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How to Use the FLEXPART Model
in Atmospheric Transport Modelling Challenges

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Introduction

- FLEXPART is a free Lagrangian particle dispersion model widely used in the CTBT community by both the PTS and NDCs.
  Extensive information, incl. code download: `https://flexpart.eu/`.
- FLEXPART has many user-definable options and possibilities for setting up simulations.
- This presentation gives hints on how to create efficient and accurate simulations (which obviously can involve some trade-offs).

Disclaimer:
The views expressed on this poster are those of the author and do not necessarily reflect the view of the CTBTO.

Forward or backward?

- Theoretically, both directions should produce identical results.
- However, there are differences in numerical implementation, therefore in practice it matters:
  - Particles can be released in any geometry (point, line, volume)
  - Particles can be sampled only in $\lambda - \phi - z$ boxes, or around a point (receptor) using a parabolic kernel
- We want as many particles as possible to be involved at both source and receptor; other particles don't contribute to the determination of the SRS!
  - Therefore, number of receptors vs. number of sources is important
  - Standard CTBT application has limited receptors (RN stations) and many (potential) sources
  - Backward simulations releasing particles from stations and sampling on a grid then is best. Receptor output may be considered.
  - If you have a known point source, or small number of sources, and a large number of relevant stations, forward simulation can be better.

Parameters in COMMAND file / 1

LOUTSAMPLE The time interval at which particle positions are sampled to generate output.

- Should not be larger than LSYNCTIME
- Should be clearly smaller than grid size / (ABL) (high) wind speed. For example, 20 km grid / 60 km/h = 1200 s. Use ≤600 s, better 300 s.

LSYNCTIME Base time step of the model.

- Note that also releases must be aligned with the temporal raster defined by LSYNCTIME.
- To be balanced with other time step parameters.

CTL defines timestep in ABL (LDT):

$CTL < 0$	:	LDT=LSYCNTIME faster, but some bias
$0 \leq CTL < 0.1$	:	undefined, do not use!
$CTL \geq 0.1$	:	$LDT = T_L/CTL$ 3 .. 5 recommended for accuracy!†

IFINE Further refinement of timestep for vertical turbulent motion

- used only if CTL > 0
- suggested value =4. Reduce if CPU time is critical.

*ABL: Atmospheric boundary layer † T_L Lagrangian time scale

Parameters in COMMAND file / 2

CBLFLAG New in v10, for skewed turbulence.

- In typical CTBT applications: CBLFLAG=0

LSUBGRID Increase of ABL heights $\propto$ to sub-grid orography variance

- Probably better LSUBGRID=1

LCONVECTION Consider moist convection

- Should be used in general for better accuracy, considered mandatory in tropics
- Significant impact on calculation time, $\propto n^3$ (number of vertical layers in input met fields). Problem to be addressed by developers.

IOUTPUTFOREACHRELEASE =1: If multiple releases are defined, separate output fields are created for each release

- Very useful for good performance: track multiple receptors in a single run, minimises the overhead of reading and processing the met input.
- Not implemented for receptor output in standard version (added for ATM Challenge 3 in private version of v10.4)
- Currently enforced for backward runs.

Parameters in COMMAND file / 3

IOUT Output type

- Use IOUT=1 concentration. =2 volume mixing ratio (pptv, gases only).

IND_SOURCE, IND_RECEPTOR

mass (=1) or (mass) mixing ratio (=2)

- *source* and *receptor* always refers to physical source and receptor, even in backward mode
- For better understanding, read
  Seibert & Frank, Source-receptor matrix calculation with a Lagrangian particle dispersion model in backward mode, `https://doi.org/10.5194/acp-4-51-2004`, Table 1 and Section 2.4
- See Slide 9 for more details!

Parameters in RELEASES file

Species Define number of species and their properties

- Note that only one single diameter of particulate species is used, even if species with different diameters are given!
- Species can be used to emulate IOUTPUTFOREACHRELEASE=1, but this is not recommended
- Usually radioactive decay is more efficiently considered in postprocessing than by specifying it in the SPECIES file (otherwise, exponential function is evaluated for every timestep).

Particle number Define number of particles for a specific release

- CPU time and memory = base value + part that is proportional to total particle number; this part is dominant for sufficiently large numbers.
- Larger partical numbers reduce numerical errors due to stochastic effects. This is more important near fringes of plume and the longer transport lasts. No general rule can be given, but test runs with nclassunc=10 to estimate these errors can be helpful (see Stohl et al., FLEXPART version 6.2, https://doi.org/10.5194/acp-5-2461-2005) for uncertainty estimation.
- Numbers between 10 000 and 10 000 000 are typically used; lower-end numbers only if several releases are added for final result

Further considerations on the ATM Challenge example

- It would be best in terms of performance to do, for example, all (backward) runs that pertain to measurements at all stations in one month in a single simulation. In ATMch3, we used FWD simulations, and scores seem to be lower than in previous ATM Challenges.
- To limit `maxpart` (used in array allocation and defined in `par_mod.f90`, maximum number of particles being in the model simultaneously), use a single ageclass with a max age, e. g. 14 d.
- If emissions are available with different temporal resolution, the LOUTSTEP (and LOUTAVER) parameters need to be set in a way that SRS can be reconstructed by adding up various output fields.
- IBDATE/IBTIME: Note that the simulation does not need to begin with the first release, it may begin earlier if that helps to find a good time raster of the output.
- If collection start / stop times do not match the temporal raster given by LSYNCTIME, we need to slightly shift them.

Setting of source and receptor units in ATM Challenge

Reminder

IND_SOURCE, IND_RECEPTOR : mass (=1), or (mass) mixing ratio (=2)

Use IND_SOURCE=1, IND_RECEPTOR=2

Then you can use a source in (T)Bq*. For the receptor, we have units of mixing ratio. In order to convert the resulting SRS to units of Bq m^{-3} (STP), we need to multiply† with

$$\rho_{\mathrm{air,STP}} = \frac{p_{\mathrm{STP}}}{R_{\mathrm{air}} T_{\mathrm{STP}}} = \frac{1013.25\ \mathrm{hPa}}{287.04\ \mathrm{J\,kg^{-1}\,K^{-1}}\ 273.15\ \mathrm{K}} = 1.292\ \mathrm{kg\ m^{-3}}$$

because the activity is reported in terms of concentration at standard pressure and temperature (taken as 1013.25 hPa, 0°C by CTBTO).
If you would take IND_RECEPTOR=1 you would get SRS for concentration at ambient conditions!
Note that this holds for both forward and backward simulations!

*FLEXPART scales results with 1E12 in forward mode. Then you either need to undo this in postprocessing, or define releases in TBq.
†Not divide, as erroneously stated in Seibert & Frank (2004), p. 55.

Suggestions for further research (please contact me if you want to do work on any)

1. Particle splitting
   - FLEXPART allows to split particles in two at intervals of ITSPLIT. Could be used to decrease stochastic noise for long transport. Has not yet been tested systematically.
2. Time step
   - Some more systematic tests for the influence of time step and related parameters would be desirable.
3. Gridded output
   - Use interpolation method of Hittmeir/Philipp/Seibert (https://doi.org/10.5194/gmd-11-2503-2018) for retrieving point values from gridded output
   - Apply spatial smoothing to gridded output for fringes of plume where stochastic numerical effects become relevant
4. Receptor output
   - Systematically compare receptor output and gridded output
   - Study possible optimisations of kernel parameters in receptor output

Conclusions

- Before designing a run or series of runs, consider carefully the parameters.
- They influence both the accuracy and the resources needed (CPU time and memory), and usually involve a trade-off.
- Most CTBT situations will best be handled with backward runs including as many stations and collection periods as possible.
- Consider using the AGECLASS feature to have the option of long runs.
- Consider the IND_SOURCE and IND_RECEPTOR in connection with the fact that station data refer to activity concentration at standard T and p.
- Further advice: • If you have many runs, just link those files which are identical for each run rather than copying them, to minimise disk usage and inode count. • Use compiler optimisation.
- If you have any further questions, please contact me at petra.seibert/at\univie.ac.at