SF_6 model intercomparison

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Initial conditions and spin-up

Modelers will be given an initial condition for January 1, 2000, called the *unoptimized* initial condition. Modelers will integrate forward for 5 years from this unoptimized initial condition. The SF_6 fields thus generated for January 2005 will then be scaled back so that they optimally match available SF_6 measurements for January 2000. These available observational constraints are dominated by surface measurements. This scaling will be achieved with a linear regression using an offset and a multiplicative scaling term. The resulting model-specific field will be used as the model-specific *optimized* initial condition for January 2000. Simulations will be conducted through January 2017, with results from 2007 through 2017 being analyzed. This gives another seven years' spin-up for each model.

Our unoptimized initial condition is based on an SF_6 curtain generated by David Nance (NOAA) for January 2000. Observed SF6 mole fractions between 1994 and 2010 are detrended to 01-Jan-2000 assuming two different linear trends before and after that date, and interpolated throughout the atmosphere to create a latitude-altitude curtain of SF_6 mole fractions. The observations include marine boundary layer observations, as well as balloon and high altitude aircraft observations up to 20 mb. This curtain covers most but not all of the atmosphere (Fig. 1, left). We extended this curtain to cover the entire atmosphere using modeled meridional SF_6 gradients in the TM5 tracer transport model over the Pacific. The simulation was spun up for 40 years using cyclostationary meteorology.

The filled SF$_6$ curtain is hosted at
https://drive.google.com/file/d/1LZZOMMQSq3xAS7qO_yYV38jQGKMTKhvv/view?usp=sharing
as a 2D field, latitude x pressure levels. This is a zonally averaged field. The recommended
method to use the curtain to initialize a model is:

1. For a given lat/lon/alt/pressure cell, look up the SF$_6$ mole fraction for that
   latitude/pressure coordinate from the curtain.

2. After filling in all model grid cells, scale the mole fraction in all cells such that the globally
   averaged dry air mole fraction, i.e., total moles SF$_6$/total moles dry air, is 4.33045
   picomoles/mole. The second step is important since the dry air mole fraction is the
   quantity measured in the atmosphere.

Please contact intercomparison organizers (sourish.basu@noaa.gov and
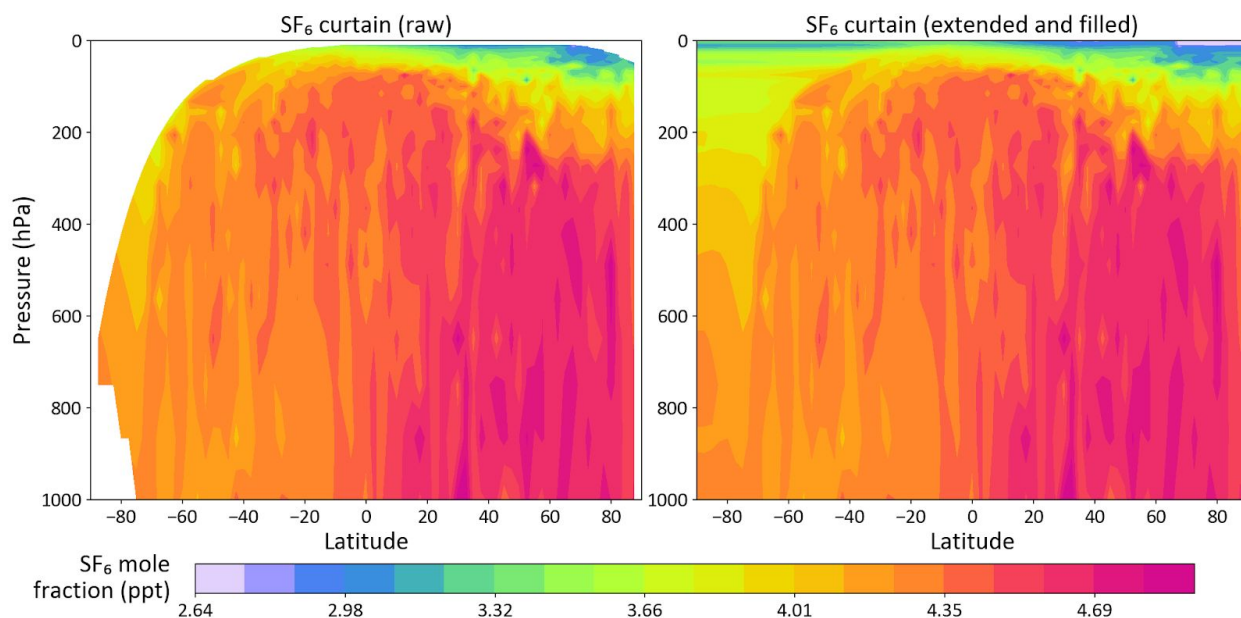andy.jacobson@noaa.gov) if you have any questions about this initialization procedure.

Figure 1: (Left) SF$_6$ mole fraction curtain for 2000-01-01 00:00 UTC, obtained by de-trending
aircraft and surface SF$_6$ observations between 1994 and 2010. (Right) The curtain extended to
fill the entire atmosphere by using TM5 modeled meridional gradients over the Pacific.

Spin-up and simulation procedures summary

- Get unoptimized initial condition for Jan 1, 2000 from Sourish Basu
- Run model forward from Jan 1, 2000 to Jan 1, 2005 using SF_6 emissions from Brad Weir
- Scale Jan 1, 2005 model SF_6 field back to Jan 1, 2000 using MBL surface constraint (to create the optimized IC)
- Run model using optimized IC from Jan 1, 2000 through Jan 1, 2017
  - Jan 1 and July 1 SF_6 global burden each year
  - Sample ObsPack measurements
  - Monthly gridded output Jan 1, 2007-Jan 1, 2017

Surface Fluxes

The EDGAR v4.2 emissions inventory of SF_6 will form the basis for fluxes between 2000 and 2017. These annual 0.1° x 0.1° emissions will be coarsened to the common 1° x 1° modeling grid and then scaled to agree with estimates of annual emissions derived from the observed global growth rate (see https://www.esrl.noaa.gov/gmd/hats/combined/SF6.html for one such product). This scaling goes from measured mole fractions to estimated atmospheric mass burden using an assumed constant atmospheric dry air mass of 5.1352×10^{18} kg (Trenberth and Smith 2005). If this is persistently different from the simulated dry air mass in a given model, participants are encouraged to scale input fluxes to their model's dry air mass. Please consult with one of the intercomparison organizers if you are interested in doing this.

To avoid discontinuities between years and to provide monthly-fluxes, a smooth linear trend model will be applied. It will be continuous from year-to-year, a linear function of month within a year, and preserve the annual total emissions. A check will be made that the resultant surface flux is nonnegative for all time and space. These emissions have been created by Brad Weir at NASA GMAO and may be downloaded at https://gmao.gsfc.nasa.gov/gmaoftp/bweir/sf6/.

Modelers may need to regrid the emissions for their particular modeling system. As total SF_6 burden will be a crucial criterion for evaluating simulations, it is vital that emissions be applied exactly and that this regridding is done conservatively. We suggest using the HEMCO emissions frontend (http://wiki.seas.harvard.edu/geos-chem/index.php/HEMCO) in standalone mode to conservatively regrid emissions to each model's emissions grid. For more complex grids, the SCRIP regridding tool (http://oceans11.lanl.gov/trac/SCRIP) can be used to perform this task. Intercomparison organizers will be available to help modelers develop emissions for their particular system. Please contact intercomparison organizers (brad.weir@nasa.gov and andy.jacobson@noaa.gov) to discuss this procedure.

Output

Modelers will sample *in situ* measurements of SF_6 from the ObsPack collection recently published by NOAA/GMD. The collection includes 221 datasets from 8 laboratories over the period 1994-2017, including measurements from surface flask, aircraft, and balloon programs. A description of this ObsPack can be found at https://www.esrl.noaa.gov/gmd/ccgg/obspack/release_notes.html#obspack_sf6_1, and the direct download link is https://www.esrl.noaa.gov/gmd/ccgg/obspack/data.php?id=obspack_sf6_1_v2.1.1_2018-08-17.

Normally, ObsPack data is provided in timeseries format, with one netCDF file per dataset. A more convenient format for modelers is the so-called "model prepped" ObsPack, in which data are provided in one file per day, containing all the measurements for that day across all available datasets. The SF_6 v2.1.1 Obspack has been reformatted into this convenient "prepped" format and is available at https://www.esrl.noaa.gov/gmd/ccgg/obspack/data.php?id=obspack_sf6_1_v2.1.1_prepped_inputs_2018-08-20.

Researchers wishing to use these SF_6 measurements should follow usage instructions provided in the release notes. Importantly, this includes citation of the DOI (https://search.datacite.org/works/10.25925/20180817).

ObsPack sampling code is available for TM5 and for GEOS-Chem and can be shared upon request. Those routines are more full-featured than is strictly needed for this exercise. For example, they are written to collect multi-hour model averages to represent flask measurements, and have the ability to also write out model meteorological variables. Modelers also can simulate ObsPack data by selecting appropriate instantaneous grid-box concentrations. Other modelers participating in the OCO-2 MIP have developed their own schemes for sampling ObsPack data, and we encourage participants to consult with others before writing new code. Contact andy.jacobson@noaa.gov if you have questions about ObsPack sampling.

Required output

The total atmospheric burden of SF_6 in units of mass will be reported by each modeler for Jan 1 and July 1 of each year of the simulation. These data should be submitted as CSV-formatted text files or netCDF files containing two variables only: the year (model time) and the total atmospheric burden of SF_6 in grams. We will use this to verify emissions and overall

simulation performance, and to determine whether the SF_6 burden within each model has any spurious seasonality. Burden output files should be named using the model name, the modeler's name, and the date of submission:

burden_sf6_<model>_<modeler>_<datestamp>.csv or
burden_sf6_<model>_<modeler>_<datestamp>.nc, for example

for example ,"burden_sf6_TM5_Jacobson_20180208.csv".

Modelers will also submit model samples of each measurement of SF_6 in the ObsPack. Modelers may submit either CSV-formatted text files or netCDF files. These should contain two pieces of information per measurement only: the 200-character "obspack_id" string used to uniquely identify each measurement, and the modeled SF_6 mole fraction in parts per trillion (pmol/mol) in dry air. ObsPack sample output files should be named using the model name, the modeler's name, and the date of submission:

obspack_sf6_<model>_<modeler>_<datestamp>.csv or
obspack_sf6_<model>_<modeler>_<datestamp>.nc,

for example, "obspack_sf6_TM5_Jacobson_20180208.csv".

Sample submission files for annual burden and ObsPack output can be found at:

ftp://aftp.cmdl.noaa.gov/user/andy/sf6_mip/burden_sf6_SAMPLE_Jacobson_20180208.csv
ftp://aftp.cmdl.noaa.gov/user/andy/sf6_mip/burden_sf6_SAMPLE_Jacobson_20180208.nc
ftp://aftp.cmdl.noaa.gov/user/andy/sf6_mip/obspack_sf6_SAMPLE_Jacobson_20180208.csv
ftp://aftp.cmdl.noaa.gov/user/andy/sf6_mip/obspack_sf6_SAMPLE_Jacobson_20180208.nc

Modelers will also be requested to produce gridded mole fractions at fixed points in time. The purpose of these gridded fields would be to diagnose differences in vertical and meridional gradients across models. With these fields, we would be able to answer questions such as (1) Where is the model stratosphere and how much SF_6 does each model put in the stratosphere? (2) How much SF_6 does each model keep in the northern hemisphere versus transport to the south? Since transport is inherently seasonal, modelers will submit monthly gridded mole fractions, on the model native grid for each model.

The gridded mole fraction files must contain, at the model grid resolution,
1. Latitude centers or edges of the grid cells (specify which)
2. Longitude centers or edges of the grid cells (specify which)
3. Enough information to reconstruct the pressure boundaries of the grid cells. This can be, e.g., surface pressure and A and B coefficients for models using hybrid sigma coefficients. The model submission must include a README file with instructions for how to reconstruct the pressure boundaries.

4. SF$_6$ dry air mole fractions, in parts per trillion (picomole/mole)
5. If geopotential heights of model interfaces cannot be reconstructed using the above information, those GPHs must also be provided. Please consult with intercomparison organizers (andy.jacobson@noaa.gov and sourish.basu@noaa.gov) if this is true for your model.

The mole fraction files must be netcdf files named according to the following convention: molefrac_sf6_<model>_<modeler>_<4 digit year><2 digit month><2digit day>_<submission datestamp>.nc, where year, month, and day are simulation time, and "submission_datestamp" is when the files are submitted/created.

References

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NOAA Carbon Cycle Group ObsPack Team. (2018). Multi-laboratory compilation of atmospheric sulfur hexafluoride data for the period 1983-2017; obspack_sf6_1_v2.1.1_2018-08-17 [Data set]. NOAA Earth System Research Laboratory, Global Monitoring Division. https://doi.org/10.25925/20180817

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