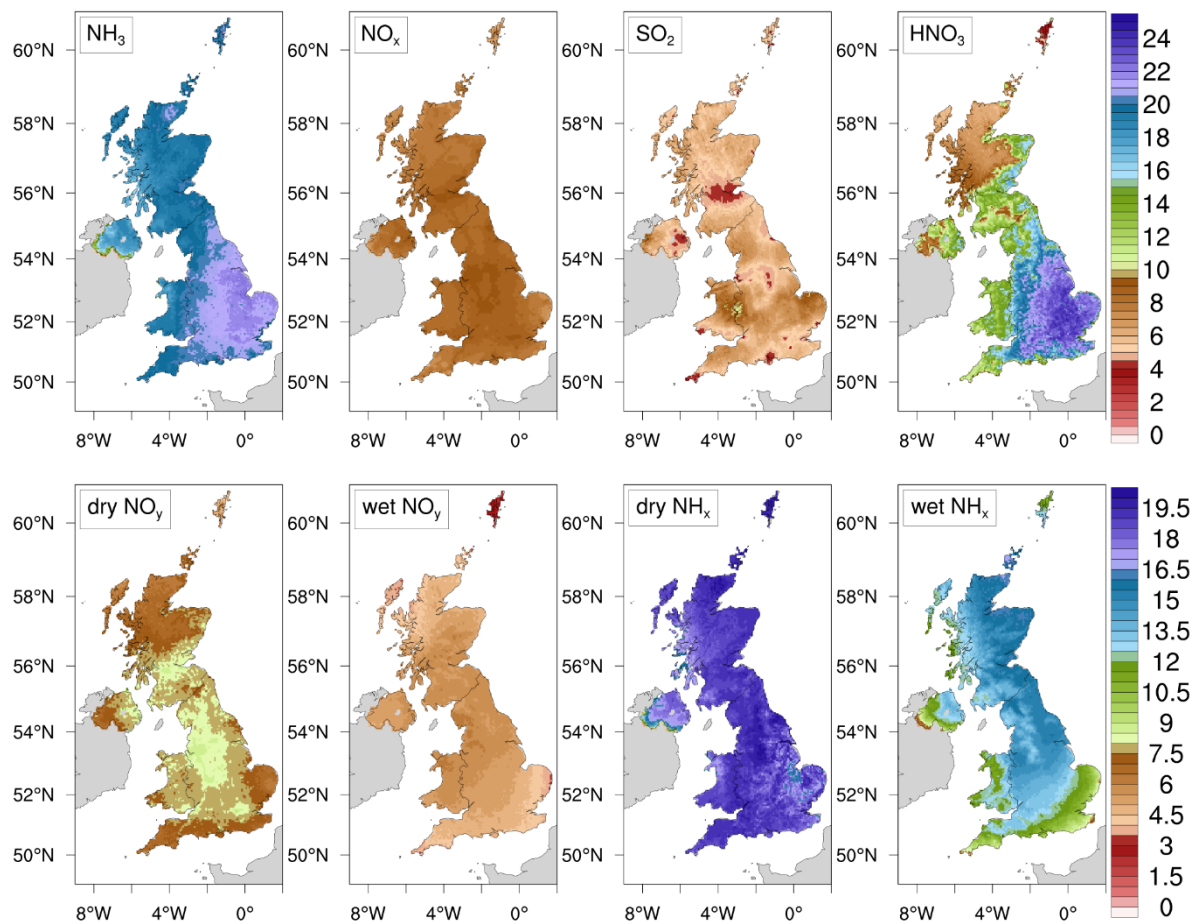
SI Figure 1 Annual average surface concentrations of particulate NH_4^+ , NO_3^- , SO_4^{2-} , and annual wet and dry deposition of SO_y calculated by the FRAME model for 2012.



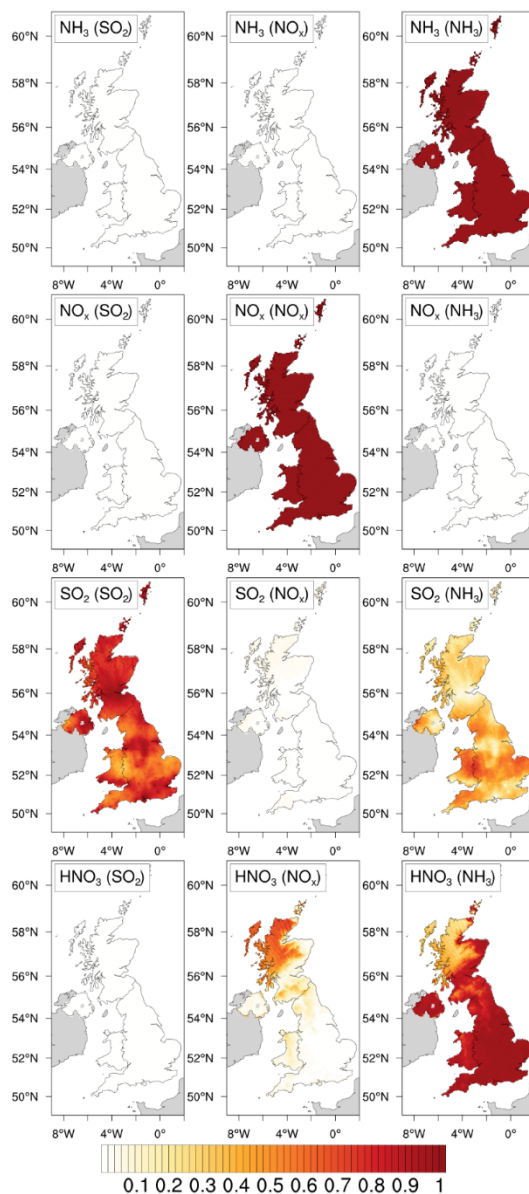
SI Figure 2 Spatial distributions (at the 5 km × 5 km model grid resolution) of RCs for NH₃, NO_x, SO₂, and HNO₃ as a function of variation in input emissions of SO₂, NO_x or NH₃. The model input emissions for which the RC quantifies the output variable sensitivity is given in the brackets in each panel.



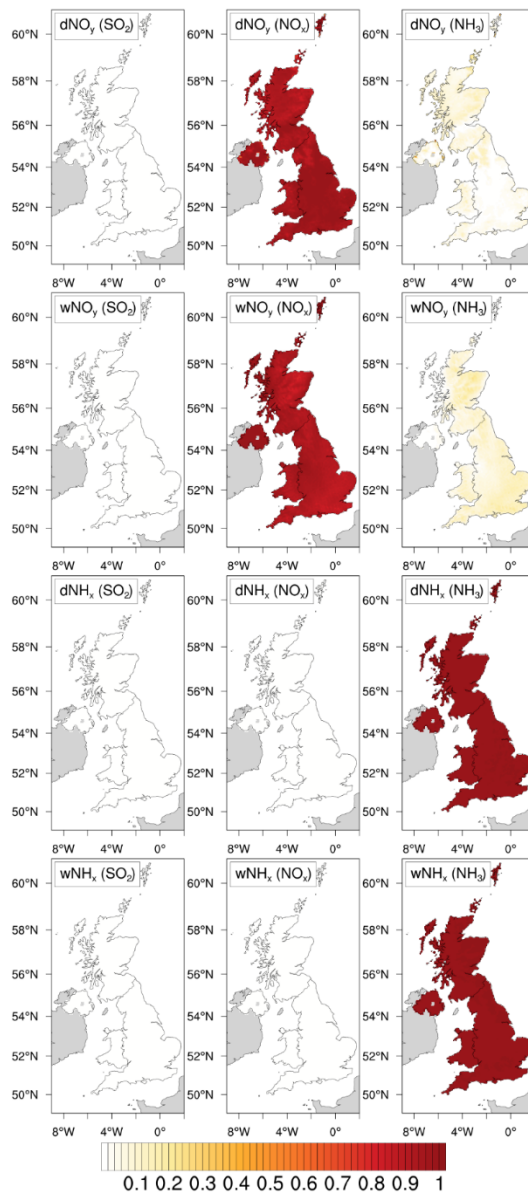
SI Figure 3 Spatial distributions (at the 5 km × 5 km model grid resolution) of RCs for wet (w) and dry (d) deposition of NO_y and NH_x as a function of variation in input emissions of SO_2 , NO_x or NH_3 . The model input emissions for which the RC quantifies the output variable sensitivity is given in the brackets in each panel.



SI Figure 4 Spatial distributions (at the 5 km × 5 km model grid resolution) of the relative uncertainties in surface concentrations of NH_3 , NO_x , SO_2 and HNO_3 and dry and wet deposition of NO_y and NH_x for uncertainties of $\pm 4\%$, $\pm 10\%$, $\pm 20\%$ in emissions of SO_2 , NO_x and NH_3 respectively. The uncertainty values are represented as a range of \pm the baseline value and represent the 95 % confidence interval.



SI Figure 5 Spatial distributions (at the 5 km × 5 km model grid resolution) of the squared SRC values which represent the fractional contribution of the uncertainty in the input emissions given in brackets to the overall uncertainty in NH₃, NO_x, SO₂ and HNO₃. The uncertainties in the input emissions are ± 4 %, ± 10 % and ± 20 % for SO₂, NO_x and NH₃ respectively.



SI Figure 6 Spatial distributions (at the $5\text{ km} \times 5\text{ km}$ model grid resolution) of the squared SRC values which represent the fractional contribution of the uncertainty in the input emissions given in brackets to the overall uncertainty in the dry and wet deposition of NO_y and NH_x . The uncertainties in the input emissions are $\pm 4\%$, $\pm 10\%$ and $\pm 20\%$ for SO_2 , NO_x and NH_3 respectively