

The Lagrangian particle dispersion model FLEXPART version 10.4

The FLEXPART Developers Team

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Introduction: FLEXPART history and recent updates

FLEXPART is an off-line model that uses meteorological fields (analyses or forecasts) as input. Since the last published version (6.4) the ECMWF and GFS versions were unified, and there were modifications in I/O, performance, physical and chemical processes. We describe here some improvements in version 10. More detailed information can be found in www.flexpart.eu and in Pissó et al., 2019 (Geosci. Model Dev., 12, 4955–4997, 2019 <https://doi.org/10.5194/gmd-12-4955-2019>)

Updated physics and chemistry

1 Boundary layer turbulence

Unresolved sub-grid motion in the input data are parameterized adding a stochastic fluctuation according to the well-mixed criteria. Gaussian perturbation are well suited only for stable to near-neutral conditions. Under unstable convective conditions, turbulence is skewed (larger area for downdrafts than for updrafts). This is modeled in FLEXPART 10 in the convective ABL, requiring for numerical stability much shorter time steps. The formulation smoothly transits to a Gaussian in neutral conditions.

2 Turbulence in the free troposphere and stratosphere

The turbulence parametrization with a random walk was updated following the latest available values. In addition, it is now possible to choose the values of the vertical and horizontal components of the turbulent diffusivity tensor as input.

Updated physics and chemistry

3 Gravitational settling for aerosols

Gravitational settling was calculated using a single dynamic viscosity of the air. The gravitational settling calculation was generalized to higher Reynolds number, including temperature dependence.

4 Wet deposition

The previous cloud definition scheme was based on relative humidity (RH of 80%). Instead, clouds and cloud water are now determined from specific Cloud Liquid Water Content (CLWC) and Cloud Ice Water Content (CIWC) mass mixing ratios read from the meteorological fields.

Wet deposition of particulates is still separated in impact scavenging (below-cloud) and nucleation scavenging (in-cloud). Below-cloud scavenging depends on aerosol size and on precipitation type (rain or snow), modeling differences in the aerosols as cloud condensation nuclei (CCN) and ice nuclei (IN). Removal efficiencies depend on cloud water phases.

Updated physics and chemistry

5 Source–receptor matrix calculation of deposited mass backward in time

For measurements of deposition on the ground, e.g., in precipitation samples or ice cores no backward simulations were possible until recently. Now an option to calculate SRR values in backward mode for wet and dry deposition exists.

6 Sensitivity to initial conditions

Since version 8.2, FLEXPART has provided an option to quantify the influence of initial conditions on the receptor in backward simulations. Then, gridded fields containing the sensitivities to background mixing ratios are produced and stored as output.

7 Chemical reactions with OH

Tracer mass can be lost by reaction with OH. The OH reaction scheme was modified to account for 1) hourly variations in OH and 2) the temperature dependence of the OH reaction rate. Monthly averaged $3^\circ \times 5^\circ$ resolution OH fields averaged to 17 atmospheric levels from the GEOS-CHEM model are now used.

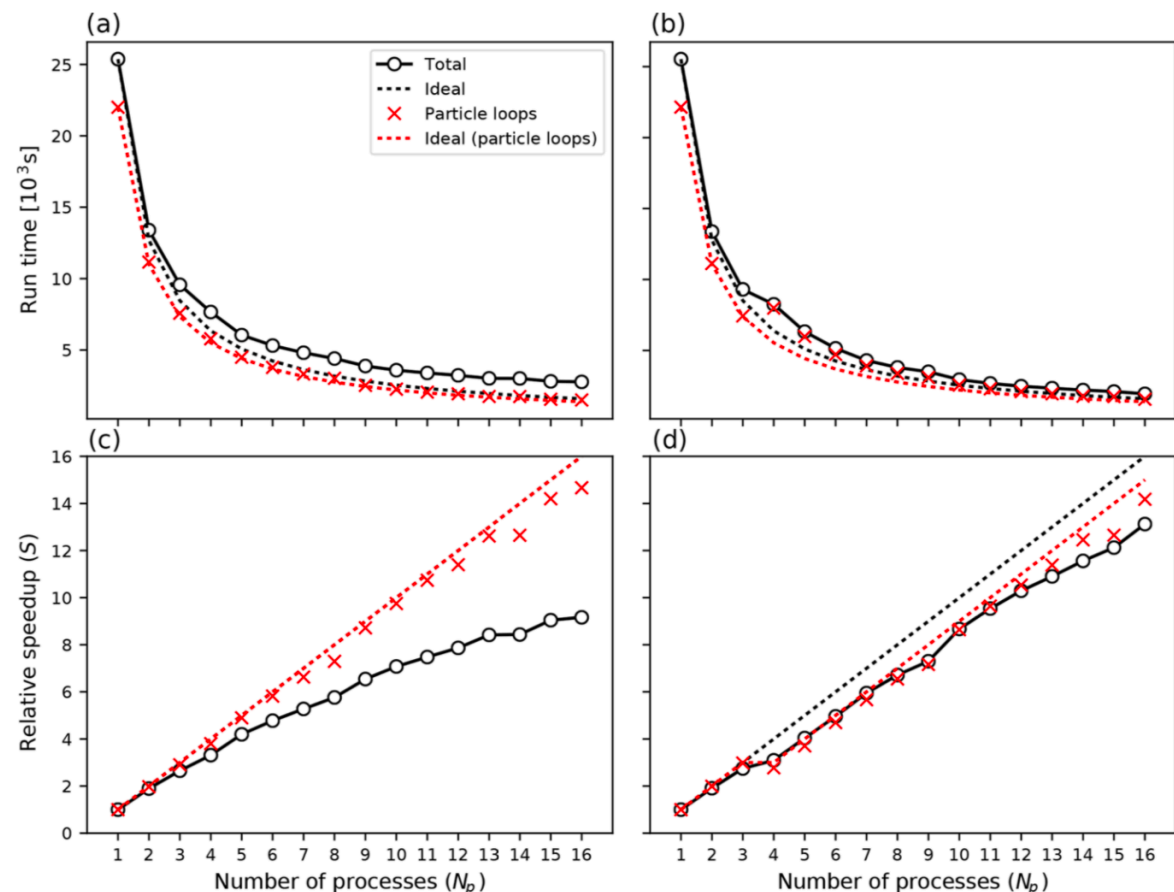
8 Dust mobilization scheme

The FLEXDUST module runs independently from FLEXPART and produces gridded output of mineral dust emissions as well as input files (RELEASES) that can be used for atmospheric simulations.

Parallelization

FLEXPART version 10 uses a pure MPI approach, as the particles do not interact while propagated in the code. The model can be run in the previous serial mode.

Computational time (a, b) and speedup (c, d) for up to 16 processes on a single node. In panels (a, c), all processes read meteorological input data, whereas in panels (b, d), a dedicated process reads and distributes input data for $N_p \geq 4$.



Input and output

1 User data

In FLEXPART version 10 the default format of the user input files is changed from fixed plain text to a namelist format.

2 Meteorological input data

FLEXPART uses meteorological fields in GRIB format commonly from the European Centre for Medium-Range Weather Forecasts (ECMWF). Optionally, GRIB data from NCEP's GFS model, available on pressure levels, can be used, now in the same executable file.

Input and output

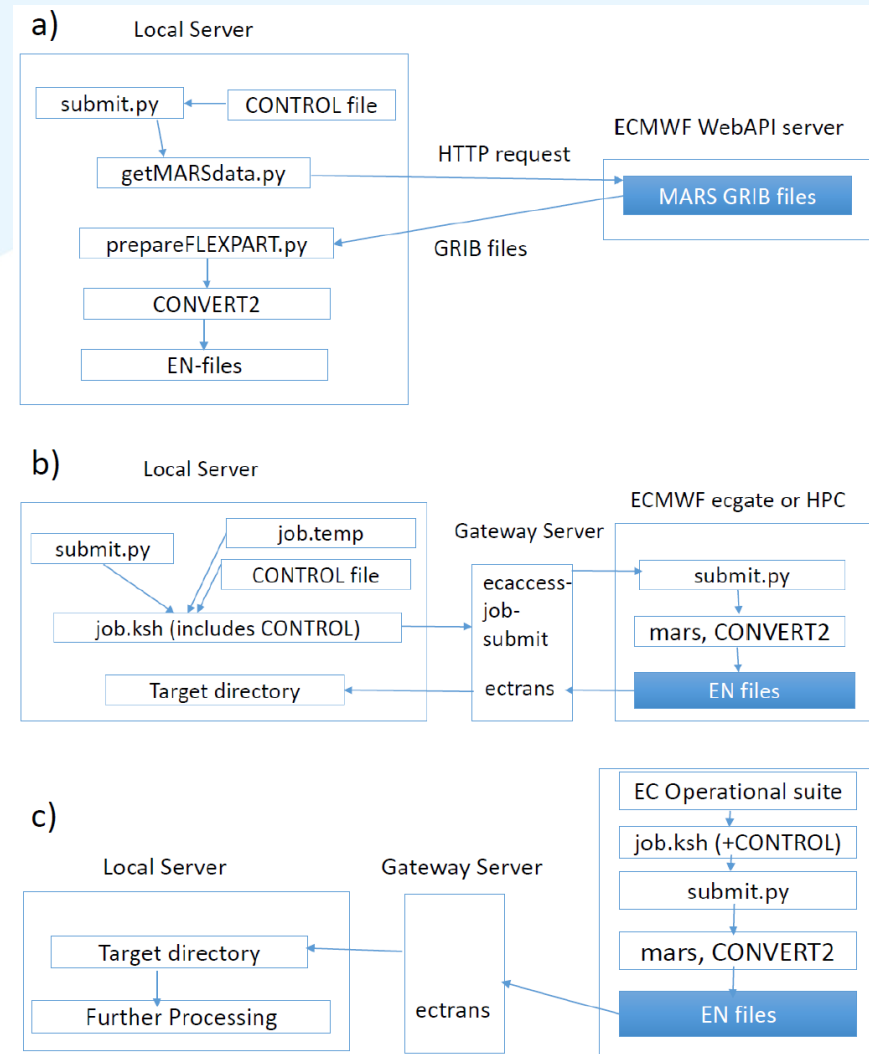
2.1 ECWMF data retrieval

An account at ECMWF is no longer required for use of the Meteorological Archival and Retrieval System (MARS). It is now possible to prepare FLEXPART input data in the users system.

2.2 NCEP data retrieval

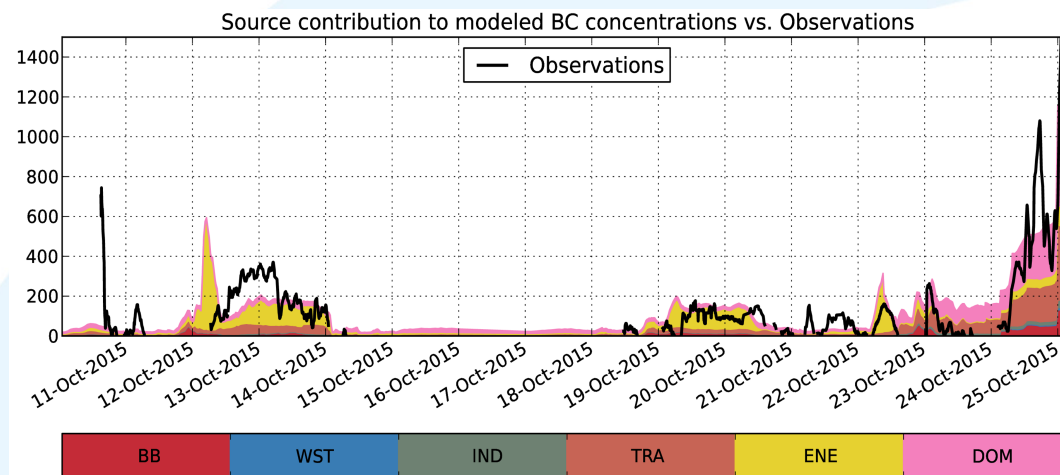
The data can be retrieved from NCEP following the instructions from the flexpart website

Figure: Summary of the flex_extract retrieval script usage scenarios. Scenario a) applies to any user worldwide. Scenario b) is for users with log in access to the ECMWF archives. Scenario c) is appropriate for operational use of (near) real time data.



Model applications

1 Source identification of Black Carbon during ship cruises in the Arctic

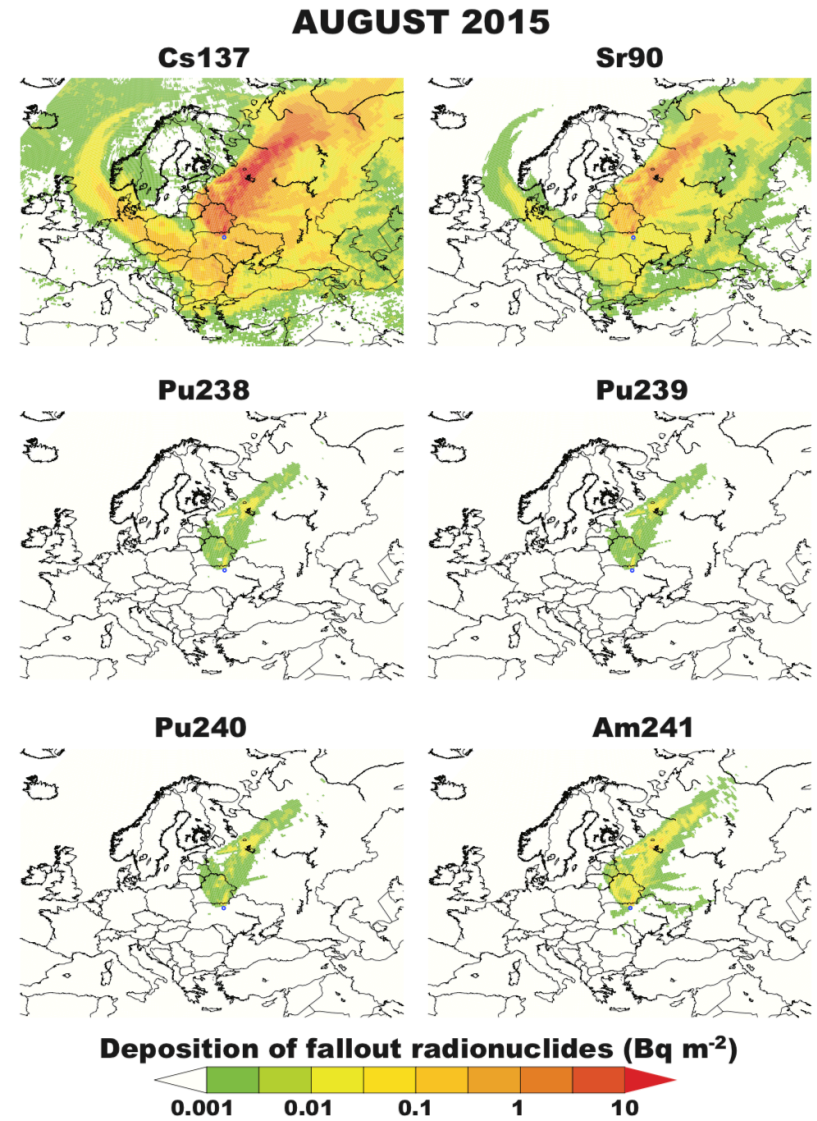


Contribution from the different sources of BC to the surface concentrations recorded during the ship cruise in White, Barents and Kara Seas. The emission sources of biomass burning (BB), waste burning (WST), industrial combustion and processing (IND), surface transportation (TRA), power plants, energy conversion, extraction (ENE) and residential and commercial (DOM) have been adopted from the ECLIPSE inventory.

Model applications

2 Transport and deposition of radionuclides from the 2015 forest fires in Chernobyl

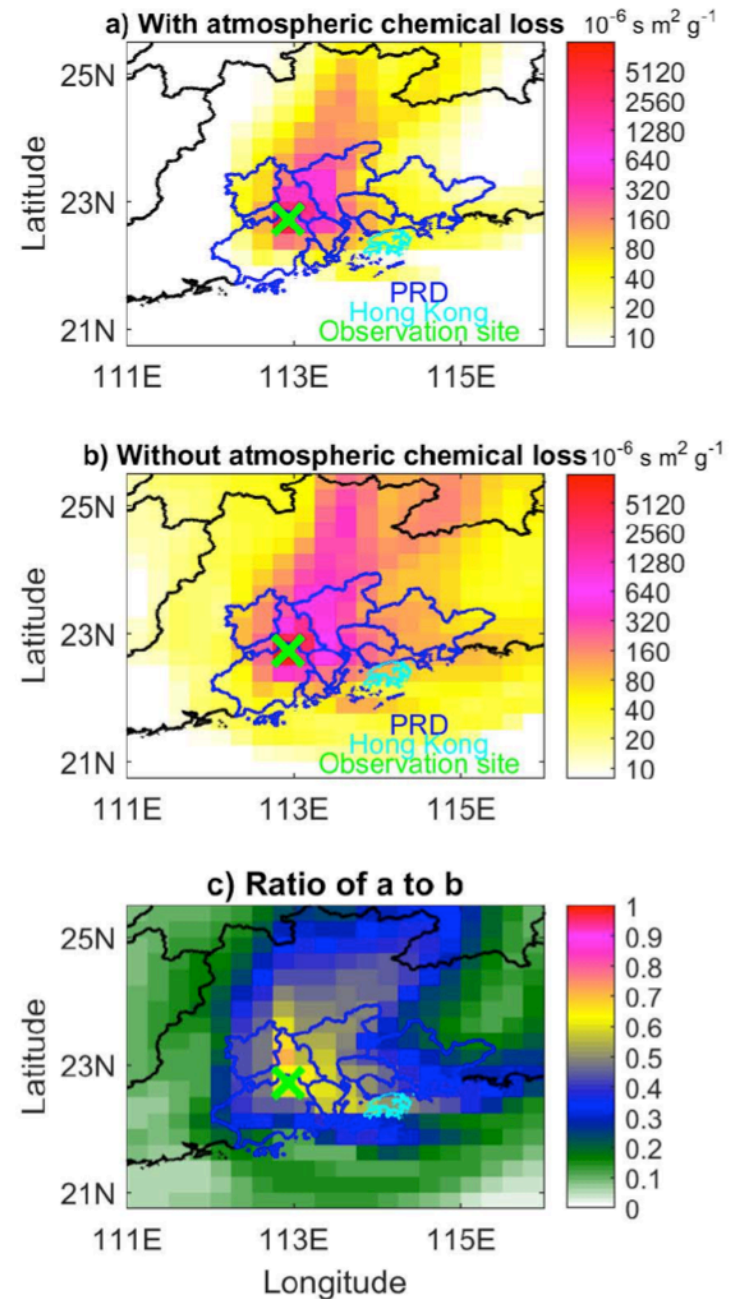
Total deposition of ^{137}Cs , ^{90}Sr , $^{238,239,240}\text{Pu}$ and ^{241}Am over Europe released after the fires in August 2015 in the exclusion zone of Chernobyl (CEZ).



Model applications

3 Footprint sensitivity for species with different lifetimes

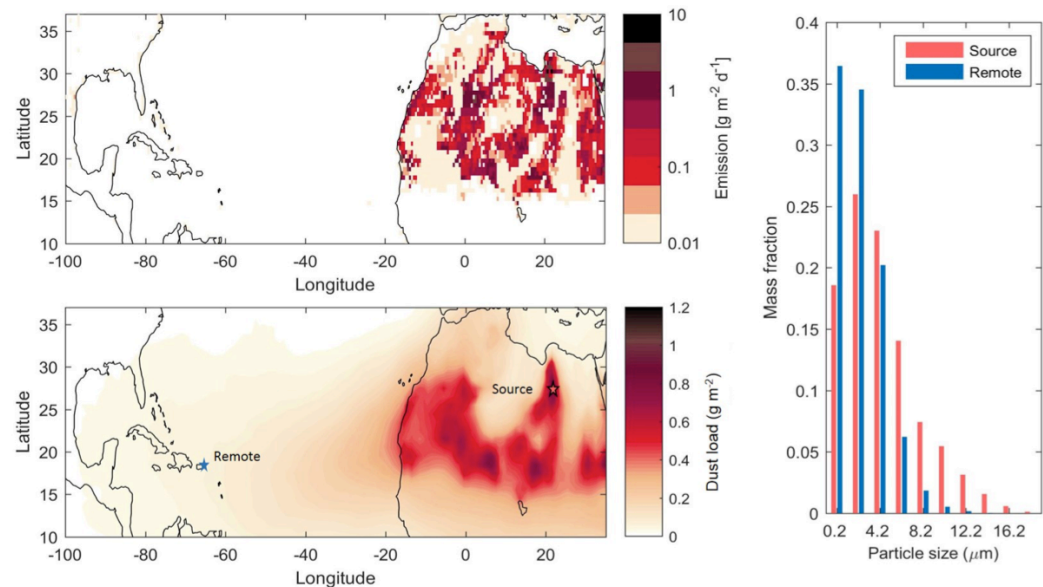
Figure: Spatial distribution of the average toluene emission sensitivities a) with and b) without atmospheric chemical loss.



Model applications

4 Dust scheme

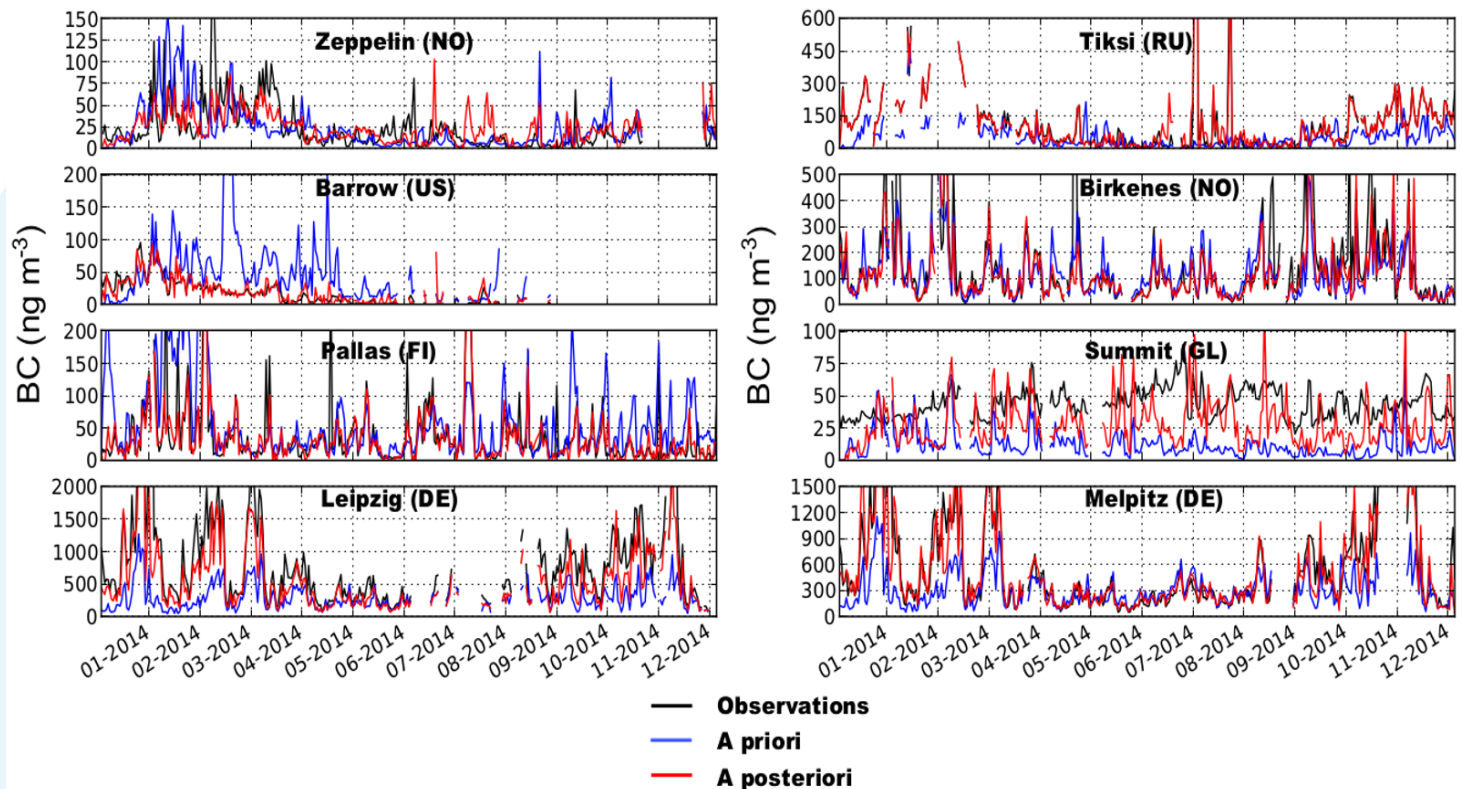
Figure: Simulated mean dust emission from source region (top left), dust load (bottom left) and particle size distribution (right) within the source region and at a remote location for the period 18 July – 17 August 2012.



Model applications

5 Inverse modelling

Time-series of surface concentrations of BC in the eight stations selected for the inversion. Surface concentrations improved significantly comparing with the use of the prior fluxes.

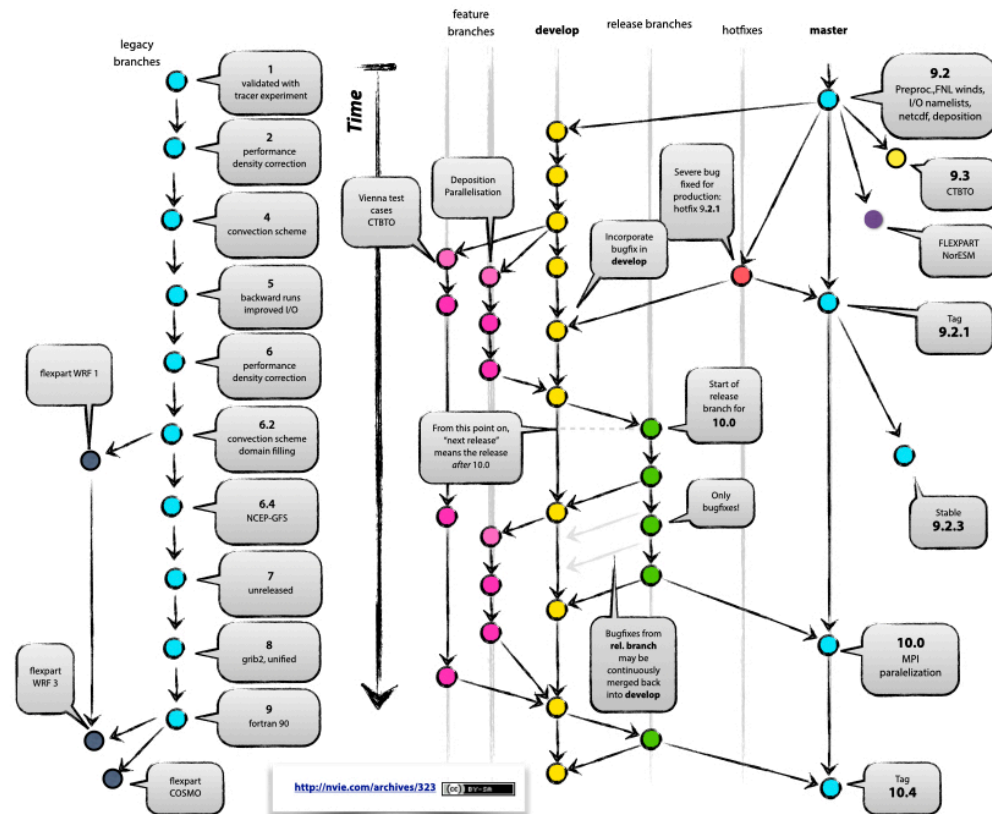


Version control and collaboration

Distributed revision control helps many developers to work on the project without requiring them to share a common network. Since version 9.2 the code was migrated from SVN to Git. Contributions are encouraged using this system.

Figure: FLEXPART
git tree schematic

flexpart branch structure schematic



Outlook

FLEXPART further version updates will be shared in the website <http://flexpart.eu>. For example full dynamical allocation of variables, Vtables approach to be able to handle in an easier way the usage of different input data and an intermediate format to avoid pre-processing of met data.

As FLEXPART is developed further, updates will continue to be made available on the FLEXPART website at <https://flexpart.eu>. We encourage established and new users to contribute to FLEXPART development by providing their code changes, as well as a description of these changes, as new feature branches of the latest commits in the FLEXPART git repository. New code should pass all test cases provided in the FLEXPART distribution and provide consistent output, unless there are specific reasons why output should be different, such as improvements in the model physics. This will expedite the integration of important new model features in the main development branch of the model.