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Using S-5p trace gas and aerosol observations of fire plumes to constrain a global composition model: a critical assessment

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The modeling of the dynamical evolution of smoke plumes from wildfires requires accurate description of its emissions together with complex chemistry. These elements challenge its representation in global atmospheric composition models, which face limitations in smoke plume chemistry, transport, and model resolution, resulting in uncertainties in the fate of key quantities such as CO, ozone, NO_x and aerosol loading.
Here we show how the S-5p observations can help to constrain the modeling of fire trace gas and aerosol emissions, and its evolution, and assess which uncertainties are introduced due to atmospheric composition modeling, as opposed to uncertainties in prior emissions.

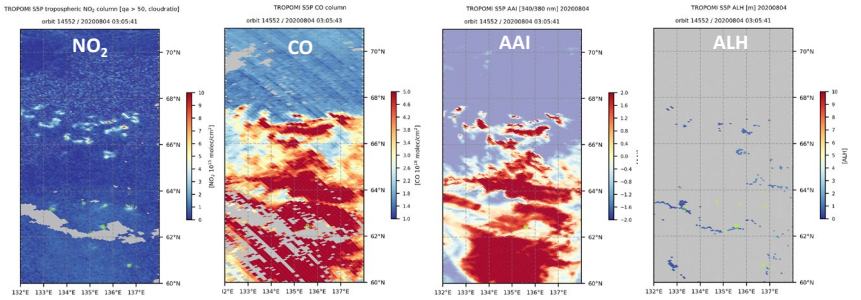
The CAMS global composition model configuration

For this study we use the CAMS global model version, based on a target CY48R1 **IFS(CB05-AER)** model configuration. The model is run on TL511 horizontal resolution (~40 km), with 137 model levels, with sectoral emissions treatment as provided by Z. Kipling, ECMWF. We use the **GFASv1.4** daily fire emissions. Here we focus on the August 2020 fires over Siberia, and September fires over the Amazon. We run sensitivity experiments with:

- varying chemistry, to assess impact of model chemistry and tracer lifetime
- varying horizontal resolution, and sub-grid scale modeling
- varying emissions treatment (injection altitude, diurnal cycle and emission factors

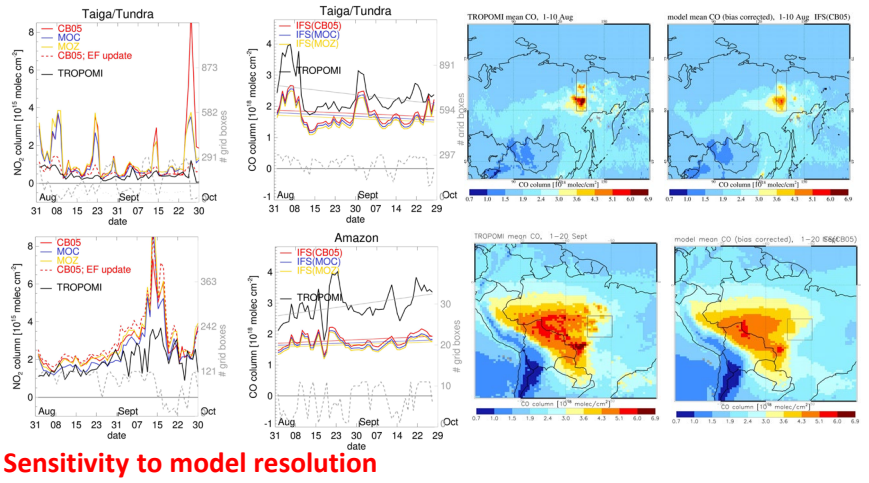
TROPOMI data for model evaluation

We compare simulations against S-5p observations for **CO** (OFFL), **NO_2** (PAL), and **ALH** (OPER). Here we use standard collocation methods and apply AK's to model profiles. We average grid boxes towards a common 0.5x0.5 deg resolution. Despite the relatively high resolution of the global model, we acknowledge a considerable discrepancy to the resolution of S-5p (up to 3.5 x 7 km). The figures show example TROPOMI data products over Siberia, 4 August 2020.



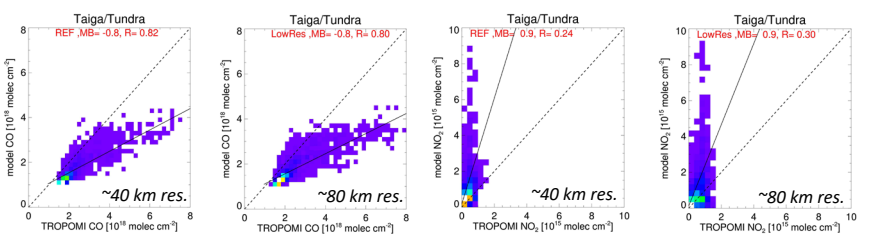
Sensitivity to model chemistry

With respect to enhancements associated to fire plumes, we find larger discrepancies between chemistry versions for NO_2 (left) than for CO (2nd -4th column). Nevertheless, the discrepancy between model configurations and observations cannot be explained from uncertainties in the respective chemistry mechanisms.



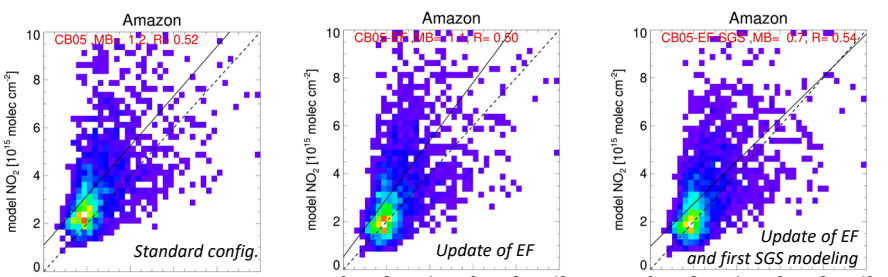
Sensitivity to model resolution

The sensitivity to model resolution appears small for CO (left) but shows changes in scores for NO_2 (right) when testing a low-resolution (~ 80 km res) configuration.



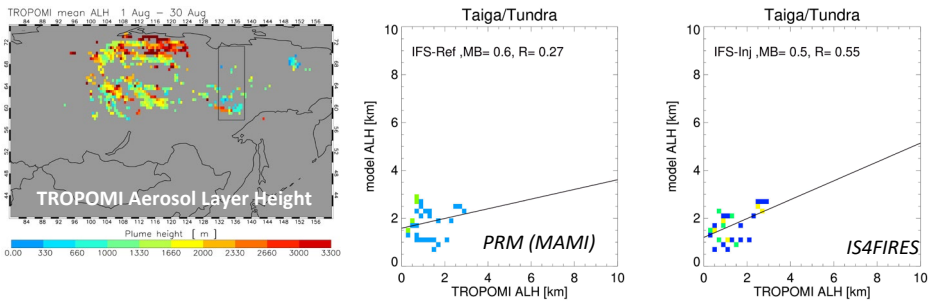
Sensitivity to emission factors and sub-grid scale modeling

Uncertainties associated to atmospheric chemistry model parameterizations turn out insufficient to explain key discrepancies between model and S-5p (left figure for Amazon).
Updates to the Emission Factors, specifying the emission of species per kg Dry Matter Burned, using updated literature values (Andreae, ACP 2019), help to further mitigate discrepancies, particularly for boreal fire cases, but less impact elsewhere (middle figure). In addition, sub-grid scale plume chemistry contributes to model discrepancies for short-lived tracers such as NO_2 (Wang et al., JGR 2021). A first attempt to model this in the CAMS system was found beneficial (improved MB, and R, see right figure) but raises the question of the minimum complexity required for such.



Sensitivity to emission parameterization

The sensitivity to emission injection altitude parameterization of wildfire emissions is tested by varying the standard parameterization (PRM, middle) with an alternative one (IS4FIRES, right), and evaluating aerosol plume altitude against TROPOMI observations of Aerosol Layer Height (left). Better performance is found for configurations using IS4FIRES, but the obs. dataset is limited. The impact of this change on performance of trace gases simulations against TROPOMI is small, though.



Implications for top-down constraints on fire emissions

The following findings are highlighted, relevant to any system that relies on large-scale atmospheric composition modeling and satellite observations to provide top-down constraints on fire emissions:

- **S-5p ALH** provides limited constraints on model plume altitude; the impact of varying assumptions on modeled composition is generally small.
- **S-5p CO** observations provide strong constraints on emission totals, also because the uncertainty due to model chemistry and resolution is small.
- **S-5p NO_2** reveals enhancements due to fire plumes on a high spatial resolution. Uncertainties in global composition modeling assumptions are insufficient to explain the discrepancies completely, but a quantitative comparison is challenging due to the resolution mismatch and fast and complex plume chemistry. Updates to EF's, along with sub-grid scale modeling helps to close the gap.

Outlook

Experience gained with this study, exploiting TROPOMI observations combined with global model simulations, helps to provide constraints on estimated fire emissions. While this has so far focused on GFAS emissions, we will exploit this to also provide constraints on alternative emission estimates developed in the **Sense4Fire** project.

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