

Evaluating the added value of multi-input atmospheric transport ensemble modeling for applications of the Comprehensive Nuclear Test-Ban Treaty Organization

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Abstract: The Comprehensive Nuclear Test-Ban Treaty Organization (CTBTO) runs to date operationally an atmospheric transport modeling chain in backward mode based on operational deterministic meteorological input data. The potential benefit of ensemble dispersion modeling for current and possible future CTBTO applications was investigated using data from the ECMWF-Ensemble Prediction System (EPS, full ensemble comprises 51 members). Five different test cases - among which are the ETEX-I experiment and the Fukushima accident - were run in backward or forward mode and - in the light of a future operational application - special emphasis was put on the performance of an arbitrarily selected 10-member versus the full ensemble.

Based on the five test cases it can be concluded that a 10-member meteorological ensemble is good enough to already benefit from useful ensemble properties. Meteorological uncertainty to a large degree is covered by the 10-member subset because forecast uncertainty is largely suppressed due to concatenating analyses and short term forecasts, as required in the operational CTBTO procedure, on which this study focuses.



Introduction: So far ensemble atmospheric transport modeling at CTBTO has been confined to multi-model ensemble modeling in case of exceptional particulate measurements (*Level-5* measurements). On the occasion of a *Level-5* event so called *Regional Specialized Meteorological Centres* (RSMCs) as designated by the *World Meteorological Organization* (WMO) run their atmospheric transport and dispersion models and provide Source-Receptor-Sensitivities to CTBTO and state signatories.

In order to investigate the added value of ECMWF-EPS based atmospheric transport modeling five test cases (three real cases, two synthetic cases) were performed:

1. **Hypothetical puff release** of $1\text{E}15$ Bq Xe-133 (default standard emission in CTBTO's operational runs) **at the DPRK test site** near Punggye-ri (129.0° E and 41.3° N) on Dec., 1st, 00:00-01:00 UTC, 2018, traced back from selected receptors. This test case covers north hemispheric winter time conditions and is favorable in terms of available pseudo-measurements.
2. **Hypothetical puff release** of $1\text{E}15$ Bq Xe-133 **at the ANSTO radiopharmaceutical production site** (151.0° E and 34.1° S) on Dec., 1st, 00:00-01:00 UTC, 2018, traced back from selected receptors. This test case covers south hemispheric summer time conditions and is unfavorable in terms of available pseudo-measurements.
3. **Real, temporally extended and vertically structured releases** of Cs-137 and Xe-133 as available from the literature **for the Fukushima-Daiichi NPP** (141.0° E and 37.4° N) **accident** starting on March, 11th, 2011, followed for 14 days (forward mode).
4. The **May 2019 Selenium-75 puff release from the Belgian research BR2 reactor** (5.1° E and 51.2° N) on the premises of SCKCEN run in backward mode. However, the transport scale (confined to Europe) is not typical for CTBTO applications.
5. The **ETEX-I release from Monterfil (France)** (2.0° W and 48.1° N) in forward mode. However, the transport scale (confined to Europe) is again not typical for CTBTO applications.

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Methods:

- Two types of ECMWF ensemble data sets were gathered: Whenever possible - in terms of necessary input variables to run FLEXPART - existing ECMWF products, i.e., **Ensemble of Data Assimilations (EDA) products** were selected. No existing data was available for the Fukushima test case dating back to 2011 and the ETEx-I test case dating even back to 1994, where an effort was undertaken to **hindcast the ensembles**. ERA5 data, providing global re-analyses from 1950 on till present, although in principle also useable since it includes 10 ensemble members, could not be considered because it is delayed in time by 5 days to the current date and thus would not be available in quasi near-real time as required by the operational needs of CTBTO. In order to neglect the forecast error which is not relevant to CTBTO's forensic post-event treaty verification tasks, **ECMWF analyses were concatenated with short term forecasts** rather than using one long-term forecast.
- **Real and synthetic measurements** were acquired or generated (the latter with FLEXPART based on NCEP-GFS data), selected and pre-processed. **Xe-133 and Cs-137 measurement data** come from the **IMS** for test case 3, **Se-75 measurements from IRSN** (national French sites) for test case 4 and **PMCH measurements** (all over Europe) from the literature for test case 5.
- **FLEXPART was set up uniformly for all five test cases except for output grid horizontal resolution**. Version 8.2.3 was used for test cases 1 and 2. For test cases 3 to 5, a subversion of version 9.3 was employed which had been specifically adapted to the operational needs of CTBTO. FLEXPART was run with 3600 seconds output time interval. Subgrid terrain effect and convection parameterization were enabled. The FLEXPART output contains a single output layer with an upper height of 150 m a.g.l. for all test cases. The output domains and their spatial resolutions were chosen to be identical to the computational domains and resolutions (the meteorological ones, respectively).

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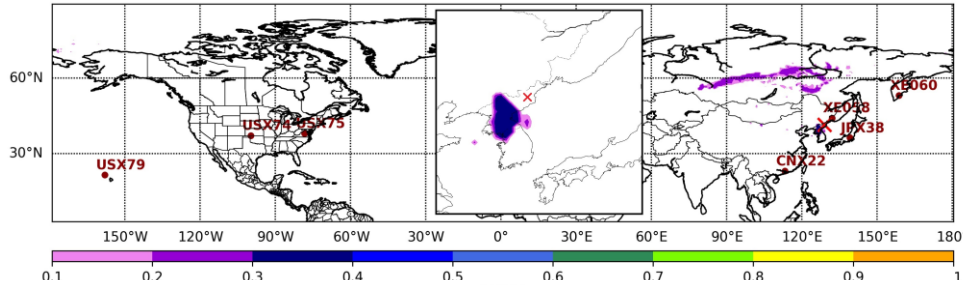
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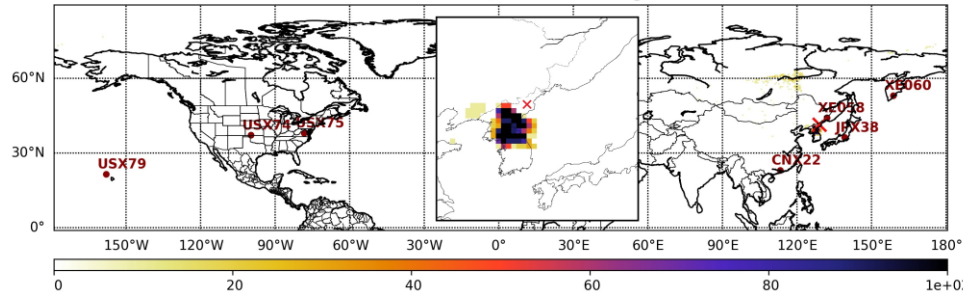
Results: DPRK test case

Minimum PSR and probability of exceedance fields can be of added value in case two relevant sites (e.g., civil radiopharmaceutical facility and known military test site with a corresponding waveform signal) fall within the deterministic PSR, but only one of them falls into the minimum PSR or probability of exceedance field. Importantly, the minimum PSR field does not diminish the correlation values uniformly.

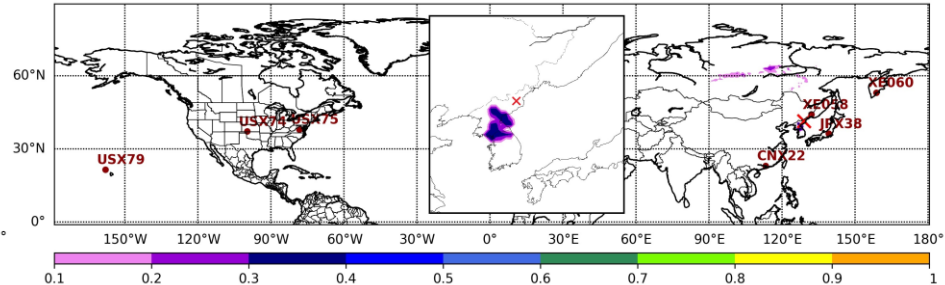
DPRK, PSR
2018-12-01_00Z
Deterministic run



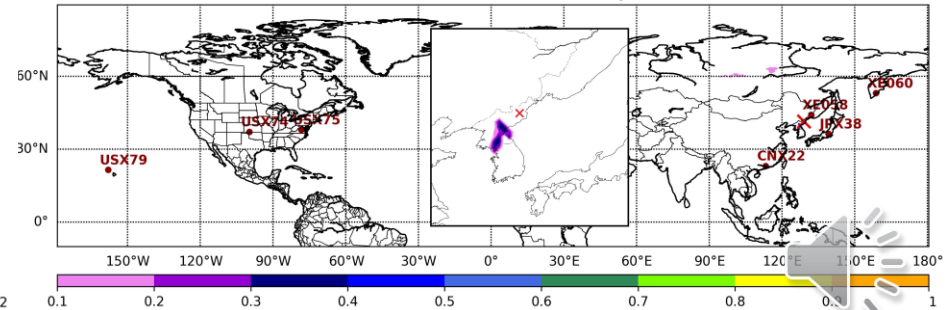
DPRK
Probability of exceeding (Agreement in threshold level) 0.27
2018-12-01_00Z
10 ECMWF-EPS-members, FO:33.38%, avAgr:68.16%



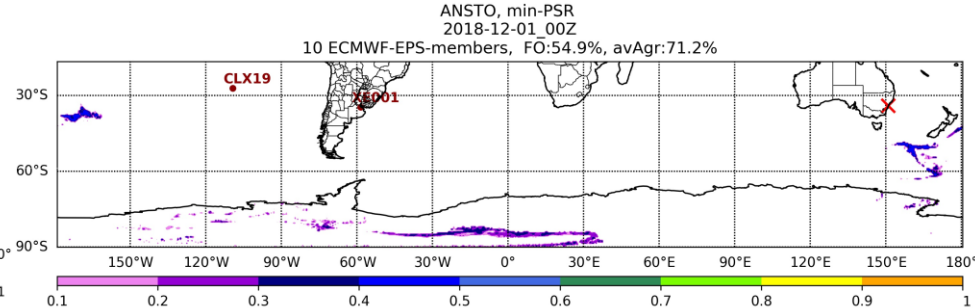
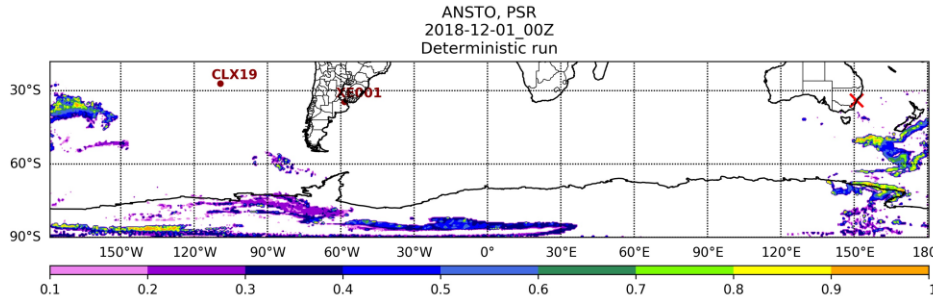
DPRK, min-PSR
2018-12-01_00Z
10 ECMWF-EPS-members, FO:33.38%, avAgr:68.16%



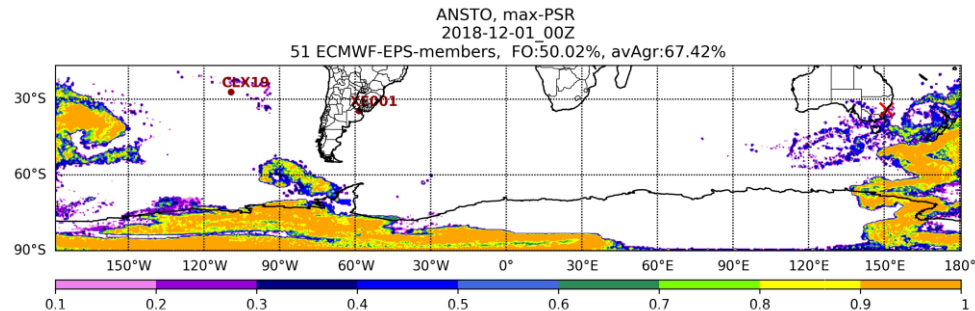
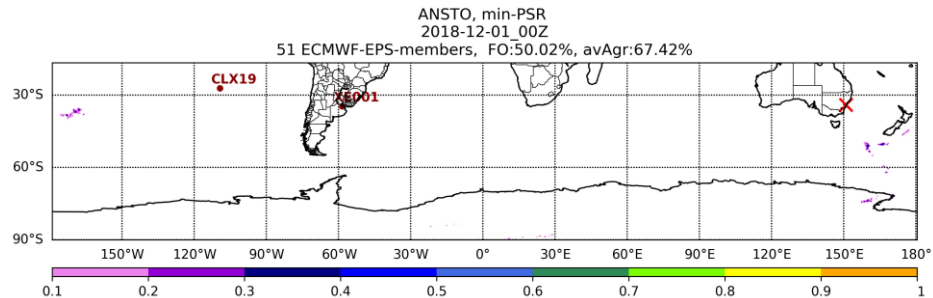
DPRK, min-PSR
2018-12-01_00Z
51 ECMWF-EPS-members, FO:32.8%, avAgr:69.65%



Results: ANSTO test case



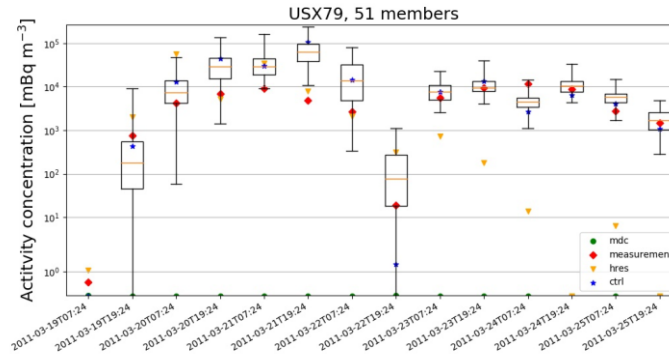
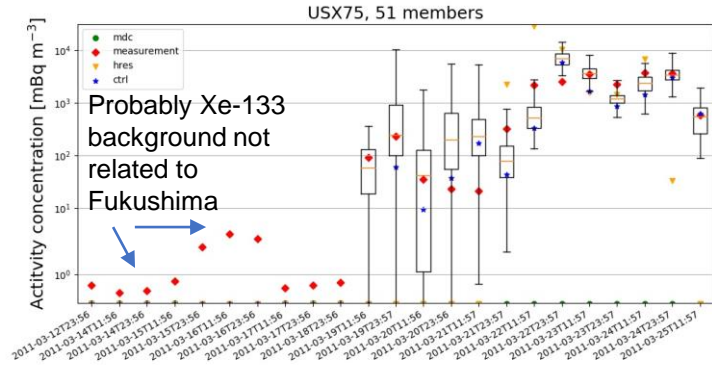
The PSR method locates the possible source location wrongly. Nevertheless, for the minimum of the reduced ensemble the PSR maxima (0.4-0.5) get confined to a region 1000 km southeast and 3000 km east of the actual source site with only a thin branch (PSR values < 0.4) stretching over Antarctica. For the minimum of the full ensemble the part of the PSR field stretching over Antarctica is further diminished (to small patches of values < 0.2). **Although one might expect a benefit from the maximum of the (full) ensemble specifically for this test case, no benefit can be demonstrated.**



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similar
very similar

IMS station	N	Rank	BS
CAX16-deterministic	5	1.81	-
CAX16-control	5	2.65	-
CAX16-10 members	5	2.97	0.41
CAX16-full ensemble	5	3.00	0.38
SEX63-deterministic	21	0.71	-
SEX63-control	21	1.97	-
SEX63-10 members	21	2.20	0.66
SEX63-full ensemble	21	2.26	0.66
USX74-deterministic	14	2.24	-
USX74-control	14	3.02	-
USX74-10 members	14	3.27	0.10
USX74-full ensemble	14	3.21	0.11
USX75-deterministic	23	1.86	-
USX75-control	23	2.68	-
USX75-10 members	23	3.07	0.44
USX75-full ensemble	23	3.01	0.44
USX77-deterministic	7	1.13	-
USX77-control	7	2.18	-
USX77-10 members	7	2.34	0.16
USX77-full ensemble	7	2.39	0.17
USX79-deterministic	14	2.21	-
USX79-control	14	1.96	-
USX79-10 members	14	2.16	0.07
USX79-full ensemble	14	2.19	0.07

"X" refers to noble gas sampling stations (for Xe-133)
 "P" to particulate sampling stations (for Cs-137)
 Deterministic (hres) ECMWF-input dates back to 2011!
Concentrations are generally highly underpredicted for Cs-137, also based on improved ECMWF input data produced in the hindcast!

Table 2

Number of involved sample pairs N, rank and Brier score for the Fukushima test case.

Results: Fukushima test case

53% and 74% of the selected samples are explained by the reduced and the full ensemble

IMS station	N ≥ thres.	N expl.	Comment on Cs-137 time series
CAX16 (Yellowknife, Canada)	3	2/3	
CAP17 (St. John's, Canada)	2	0/0	Modelled Cs-137 too diluted when reaching the station
SEX63 (Stockholm, Sweden)	9	3/5	
SEP63 (Stockholm, Sweden)	2	1/1	Timing of the plume arrival reproduced
USX74 (Ashland, US)	13	5/9	
USP74 (Ashland, US)	6	1/5	For 5/1 samples the ensemble maximum comes close to the measurements
USX75 (Charlottesville, US)	16	10/12	
USP75 (Charlottesville, US)	4	1/3	Timing of the plume arrival reproduced
USX77 (Wake Island, US)	6	3/3	
USP77 (Wake Island, US)	3	0/0	
USX79 (Ohau, US)	13	9/12	
USP79 (Ohau, US)	6	0/1	Timing of the plume arrival reproduced

Table 1

Number of samples N greater than or equal to selected threshold value and number of explained samples N for the reduced and the full ensemble for the six selected IMS sampling site time series for each of the two isotopes.

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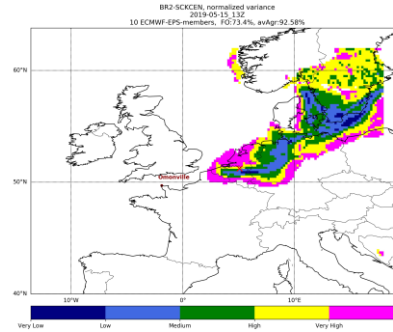
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Results: Se-75 test case

Known source
term: $4E10$ Bq

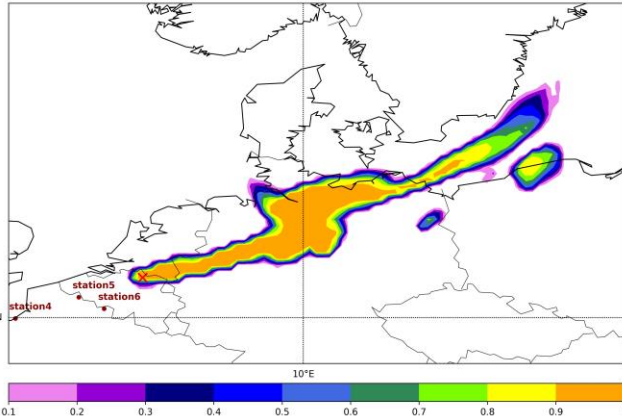
(Ensemble) metric	SRS value [$1/m^3$] or probability [%]	Source estimate [Bq]
Deterministic run	$1.59E-16$	$1.26E10$
Probability of exceeding $1E-18$ – reduced ensemble	100	$2.00E12$
Minimum – reduced ensemble	$2.23E-18$	$8.97E11$
Median – reduced ensemble	$1.32E-16$	$1.52E10$
Maximum – reduced ensemble	$6.50E-16$	$3.08E9$
Probability of exceeding $1E-18$ – full ensemble	94	$2.00E12$
Minimum – full ensemble	$1.15E-19$	$1.74E13$
Median – full ensemble	$1.59E-16$	$1.26E10$
Maximum – full ensemble	$1.08E-15$	$1.85E9$

Table 3
(Reduced and full ensemble) metrics names, corresponding SRS values interpolated to $51.2^\circ N$ and $5.0^\circ S$ (grid point closest to the BR2 reactor) and estimated source term resulting from scaling with the scaled Omonville measurement.

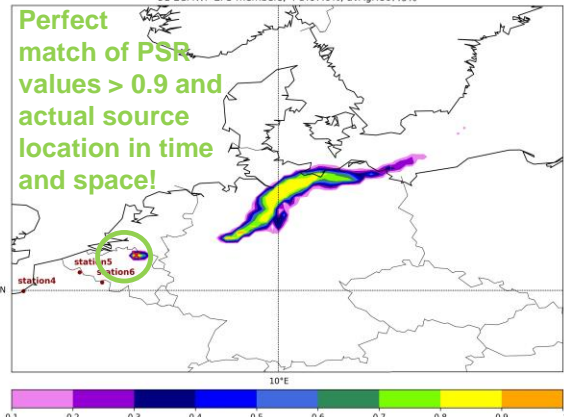
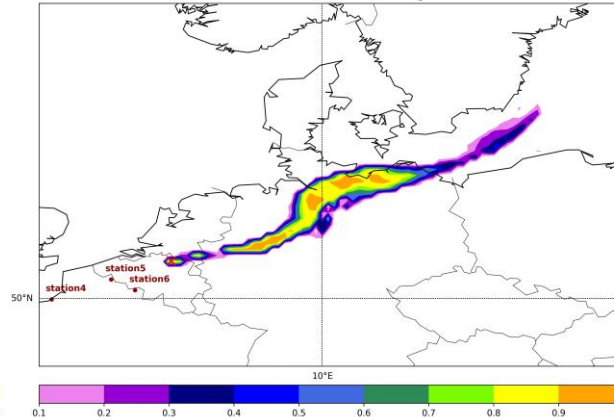


The degree of uncertainty in source term estimates related to ECMWF input data based on median, minimum and maximum SRS values is reflected by a medium to high normalized variance.

BR2-SCKCEN, PSR
2019-05-15 13Z
Deterministic run



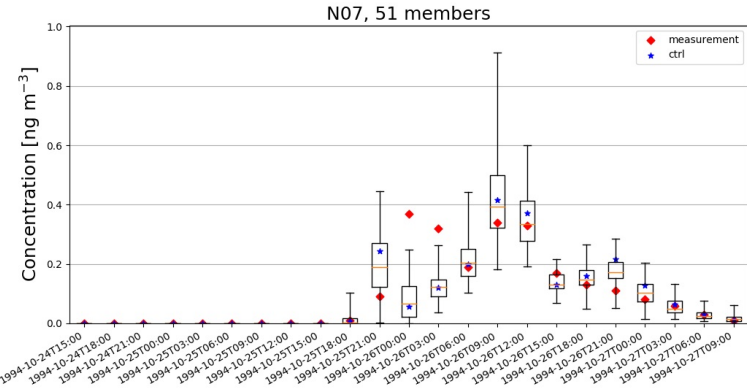
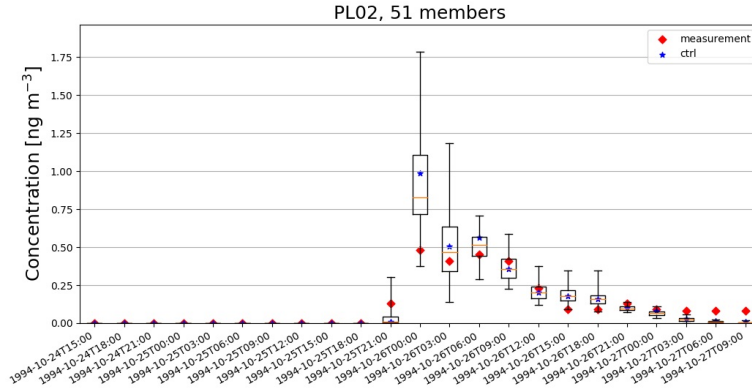
BR2-SCKCEN, min-PSR
2019-05-15 13Z
10 ECMWF-EPs-members, FO:65.29%, avAgr:80.15%



Perfect
match of PSR
values > 0.9 and
actual source
location in time
and space!

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Results: ETEX-I test case

Sampling station	N > 0.0	N > 0.0 expl. – 10/51 mem	Rank control/10-men med./51-men med.
A02	20	4/5	1.62/1.60/1.64
CR01	18	3/7	2.99/3.11/3.05
DK01	13	3/4	2.86/2.90/2.89
DK05	16	1/1	2.40/2.40/2.40
DK06	14	4/5	2.25/2.23/2.28
DK10	14	1/1	2.72/2.74/2.72
F02	9	3/3	3.19/3.18/3.14
H01	14	3/3	3.19/3.24/3.18
H02	13	5/10	2.95/3.04/3.06
N07	14	11/12	3.43/3.46/3.44
PL02	13	6/9	3.59/3.59/3.62
PL03	16	5/7	2.89/2.90/2.89
PL08	15	1/3	2.44/2.41/2.46
SR01	15	3/5	3.01/2.90/2.95
SR03	14	3/4	3.01/3.12/3.07

Table 4

Number of samples N > 0.0, number of explained samples N > 0.0 for the reduced and the full ensemble and rank for the control run as well as the reduced and the full ensemble medians for the 15 selected ETEX-I sampling sites time series.

Performance of control run and reduced as well as full ensemble medians are again (like for the Fukushima test case) very similar. However, there are less explained measured samples (27% and 37% for the reduced and the full ensemble), but overall plume passages are well captured.

Conclusions:

- Analyzing **FLEXPART ECMWF-EPS based ensemble products in addition to results based on the deterministic ECMWF run is of added value.**
- For the FOR fields**, ensemble products considered suitable are the **median, minimum, maximum, probability of exceedance and normalized variance**. The minimum, median and maximum products as a function of space and time can indicate the possible spread in estimated (puff) release source terms, whereas a high probability of exceedance given a specific FOR threshold value allows to estimate the upper bound of the source terms under investigation.
- For the PSR fields** the selected metrics include **minimum and probability of exceedance**, which were **demonstrated to better constrain a possible source region via enhancing contrasts between less likely and more likely source regions.**
- Ensemble time series can help explaining measured samples** of the IMS if the underlying source term is known.
- An arbitrarily selected 10-member ensemble is sufficient in order to benefit to a large degree from desirable ensemble properties.** The gain of using the full 51-member ensemble is visible, but rather small compared to the computational efforts.
- Model performance** when trying to predict measured samples **is similar for the control run when compared to the ensemble medians, and even more for the reduced and the full ensemble medians** in the present study, which may reflect the fact that **forecast uncertainty was largely suppressed by concatenating analyses and short term forecast. Besides**, e.g., member #1 from the analysis started at 12 UTC on average does not "know" the history of member #1 started at 00 UTC due to the **randomness of perturbations introduced during data assimilation**. This may contribute to the fact that a lot of uncertainty is already covered by a 10-member subset. **The added value of the ensemble is rather in giving** an indication of possible **concentration ranges and stating their likelihood** rather than yielding a more accurate forecast.
- It was recommended to the CTBTO to run the ensemble software created in the frame of the work at least on an ad-hoc basis. If computational and storage constraints are a limiting factor runs should be performed with 10 ECMWF-EPS members only.

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