

Supplementary dataset for *A multi-method assessment of the regional sensitivities between flight altitude and short-term O_3 climate warming from aircraft NO_x emissions*

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Introduction

This dataset accompanies the journal article entitled *A multi-method assessment of the regional sensitivities between flight altitude and short-term O₃ climate warming from aircraft NO_x emissions* and has been generated from 74 simulations performed with the ECHAM/MESSy Atmospheric Chemistry model (EMAC). The impact on atmospheric ozone (O₃) from aircraft nitrogen oxide (NO_x) emissions is estimated for five regions (North America, Eurasia, South America, Africa and Australasia), three pressure altitudes (200, 250 and 300 hPa) and two seasons (July 1, 2014 representing the Northern summer and January 1, 2014 representing Northern winter) using three calculation methods: Eulerian tagging, Lagrangian tagging and perturbation. Each region has 28 points at which 0.5 Gg of NO are introduced in the form of a 15-min pulse emission (see Figure 1 of main article). For further information regarding the differences between each method, please refer to the main article as well as the Supplement.

Simulations per method (total of 74 simulations):

- Lagrangian tagging → 5 regions × 2 seasons × 3 pressure altitudes = 30 simulations
- Eulerian tagging → 5 regions × 2 seasons × 3 pressure altitudes = 30 simulations
- Perturbation → Requires 2 additional reference cases, 1 per season = 2 simulations
- Emission strength sensitivity → 4 emission strengths × 3 pressure altitudes = 12 simulations

EMAC model grid resolutions

Resolution used for the Lagrangian tagging simulations:

- ❖ T42L41 resolution
 - T42: horizontal discretization of the grid space into 128 longitudes and 64 latitudes, corresponding to a $2.8^\circ \times 2.8^\circ$ quadratic Gaussian grid.
 - L41: 41 vertical hybrid pressure levels ranging from the surface up to 5 hPa.

Resolution used for the Eulerian tagging and perturbation simulations:

- ❖ T42L90MA resolution
 - T42: same as above.
 - L90MA: 90 vertical hybrid pressure levels ranging from the surface up to 0.01 hPa.

Description of data files

The net NO_x-induced O₃ production [kg] as well as the associated instantaneous radiative forcing (iRF), measured in W/m², have been calculated using all three methods (Eulerian tagging, Lagrangian tagging and perturbation). All output files are provided in NetCDF (.nc) format. We note that “emission region” can refer to the options [NA=North America, EU=Eurasia, SA=South America, AF=Africa and AU=Australasia], “emission altitude” to the options [200, 250, 300], “emission time” to [Jan=January 1, 2014 or Jul=July 1, 2014] and lastly, for the Lagrangian tagging method, “emission point (EP)” varies from calls 1 to 30. The first call does not refer to a specific emission scenario, rather it specifies the required inputs for the quasi-chemistry-transport model (QCTM) climatology. The second call calculates the long and shortwave radiative fluxes only for the background O₃ concentration. Calls 3 – 30 then refer to the emission points displayed in Figure 1 of the main article (i.e., call 3 calculates the radiative fluxes for the NO_x-induced O₃ field as well as the background O₃ when emitting at emission point 1 in Figure 1). We emit 5×10^5 kg(NO) at each of the 28 points per region, the main difference between the Eulerian and Lagrangian simulations is that the latter does not consider chemical interactions between the emitted NO.

Eulerian tagging (Eul)

NO_x-induced O₃ mass

Relevant files:

- Eul_{emission region}_{emission altitude}_{emission time}_tracer_pdef_gp.nc

Relevant variables:

- *MP_O3_air*{emission region}_ave[time], in kg of O₃
- *Time*, in days

NO_x-induced O₃ iRF

Relevant files:

- Eul_{emission region}_{emission altitude}_{emission time}_viso.nc

Relevant variables:

- *Flxs_tp_02_ave*[time,lat,lon], shortwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m²
- *Flxt_tp_02_ave*[time,lat,lon], longwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m²
- *Flxs_tp_03_ave*[time,lat,lon], shortwave radiative flux relative to the climatological tropopause based on background and additional O₃ produced from NO emissions simultaneously introduced at 28 emission points, in W/m²
- *Flxt_tp_03_ave*[time,lat,lon], longwave radiative flux relative to the climatological tropopause based on background and additional O₃ produced from NO emissions simultaneously introduced at 28 emission points, in W/m²
- *Time*, in days

We note that the net radiative flux using Eulerian tagging, iRF_{Net}^{Eul} , may be computed as follows:

$$iRF_{Net}^{Eul} = [flxt_tp_03_ave + flxs_tp_03_ave] - [flxt_tp_02_ave + flxs_tp_02_ave]$$

Lagrangian tagging (Lg)

NO_x-induced O₃ mass

Relevant files:

- Lg_{emission region}_{emission altitude}_{emission time}_tracer_pdef_lggp.nc

Relevant variables:

- *MP_airO3_{emission point}_ave[time]*, in kg of O₃
- *Time*, in days

NO_x-induced O₃ iRF

Relevant files:

- For an NO emission at 250 hPa:
 - Lg_{emission region}_{emission altitude}_{emission time}_{emission point}_fluxes_tp.nc
- For an NO emission at other levels (200 and 300 hPa):
 - Lg_{emission region}_{emission altitude}_{emission time}_viso.nc

Relevant variables:

- *Flxs_tp_02[time,lat,lon]*, shortwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m²
- *Flxt_tp_02[time,lat,lon]*, longwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m²
- *Flxs_tp_EP[time,lat,lon]*, shortwave radiative flux relative to the climatological tropopause based on background O₃, NO emission at a specific emission EP only, units in W/m², for a specific call (EP between 3 and 30)
- *Flxt_tp_EP[time,lat,lon]*, longwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions at a specific emission EP only, units in W/m², for a specific call (EP between 3 and 30)
- *Time*, in days

We note that the total net radiative flux using Lagrangian tagging, iRF_{Net}^{Lg} , may be computed as follows:

$$iRF_{Net}^{Lg} = \sum_{EP=3}^{30} ([flxt_tp_EP + flxs_tp_EP] - [flxt_tp_02 + flxs_tp_02]).$$

EP may vary from 1 – 30, where each call represents a specific scenario:

- Call 1 (EP01): input variables for QCTM climatology, useful for ensuring identical background meteorology and chemistry across all 28 emission points.
- Call 2 (EP02): background O₃
- Call 3 (EP03): background O₃ + O₃ produced from NO emission at point 1 (Figure 1 of main article)
- Call 4 (EP04): background O₃ + O₃ produced from NO emission at point 2 (Figure 1 of main article)
- Call 5 (EP05): background O₃ + O₃ produced from NO emission at point 3 (Figure 1 of main article)
- ...
- Call 30 (EP30): background O₃ + O₃ produced from NO emission at point 28 (Figure 1 of main article)

Perturbation (Pert)

NO_x-induced O₃ mass

Relevant files:

- Eul_{emission region}_{emission altitude}_{emission time}_tracer_pdef_gp.nc (Perturbed simulation)
- Eul_ref_{emission time}_tracer_pdef_gp.nc (Unperturbed, reference simulation)

Relevant variables:

- *MP_O3_ave[time]*, in kg of O₃
- *Time*, in days

We note that the net O₃ mass production using the perturbation method is calculated as follows:

$$O_{3,Net}^{Pert} = \underbrace{MP_{O3_ave}}_{\text{Perturbed}} - \underbrace{MP_{O3_ave}}_{\text{Reference}}$$

NO_x-induced O₃ iRF

Relevant files:

- Eul_{emission region}_{emission altitude}_{emission time}_viso.nc (Perturbed simulation)
- Eul_ref_{emission time}_viso.nc (Unperturbed, reference simulation)

Relevant variables:

- *Flxs_tp_02_ave[time,lat,lon]*, shortwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m² (Perturbed)
- *Flxt_tp_02_ave[time,lat,lon]*, longwave radiative flux relative to the climatological tropopause based on background O₃, NO emissions are absent, units in W/m² (Perturbed)
- *Flxs_tp_03_ave[time,lat,lon]*, shortwave radiative flux relative to the climatological tropopause based on background and additional O₃ produced from NO emissions, in W/m² (Perturbed)
- *Flxt_tp_03_ave[time,lat,lon]*, longwave radiative flux relative to the climatological tropopause based on background and additional O₃ produced from NO emissions, in W/m² (Perturbed)
- The same 4 variables above are of interest in the reference simulation (Eul_ref_...viso.nc)
- *Time*, in days

We note that the net radiative flux using the perturbation method, iRF_{net}^{Pert} , may be computed as follows:

$$iRF_{Net}^{Pert} = iRF_{Net}^{Perturbed} - iRF_{Net}^{Reference},$$

where iRF_{Net} must be found for both the perturbed and reference simulations as follows:

$$iRF_{Net} = [flxt_tp_03_ave + flxs_tp_03_ave] - [flxt_tp_02_ave + flxs_tp_02_ave].$$

Emission strength sensitivity simulations

We have also performed an additional 12 simulations to investigate the influence of altitudinal variation on the degree of $\text{NO}_x\text{-O}_3$ non-linearities. Emission strength of NO assumes values of 1%, 50%, 100%, 150% and 200% where the 100% scenario equates to a 5×10^5 kg (NO) emission at each of the 28 points of Figure 1 (main article). These simulations apply only to North America during the Northern summer season. Therefore, “emission strength” may refer to 1%, 50%, 150% or 200%. The Eulerian tagging and perturbation methods were again applied to these 12 simulations, the variables and calculation methods themselves are identical to the ones described in the “Eulerian tagging” and “Perturbation” sections of this document. The perturbation method once again relies on the reference simulations from before (“Eul_ref..”). The Lagrangian method cannot be used in this context due to its linearization of reaction rates.

Relevant files:

- Eul_NA_{emission altitude}_{emission strength}_July...tracer_pdef_gp.nc
- Eul_NA_{emission altitude}_{emission strength}_July...viso.nc