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The Lagrangian particle dispersion model FLEXPART version 10.4

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Following its release and corresponding publication in GMD, we present the Lagrangian model FLEXPART 10.4, which simulates the transport, diffusion, dry and wet deposition, radioactive decay and first order chemical reactions of atmospheric tracers. The model has been recently updated, both technical and in the representation of physico-chemical processes.

FLEXPART was in its original version in the mid-1990s designed for calculating the long-range and mesoscale dispersion of hazardous substances from point sources, such as released after an accident in a nuclear power plant. Given suitable meteorological input data, it can be used for scales from dozens of meters to the global scale. In particular, inverse modelling based on source-receptor relationships from FLEXPART has become widely used. In this paper, we present FLEXPART version 10.4, which works with meteorological input data from the European Centre for Medium-Range Weather Forecasts' (ECMWF) Integrated Forecast System (IFS), and data from the United States' National Centers of Environmental Prediction (NCEP) Global Forecast System (GFS). Since the last publication of a detailed FLEXPART description (version 6.2), the model has been improved in different aspects such as performance, physico-chemical parametrizations, input/output formats and available pre- and post-processing software. The model code has also been parallelized using the Message Passing Interface (MPI). We demonstrate that the model scales well up to using 256 processors, with a parallel efficiency greater than 75% for up to 64 processes on multiple nodes in runs with very large numbers of particles. The deviation from 100% efficiency is almost entirely due to remaining non-parallelized parts of the code, suggesting large potential for further speed-up. A new turbulence scheme for the convective boundary layer has been developed that considers the skewness in the vertical velocity distribution (updrafts and downdrafts) and vertical gradients in air density. FLEXPART is the only model available considering both effects, making it highly accurate for small-scale applications, e.g. to quantify dispersion in the vicinity of a point source. The wet deposition scheme for aerosols has been completely rewritten and a new, more detailed gravitational settling parameterization for aerosols has also been implemented. FLEXPART has had the option for running backward in time from atmospheric concentrations at receptor locations for many years, but this has now been extended to work also for deposition values. To our knowledge, to date FLEXPART is the only model with that capability. Furthermore, temporal variation and temperature dependence of chemical reactions with the OH radical have been included, allowing more accurate simulations for species with intermediate lifetimes against the reaction with OH, such as ethane. Finally, user settings can now be specified

in a more flexible namelist format, and output files can be produced in NetCDF format instead of FLEXPART's customary binary format. In this paper, we describe these new developments. Moreover, we present some tools for the preparation of the meteorological input data and for processing of FLEXPART output data and briefly report on alternative FLEXPART versions.

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