DECSO emission versions

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The DECSO algorithm (Daily Emission estimation Constrained by Satellite Observations) has been applied successfully for NOx emission estimation in East Asia, Middle East, South Africa, and India. As the algorithm is further improved, emission estimations are updated accordingly. Below you can find an overview of the different algorithm versions. An extensive algorithm description can be found in Mijling and Van der A (2012), and the GlobEmission ATBD.

Version 1

- CHIMERE V2006
- No biogenic emissions
- INTEX-B emission inventory
- Landuse by GLCF database (1993)
- European diurnal cycle
- Boundary conditions LMDzINCA (gas), GOCART (aerosol)

Used in:

- Mijling and Van der A (2012)
- GlobEmission, phase 1 (East Asia)

Version 2

- Modelling CHIMERE with sector-dependent emission injection heights
- Fast back-trajectory calculations
- Adjusted retrieval error tropospheric NO2
- Update of NOx-correlated pollutants
- Noise and bias reduction in remote areas
- Full Kalman matrix inversion using LDL decomposition
- Initial emission inventories:
    - South Africa: EDGAR v4.2, 2008
    - India: EDGAR v4.2, 2008

Used in:

- Mijling et al. (2013)
- GlobEmission, phase 1 (India, South Africa)

Version v3a

- CHIMERE V2006.
- Initial emission inventories:
    - East Asia: MEIC 2008 (China) + INTEX-B (outside China)
    - South Africa: EDGAR v4.2, 2008
    - Middle East: EDGAR v4.2, 2008
- Diurnal cycle: flattened for China, European for other regions.
- Calculation speed: switching from g95 to ifort compiler, and calculating matrix inversions with LAPACK

Used in:

- GlobEmission, phase 2 (East Asia, Middle East, South Africa)

The emission estimates show unrealistic day-to-day (and possibly month-to-month) fluctuations of emissions. Emission noise in low-emitting areas (introduction of positive emission bias, and unrealistic seasonal cycle when assimilating OMI measurements).

Version v3b

- CHIMERE V2013: new transport schemes, secondary organic aerosol chemistry, updated chemical reaction rates.
- New land use data: GlobCover Land cover (2009).
- Biogenic emissions by MEGAN
- Initial emission inventories:
    - East Asia: MEIC 2010 (China) + INTEX-B (outside China), regridded.
    - Middle East: HTAP v2 (EDGAR v4.3)
- Reduction of day-to-day emission fluctuations by OmF criterium [-5,10].
- Diurnal cycle: flattened for Middle East, European for East Asia.

Used in:

- Ding et al. (2015)
- GlobEmission, phase 2 (East Asia, Middle East)

Version 4

- Reduction of day-to-day emission fluctuations by 3-sigma (emission error) criterion
- New parametrization of R matrix
- Diurnal cycle: flattened
- OmF criterion has been removed

Used in:

- GlobEmission, phase 2 (East Asia)

The emission noise is greatly reduced. The regional emission totals go down, but this is mainly related to the emission noise reduction (reduction of positive bias). Individual hot-spots, especially when undersampled, can disappear (e.g. Ulaanbaatar, and some power plants in North-East China). A slower convergence rate at changing emission signals. But 10% more observations have been used in this version compared with DECSO v3b.

Version 5

- Switch off biogenic emissions from MEGAN in CHIMERE, estimate total surface emissions instead of anthropogenic emissions
- Change the threshold of the sensitivity matrix from 0.05 h to 0.1 h.

Used in:

- GlobEmission, phase 2 (East Asia)
- Ding et al. (2017a, 2017b)

The total emissions are more realistic and we reduce the uncertainties in biogenic emissions from CHIMERE. The change of H threshold helps to reduce biases coming from the uncertainties occurring at the edge of a NO_2 plume.

This version is extensively validated for East China in Ding et al. (2017b)

Version 5.1

- Set maritime inject height of newly-found maritime at 40 m.
- Exclude the observations with a large pixel size by filtering out 8 pixels at each side of the swath
- Exclude the observations with a cloud fraction larger than 50%

Used in:

- Ding et al. (2018)
- For QA4ECV data: Ding et al. (2022)

With the new settings, we get more clear shipping tracks near Chinese coast areas.

Version 5.2-TROPOMI

- Results are generated on 0.125 degree resolution for a smaller domain.
- Timestep of the CHIMERE decreased to 7.5 min.
- The lifetime fit of NOx has been optimized for more precise local lifetimes.
- New parametrization of the R-matrix for TROPOMI
- The value of the minimum of H-elements has been set to 0.05 to avoid amplification of noise in the inverse calculation.
- The correlation length of Q is set to 1 km.
- Improved regularisation of the inverse calculation of (KSK+R).
- The NO2 climatology for the free troposphere has been corrected.

Used in

- Van der A et al. (2020)

This version is developed for using TROPOMI NO2 data. Since TROPOMI observations have a much higher resolution, we can also switch to higher resolution output.

Version 5.2-TROPOMI-superobservations

- In this variant of version 5.2 (1) TROPOMI data have been regridded into super-observations before using as input and (2) Results are generated on 0.25 degree resolution.
- Because of the different resolution, different parametrizations are used for the R-matrix and Q_matrix that describe the errors due to the model, measurements and representation.

Used in:

- Ding et al. (2020)

Since this version use super observations and generates output on the lower resolution of 0.25 degree it is much faster and can easily calculate emissions for large regions.

Version 5.5-TROPOMI-superobservations

- In this version superobservations are generated for columns till 700 hPa to remove upper-tropospheric effects.
- No error correction for negative obs.
- Correlation length of emissions is 2 km (i.o. 10 km)
- Radius of taking correlation length into account is 50 km (i.o. 300 km)
- Shorter steps in lifetime fit to reach more often convergence (dk=0.2k instead of 0.5k.)
- Lifetime fit: if the last iteration is resulting in a worse cost function, then take the previous iteration.
- New landuse data base: Copernicus Landcover 2019.
- Use of PAL data for TROPOMI NO2 data

Used in:

- Used as SEEDS deliverable for Europe

Version 6.0-TROPOMI-superobservations

- superobservations till 700 hPa
- CHIMERE 2020r3
- timeRes=8

Used in:

- Used as SEEDS deliverable for High-Resolution output (Lowlands)

Version 6.1-TROPOMI-superobservations (not released)

- Combined NH3 and NOx inversion.
- maximum distance in H is 200 km.
- new start -field HTAP3-2018
- Minimum value of H_min becomes 0.01 (was 0.05)
- 3-sigma limit turned off

Used in:

- Used in X. Zhang et al. (2023)

Version 6.2-TROPOMI-superobservations

- Timeres=8 for 0.2x0.2 ° (default), timeres=12 for 0.1x0.15 ° (Spain) and timeres=30 for 0.05 x0.05 (lowlands)
- The range *Hdistance_max* of the sensitivity function H is reduced to 150 km for 0.2x0.2° (default), and 50 km for lower resolutions (Spain, Lowlands)
- Number of iterations for the lifetime fit is limited to reduce the calculation time.
- R is based on the level2 error estimates (about.0.3), Q_{abs}=0.025, Q_{rel}=0.02
- The subgridding over a satellite pixel is based on 16x16 subgrids (instead of 32x8)
- The NO_2 observations are based on TROPOMI retrieval version 2.4. For the highest resolution of 0.05° no superobservations are used.
- In the calculated emissions negative emission are set to zero without compensation the neighbouring grid cells.
- TROPOMI version 2.4

Used in:

- Used as SEEDS deliverable for Europe and Lowlands(?)

Future steps: no boundary conditions in Chimere.

Version 6.2HR-TROPOMI- normal observations

Same as version 6.2 except:

- Applied to normal TROPOMI observations (i.e. no superobservations used)
- The resolution of the grid is 0.05x0.05 degree
- A reduced number of observations (less than 4000) is used per day
- More model steps in trajectories. N=30
- Because of calculation speed: no iterations for the lifetime fit

Version 6.3-TROPOMI-superobservations

Same as version 6.2 except for a post-processing step:

- This version includes a new split up in soil NOx emissions and anthropogenic NOx emissions

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SOFTWARE and KEY DATA of Version 6.1

Software/data	Version	Ref
Inverse algorithm	DECSO v6.1	
Chemical Transport Model	CHIMERE v2020r3	
NO2 observations	TROPOMI v.2.4	
Meteorological data	ECMWF operational model	
Land-use database	Copernicus LandCover	
Start field emissions	HTAP v3	

PARAMETERS in Version 6.2

Parameter	**Value**
Time resolution transport kernel	7.5 minutes or less
Initial lifetime	6 hours
Initial maximum lifetime	6 hours
Maximum lifetime during iterations	100 hours
Minimum Lifetime	0.5 hour
Maximum Lifetime	24 hours
Smallest allowed value for matrix H elements	0.01
Alpha (Regularisation factor for lifetime fit)	0.01
Emission correlation length	0.5 km
Q_{abs} Absolute error of emissions	0.025 [1e15 molec/cm2/h]
Q_{rel} Relative error of emissions	0.02
OmF correlation length (default)	10 km
Pa_radius (Max. distance for cov. analysis)	50 km
absMsigma (absolute error of σ_R)	0.1
relMsigma (relative error of σ_R)	0.05
Tikhonov_threshold	0.01
Error of start-field Pa of emissions on day 1	0.3 [1e15 molec/cm2/h]
Maximum distance for emission-concentration relationship	150 km or less for higher resolution emissions

Version	**Year of release**	**Study using this data version**
1	2012	Mijling and Van der A (2012)
2	2013	Mijling et al. (2013)
3a	2014	GlobEmission, phase 2 (East Asia, Middle East, South Africa)
3b	2015	Ding et al. (2015), GlobEmission, phase 2 (East Asia, Middle East)
4	2016	GlobEmission, phase 2 (East Asia)
5.0	2017	Ding et al. (2017a, 2017b)
5.1	2018	Ding et al. (2018)
5.2	2019	Van der A et al. (2020)
5.2-superobs	2020	Ding et al. (2020)
5.6	2022	SEEDS, first phase, 0.2x0.2 degree
6.0	2022	SEEDS, first phase, 0.05x0.05
6.1	2022	Zhang et al. (2023)
6.2	2023	SEEDS, second phase