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1. The 16 participants of the 3rd ATM-Challenge and their model set-ups

Main aims:	Name	Institution	ATM	Meteorology	Simulation	Minor
Investigate					length	included
the added	Kihyun Park (Korea)	KAERI	LADAS	UM-GDAPS (KMA)	6 months	Yes
of:	Arnaud Quérel (France)	IRSN	IdX-C3X (Eulerian)	ARPEGE (Météo France)	6 months	No (ZAMGʻs)
	Akiko Furuno (Japan)	JAEA	WSPEEDI-II (WRF+GEARN)	GPV- Global (JMA)	3 months	No (ZAMGʻs)
1) STACK	Alain Malo (Canada)	CMC	MLDP	GDPS (CMC)	6 months	Yes
emission	Donald Lucas (USA)	LLNL	LODI	NCEP-GFS/ADAPT	6 months	Yes
data	Paul Eslinger (USA)	PNNL	HYSPLIT	NCEP-GDAS	6 months	Yes
	Yuichi Kijima (Japan)	JAEA	HYSPLIT	NCEP-GDAS	3 months	No (ZAMGʻs)
R	Rich Britton (UK)	UK-NDC/AWE	HYSPLIT	NCEP-GDAS	6 months	Yes
and	Blake Orr (Australia)	ARPANSA	HYSPLIT	ACCESS-G (BoM)	6 months	No (ZAMGʻs)
	Alice Crawford (USA)	NOAA-ARL	HYSPLIT (-GEM)	NCEP-GDAS & ERA5	6 months	Yes
2) training	Anders Axelsson (Sweden)	FOI	HYSPLIT	NCEP-GDAS	6 months	Yes
z) training	Jolanta Kusmierczyk-Michulec (CTBTO)	CTBTO/IDC	FLEXPART 9.3.2	ECMWF-IFS	6 months	Yes
an	Christian Maurer (Austria)	ZAMG	FLEXPART 10.3	ECMWF-IFS	6 months	Yes
optimum	Michael Schoeppner (CTBTO)	CTBTO/OSI	FLEXPART 9.3.2	ECMWF-IFS	3 months	Yes
oncomble	Petra Seibert (Austria)	BOKU	FLEXPART	ECMWF-IFS	6 months	Yes
ensemple Pr	Pham Kim Long (Vietnam)	VINATOM	FLEXPART	NCEP-GFS	6 months	Yes 📃





2. A first glimpse on important statistics

What is the <u>average benefit</u> (over all four investigated stations CAX17, DEX33, SEX63, USX75 and all samples for June to December 2014 and all submitted runs) of:

- using actual historic daily stack emission¹ versus average literature emission data for IRE and CNL facilities?
- including rough estimates for NPPs' & and other facilities' emissions?

Ra	$ank = R^2 + \left(1 - \frac{1}{2}\right) $	$\frac{ FB }{2} + F5 + ACC$ 1) "Rank" according to 2 nd 2) "Rank" amended by dist 3) "Seibert's Skill Score ("Second Score")	ATM-Challenge ("R_2nd_Challenge"; 4 metrics combined) ribution metric ("R_KS"; 5 metrics combined) S"; 4 metrics combined)
	Rank ²	Actual daily stack emissions	Average literature emissions
	NPP emissions included	2.33 [1.45,2.70]; 3.08 [2.01,3.56]; 0.46 [0.20,0.61]	2.39 [1.47,2.73]; 3.17 [2.04,3.62]; 0.45 [0.19,0.60]
	NPP emissions not included	1.92 [0.91,2.45]; 2.56 [1.37,3.21]; 0.35 [0.07,0.58]	2.09 [1.08,2.59]; 2.78 [1.56, 3.39]; 0.39 [0.09,0.59]
¹ acc ² Rev acce altitu	essed via vDEC viewed IMS data set ssed via vDEC + DEX33 ude correction applied	Answers: • <u>No average benefit</u> from daily stack data of • Indication of a <u>positive impact of roughly</u> • that adds up to ~20%	over all samples, independent of the score used estimated emissions of NPPs and other facilities





3. Statistics per station – flagging main emitters' influence based on ATM



S: stack emissions outperform literature emissions based on all metrics

L: literature emissions outperform stack emissions based on Rank, but not on SS

L: literature emissions outperform stack emissions based on all metrics





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SEX63, stack

emissions

SEX63.

literature

emissions

USX75. stack

emissions

USX75.

literature

emissions

DEX33, stack

emissions

DEX33,

literature

emissions

flagged_bwd, >= MDC, 50% influence (IRE & CNL)

■ R 2nd Challenge ■ R KS ■ SS

0

CAX17, stack

emissions

CAX17,

literature

emissions





4.1 A different perspective: Selecting samples based on the emission profile: CNL-USX75 • In 2/3 of the cases the CNL



— Daily stack Xe-133 Emission [Bq] —— Mean daily Xe-133 value (Bq, disaggregated annual sum) – – – Literature Xe-133 value (Bq, disaggregated annual sum)

- In 2/3 of the cases the CNL contribution alone does not explain the signal -> Something is missing!
- NPPs+NRRs+other facilities' contributions are always and up to two orders of magnitude smaller than CNL stack emission based contributions -> CNL is the driving force
- Stack data are beneficial in 2/3 of the cases

Collection start [UTC]	Measured value [mBq/m3]	MIPFs contribution stack	MIPEs contribution literature	NPPs+NRRs+other facilites	Sum stack	Sum literature
20141102160000	0,53	0,88	20,70 <mark>S</mark>	0,36 S!	1,24	21,06
20140802160000	18,51	3,92	1,07 S?	0,09 <mark>S</mark>	4,01	1,16
20140620160000	5,6 3	4,82	3,57 S?	0,13 S	4,95	3,71
20140820160000	0,80	0,17	0,23 L?	0,10 L	0,27	0,33
20141001160000	4,80	6,85	2,61 L	0,67 L	7,52	3,28
20141014160000	0,9 5	0,38	0,15 S?	0,05 S	0,43	0,20

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USX75





4.2 A different perspective: Selecting samples based on the emission profile: IRE-SEX63 • For all cases the IRE (+CNL)



- For all cases the IRE (+CNL) contribution alone does not explain the signal -> *Something is missing!*
- NPPs+NRRs+other facilities' contributions are in 2/3 of the cases and up to two orders of magnitude bigger than IRE stack emission based contributions -> <u>IRE is not</u> <u>the driving force for these samples</u>
- Stack data are beneficial in 2/3 of the cases

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SEX63

Collection start [UTC]	Measured value [mBq/m3]	MIPFs contribution stack	MIPFs contribution literature	NPPs+NRRs+other facilites	Sum stack	Sum literature
20140707000000	1,71	0,16	0,09 S ?	0,115	0,2	7 0,20
20140727000000	0,60	0,05	0,08 L?	0,54 <mark>S</mark>	0,60	0 0,62
20140903000000	0,41	0,12	0,41 S?	0,29 S	0,4	2 0,70
20141024000000	1,36	0,02	2 0,03 L?	1,02 <mark>L</mark>	1,04	4 1,25
20141003000000	1,01	0,30) 0,34 L?	1,52 S	CNL influence! 1,8	2 1,8a
20141013000000	0,72	0,19	0,48 L?	0,15 L	0,3	30,62





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5. To remember: Monthly Xe-background in 2014 (PTS pilot study)





Gueibe et al. (2017): IRE: 2E15 Bq/y CNL: 1.5E16 Bq/y

- CNL had highest annual values!
- Knowing exact IRE emissions is clearly not enough for DEX33 and SEX63!

Percentage values are based on actual concentrations in Bq/m3







6. Redundancy of the ensemble



Prominent Features:

- High redundancy within the ensemble: Talagrand diagram is not evenly populated!
- Ensemble is highly overpredictive for very small concentrations. Likely due to setting below MDC concentrations to 0.

Number of effective members (that are sufficient to cover the variability of the observations):

- Define metric $d = e_m R * MME$; e_m : error of model m, R: Pearson correlation coefficient between multi-model average error *MME* and error e_m of model m
- Calculate eigenvalues λ of $corr(d_i, d_j)$ with $i, j = 1 \dots N$ ensemble members
- Calculate $N_{eff} = \frac{\left(\sum_{i=1}^{N} \lambda_i\right)^2}{\sum_{i=1}^{N} \lambda_i^2}$ for period 20140601-20141201
- 3.5 (out of 26 models) for CAX17
- 2.5 (out of 27 models) for DEX33
- 3.5 (out of 25 models) for SEX63
- 1.7 (out of 25 models) for USX75
- But not necessarily the very same 2 to 4 members at every station!





A sophisticated analysis performed by

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7. A first outlook on optimized ensemble results



(12/4.10)

stations





8.1 Conclusions

- A huge data pool of modelling results has been created. Please request it from ZAMG/CTBTO (i.e., contact <u>christian.maurer@zamg.ac.at</u> and <u>jolanta.kusmierczyk-michulec@ctbto.org</u>). A more thorough statistical analysis (Phd?) would be desirable.
- It seems to be important to select samples appropriately to demonstrate an on average small added value of stack emissions from IRE and CNL alone. However, there is considerable benefit from these stack data for individual samples.
- It is interesting to note that the mere selection of samples partly (at least to 50%) or predominantly (at least to 80%) influenced by IRE and/or CNL pushes the scores up most. The relative increase in scores on average adds up to ~15% when switching from all above MDC samples to those with 50% or 80% IRE and/or CNL influence using literature emissions compared to 7% when additionally switching from literature to stack emissions for 50% or 80% influence samples. This demonstrates that 1) knowing a large emitter and its location as well as 2) a proper average emission is more important than knowing the exact emission profile. Implicitly suppressing samples with overprediction > 50% or 20% in the sample selection process (via an absolute difference metric) can further enhance the scores which demonstrates the effects of the transport error on scores.





8.2 Conclusions II

- Simulating the radioxenon background at CAX17 without selecting samples according to CNL influence seems to be especially promising since CAX17 is a remote station with (at the time of 2014) dominating CNL influence.
- It seems to be very important to gain more knowledge about non IRE- and CNL-related emissions (for 2014). These emissions may be small individually (but can also be big, see MIPF Dimtrovgrad for SEX63), but in any case their sum (e.g., for DEX33) – depending on the predominant synoptic situation – is a decisive factor in accurately predicting the radioxenon background at IMS stations.
- The existent, full ensemble is highly redundant. If individual members cannot be made more diverse, a few submissions are good enough to forecast the Xe-133 background. This characteristic is related, e.g., to dominating transport models (FLEXPART & HYSPLIT), dominant meteorological input (ECMWF-IFS, NCEP-GFS) or to the fact that meteorological input consists of analyses concatenated with short-term forecasts thus reducing forecast uncertainty. The effective ensemble size is below five, however, depending on the station investigated, the time period considered and the individual members involved.
- A preliminary study shows that a reduced, optimized ensemble at each station has slightly higher skill compared to the full ensemble also for an independent evaluation period.





5. References

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- vDEC-Virtual Data Exploitation Centre. CTBTO, https://www.ctbto.org/specials/vdec/

THANK YOU FOR YOUR ATTENTION!

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Results of the 3rd ATM-Challenge 2019

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Auxiliary material





An example: Time series for CAX17

- A lot of valuable data for half a year
- 28 to 31 runs per station (CAX17, DEX33, SEX63 & USX75)



Ensemble approach has started: Appropriate files were sent to S. Galmarini (JRC, ensemble expert).
 Results will demonstrate how much independent and redundant information is inherent in the

runs.





Correcting DEX33 results to STP conditions

- CTBTO-IMS Xe-measurements are valid with respect to STP (standard temperature and pressure, T = 288.15 K, p =1013.25 hPa)
- All but BOKU and VINATOM submissions were referenced to ambient conditions -> simulations at DEX33 (~1200 m a.s.l.) are biased low due to reduced air density.
- Rough correction of activity concentrations via multiplying with the density quotient of STP density and average ambient density in the respective output layer.
- Average ambient density in the output layer calculated according to:

$$\rho = \rho_0 (T_0 / (T_0 + \gamma h))^{(1 + g_0 M / R\gamma)}$$
(1)

$$p_0 = 1.225 \text{ kg/m}^3$$
, $T_0 = 288.15 \text{ K}$, $\gamma = -0.0065 \text{ K/m}$, $R = 8.314 \text{ kg m}^2/\text{K mol s}^2$,
 $M = 0.029 \text{ kg/mol}$, $g_0 = 9.81 \text{ m/s}^2$

- Correction on average improves scores just slightly (7% for one metric).
- Not unexpected, a positive effect is only pronounced for those runs, where upper output layers were sampled (e.g., ZAMG and CMC runs) and not just the first 100 or 200 m above model topography.





Different approaches for selecting samples

Hypothesis: Benefit of stack emission data depends on the samples selected

Selection methods applied:

• (1)
$$\frac{|\text{measurement} - \text{MIPFs' contribution}|}{\text{measurement}} \le 50\% \text{ or } 80\%$$

or (1a) $\frac{\text{measurement} - \text{MIPFs' contribution}}{\text{measurement}} \le 50\% \text{ or } 80\%$

measurement

Contributions are calculated based on (A1) FLEXPART V9 bwd runs or a (B1 & B1a) FLEXPART V9-CTBTO fwd run and (A1) 1° or (B1 & B1a) 0.5° meteorological input and output resolution (operational CTBTO/IDC set-up as of 2014 or set-up for 3rd ATM-Challenge 2019).

• (2)
$$\frac{NPPs' + NRRs' + other facilities' contributions}{simulated value} \le 50\% \text{ or } 80\%$$

Contributions are calculated based on a FLEXPART V9-CTBTO fwd run and 0.5° meteorological input and output resolution (set-up for 3rd ATM-Challenge 2019).

• (3) Select subjectively a few outstanding daily stack emissions (outstanding with respect to the mean daily value as deduced from disaggregating the annual sum) and related samples predicted by the CTBTO fwd run.





A detailed look on the scores: all stations

Table 1: Average statistics per institution over all stations over all and for individual run-IDs ordered by Rank

	Institution		R	\mathbf{FB}	F5 [%]	RMSE	NMSE	KS [%]	ACC [%]	NAAD [%]	CRmax (\hat{t})	Rank	Rank KS	\mathbf{SS}
	AWE-1	Devilian	0.18	-1.07	30	5.17	40	47	51	99	0.18 (-1)	< 1.30	1.83	0.19
	AWE	Ranking	0.16	-0.63	36	7.01	31	44	58	294	0.18(-1)	1.45	2.01	0.20
	AWE-2		0.14	-0.18	41	8.84	22	40	65	489	0.19(-1)	1.59	2.19	0.22
	LLNL	according to	0.35	-0.51	63	4.52	11	33	66	92	0.35(0)	2.09	2.77	0.27
	FOI		0.36	-0.20	60	4.81	9	28	67	108	0.36(-1)	2.15	2.88	0.39
	VINATOM	one metric	0.27	0.48	56	11.80	18	21	70	181	0.27(0)	2.16	2.95	0.46
	PNNL	one metric	0.35	-0.20	60	4.61	8	34	69	100	0.35(0)	2.18	2.84	0.40
	JAEA	door not	0.40	-0.15	61	4.37	6	25	65	101	0.40(0)	2.19	2.93	0.45
	CTBTO	ubes not	0.47	-0.57	65	2.79	5	31	66	76	0.49(0)	2.25	2.94	0.45
	ARPANSA-1	necessity	0.41	-0.55	68	4.58	10	24	68	76	0.44(-1)	2.28	3.04	0.37
	ARPANSA	necessarily	0.47	-0.57	70	3.90	9	25	67	74	0.49(-1)	2.33	3.09	0.35
	BOKU	and the second second	0.32	-0.12	69	5.29	9	17	72	98	0.32(0)	2.38	3.21	0.58
1	KAERI-6	do justice to	0.39	0.34	67	5.71	7	24	75	132	0.41(-1)	2.40	3.17	0.62
C	KAERI-5		0.37	0.30	68	5.76	7	22	75	126	0.40(-1)	2.42	3.21	0.62
	ZAMG	the	0.48	-0.44	70	4.19	8	25	71	70	0.48(0)	2.45	3.20	0.49
	KAERI-8	the	0.40	0.23	69	5.73	8	19	74	117	0.43(-1)	2.46	3.27	0.61
	KAERI-7	submissionsl	0.39	0.27	69	5.69	7	21	75	119	0.42(-1)	2.46	3.26	0.62
	JAEA1	5001115510115:	0.45	0.05	71	4.10	4	18	73	108	0.54(0)	2.47	3.30	0.55
	NOAA-ARL-1		0.41	-0.00	69	4.76	6	28	76	91	0.42(0)	2.51	3.23	0.50
	NOAA-ARL		0.44	-0.23	71	4.56	8	24	75	79	0.46(-1)	2.52	3.28	0.49
	NOAA-ARL-3		0.47	-0.39	73	4.44	9	23	75	71	0.49(-1)	2.52	3.29	0.45
	KAERI		0.43	0.25	70	5.24	6	20	77	111	0.44(-1)	2.52	3.32	0.61
	NOAA-ABL-2		0.45	-0.30	72	4.49	8	22	75	74	0.49(-2)	2.53	3.31	0.52
	ARPANSA-2		0.70	-0.67	74	1.18	4	28	65	65	0.70(0)	2.56	3.28	0.26
	CTBTO1-1		0.48	0.07	72	5 20	11	16	78	100	0.49 (0)	2.56	3.41	0.47
	CMC-3		0.43	0.03	76	4 47	6	21	78	92	0.43(0)	2.59	3.38	0.55
	KAERI-2		0.47	0.25	72	4 77	5	22	78	103	0.47(0)	2.60	3.38	0.60
	KAERL4		0.48	0.19	72	4 75	5	19	79	98	0.48(0)	2.61	3 42	0.58
	KAERL3		0.47	0.21	72	4 75	5	19	79	99	0.47(0)	2.61	3 42	0.60
	KAFRI-1		0.47	0.19	73	4.73	5	18	79	96	0.47(0)	2.62	3 44	0.61
/	CMC		0.48	-0.09	78	4.35	6	17	80	79	0.48(0)	2.68	3 51	0.56
	CTBTO1		0.40	-0.03	74	4.33	8	15	79	80	0.48(0)	2.08	3 54	0.60
	IRSN		0.51	-0.36	77	4.04	7	14	78	66	0.52(0)	2.03	3 56	0.00
	CMC 1		0.55	-0.30	77	4.00	5	19	80	70	0.55 (0)	2.10	9.54	0.40
(CMC 2		0.30	-0.03	80	4.20	7	10	81	19	0.30(0)	2.12	0.04	0.00
ſ	CTRTO1 2		0.49	-0.28	78	4.30	2	12	83	60	0.49 (0)	2.74	2.91	0.55
	TBIOI-		0.00	-0.03	10	2.00	0	19	02	09	0.08 (0) (4.04	5.81	0.00
<	Average over	all institutions	0.40	-0.20	66	4.99	10	24	71	108	0.42(-1)	(2.33)	3.08	0.46
_	Median over	all institutions	0.44	-0.20	69	4.44	8	24	70	95	0.45(0)	2.35	3.14	0.47
_	Maximum ov	er all institutions	0.53	0.48	78	11.80	31	44	80	294	0.54(0)	2.70	3.56	0.61
	Minimanna or	on all institutions	0 16	0 69	96	2 70	4	14	EO	66	0 19 (1)	1 45	2 01	0.20

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Average Rank of 2nd ATM-Challenge was 2.06. However, the metrics of the two Challenges should not be compared because of different:

- participants, model set-ups (uniform vs. non-uniform output grid!), model versions
- coverage of seasons, hemispheres
- number of samples above MDC for the 2nd Challenge (very low)





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A detailed look on the scores: CAX17

Table 2: Average statistics and individual statistics for station CAX17 per institution over all run-IDs and for individual run-IDs ordered by Rank

Institution	\mathbf{R}	\mathbf{FB}	F5 [%]	RMSE	NMSE	KS [%]	ACC [%]	NAAD [%]	$CRmax(\hat{t})$	Rank	Rank KS	SS
AWE-1	0.42	-1.46	23	5.25	25	46	54	86	0.42(0)	1 22	1.76	0.12
AWE	0.43	-1.41	28	5.21	23	45	58	85	0.43(0)	1.33	1.89	0.13
AWE-2	0.44	-1.37	32	5.17	20	43	61	83	0.44(0)	1.44	2.01	0.13
JAEA1	0.12	-0.04	52	6.99	5	7	68	112	0.44(-1)	2.19	3.12	0.74
LENE	0.47	-0.89	74	4.87	9	29	78	69	0.47(0)	2.29	3.00	0.24
VINATOM	0.23	0.03	54	8.04	9	21	74	111	0.23(0)	2.32	3.11	0.77
CTBTO	0.48	-0.74	71	5.63	7	22	79	69	0.48(0)	2.36	3.14	0.25
JAEA	0.42	-0.08	59	5.89	4	7	73	87	0.42(0)	2.45	3.38	0.79
KAERI-4	0.43	0.46	69	6.38	4	14	88	125	0.43(0)	2.51	3.37	0.50
KAERI-1	0.43	0.46	69	6.32	4	14	87	124	0.43(0)	2.52	3.38	0.51
KAERI-3	0.43	0.46	70	6.32	4	14	87	124	0.43(0)	2.52	3.38	0.51
KAERI-2	0.44	0.47	70	6.32	4	14	87	125	0.44(0)	2.52	3.38	0.50
KAERI	0.45	0.42	71	6.22	4	13	87	118	0.45(0)	2.57	3.45	0.53
KAERI-6	0.47	0.41	71	6.25	4	11	87	114	0.47(0)	2.60	3.49	0.54
FOI	0.48	-0.34	75	4.79	5	16	80	69	0.48(0)	2.61	3.45	0.57
PNNL	0.59	-0.53	70	4.31	5	18	83	63	0.59(0)	2.62	3.44	0.45
KAERI-5	0.46	0.37	72	6.10	4	11	88	111	0.46(0)	2.62	3.51	0.57
BOKU	0.37	-0.12	73	6.19	6	11	82	90	0.37(0)	2.63	3.52	0.77
KAERI-7	0.47	0.37	72	6.09	4	11	88	111	0.47(0)	2.63	3.52	0.57
ZAMG	0.53	-0.42	79	4.58	5	20	80	64	0.53(0)	2.66	3.46	0.52
KAERI-8	0.46	0.34	73	5.98	4	11	89	109	0.46(0)	2.66	3.55	0.59
ARPANSA	0.59	-0.39	78	4.28	4	13	83	65	0.59(0)	2.76	3.63	0.54
NOAA-ARL-3	0.60	-0.31	79	4.24	4	12	84	63	0.60(0)	2.84	3.72	0.61
NOAA-ARL-1	0.63	-0.08	70	4.11	3	26	79	72	0.63(0)	2.85	3.59	0.72
NOAA-ARL	0.62	-0.20	76	4.16	3	17	83	66	0.62(0)	2.87	3.71	0.69
NOAA-ARL-2	0.64	-0.21	79	4.12	3	12	84	63	0.64(0)	2.94	3.82	0.74
CMC-2	0.56	-0.13	87	4.45	3	6	89	64	0.56(0)	3.01	3.95	0.80
IRSN	0.62	-0.20	84	4.09	3	5	89	59	0.62(0)	3.02	3.97	0.71
CMC-3	0.56	0.03	87	4.85	3	6	91	71	0.56(0)	3.07	4.01	0.89
CMC	0.57	-0.03	88	4.59	3	5	91	68	0.57(0)	3.09	4.04	0.86
CTBTO1-1	0.74	-0.15	79	3.53	2	11	87	58	0.74(0)	3.13	4.02	0.83
CTBTO1	0.74	-0.12	79	3.53	2	10	87	58	0.74(0)	3.15	4.05	0.86
CMC-1	0.60	0.01	90	4.47	3	3	93	68	0.60(0)	3.17	4.14	0.90
CTBTO1-2	0.75	-0.09	79	3.53	2	9	88	58	0.75 (0)	3.18	4.09	0.89
Average over all institutions	0.48	-0.32	69	5.21	6	16	80	78	0.50(-1)	2.56	3.40	0.59
Median over all institutions	0.48	-0.20	74	4.83	5	15	81	69	0.48(0)	2.61	3.45	0.63
Maximum over all institutions	0.74	0.42	88	8.04	23	45	91	118	0.74 (0)	3.15	4.05	0.86
Minimum over all institutions	0.12	-1.41	28	3.53	2	5	58	58	0.23(-1)	1.33	1.89	0.13

However, the highest Ranks tend to come with high "Seibert Scores"





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A detailed look on the scores: DEX33

Table 3: Average statistics and individual statistics for station DEX33 per institution over all run-IDs and for individual run-IDs ordered by Rank

Institution	R	FB	F5 [%]	RMSE	NMSE	KS [%]	ACC [%]	NAAD [%]	$CRmax(\hat{t})$	Rank	Rank_KS	gg
AWE-2	-0.17	1.79	10	16.44	22	90	63	1682	-0.07 (-3)	0.87	0.97	0.04
AWE	-0.13	0.99	34	9.03	13	61	64	903	-0.08(-2)	1.51	1.90	0.28
VINATOM	-0.02	1.02	48	4.08	8	32	64	296	-0.02(0)	1.61	2.29	0.16
FOI	0.16	0.72	45	3.01	6	29	57	213	0.16(0)	1.69	2.40	0.27
PNNL	0.10	0.71	55	2.01	3	50	65	176	0.10(0)	1.85	2.35	0.36
CMC-3	0.25	0.72	59	1.97	3	47	66	159	0.25(0)	1.95	2.48	0.39
KAERI-6	0.45	0.98	58	2.78	4	48	66	223	0.45(0)	1.95	2.47	0.30
LLNL	0.08	0.47	60	1.79	3	30	64	145	0.08(0)	2.01	2.71	0.41
KAERI-5	0.39	0.87	62	2.98	5	36	69	203	0.39(0)	2.02	2.66	0.27
JAEA	0.46	-0.71	65	1.60	4	39	59	70	0.46(0)	2.10	2.71	0.30
ARPANSA-1	0.42	-0.55	66	1.31	4	19	58	81	0.42(0)	2.14	2.95	0.29
AWE-1	-0.10	0.18	58	1.62	3	32	64	123	-0.10(0)	2.14	2.82	0.52
CTBTO1-1	0.36	0.77	72	4.48	13	16	74	167	0.37(3)	2.20	3.04	0.17
KAERI-7	0.47	0.78	68	2.70	5	33	69	174	0.47(0)	2.20	2.87	0.30
KAERI-8	0.50	0.71	68	3.02	6	25	65	169	0.50(0)	2.22	2.97	0.27
KAERI	0.55	0.70	63	2.10	3	38	67	153	0.55(0)	2.26	2.88	0.41
BOKU	0.30	0.33	70	1.93	4	16	64	121	0.30(0)	2.26	3.10	0.55
CMC-1	0.49	0.43	61	1.34	2	38	69	110	0.49(0)	2.32	2.94	0.51
KAERI-2	0.63	0.66	60	1.43	2	50	66	129	0.63(0)	2.34	2.84	0.50
ARPANSA	0.56	-0.61	70	1.24	4	24	62	73	0.56(0)	2.35	3.11	0.27
CMC	0.44	0.34	67	1.48	2	31	72	111	0.44(0)	2.39	3.09	0.54
KAERI-3	0.64	0.56	62	1.34	1	39	68	113	0.64(0)	2.43	3.04	0.53
NOAA-ARL-1	0.54	0.37	65	1.23	2	49	68	104	0.54(0)	2.43	2.94	0.44
CTBTO1	0.38	0.38	74	3.11	9	17	75	123	0.39(1)	2.45	3.28	0.50
KAERI-4	0.65	0.53	62	1.31	1	37	67	109	0.65(0)	2.45	3.08	0.54
KAERI-1	0.63	0.47	64	1.25	1	36	68	103	0.63(0)	2.49	3.13	0.56
NOAA-ARL	0.55	0.15	64	1.19	2	36	68	89	0.55(0)	2.54	3.18	0.65
ARPANSA-2	0.70	-0.67	74	1.18	4	28	65	65	0.70(0)	2.56	3.28	0.26
NOAA-ARL-2	0.54	0.06	63	1.17	2	29	67	83	0.54(0)	2.57	3.28	0.75
CTBTO	0.34	-0.11	78	1.64	2	21	73	84	0.34(0)	2.58	3.37	0.74
ZAMG	0.50	-0.25	74	1.28	3	18	73	71	0.50(0)	2.59	3.41	0.65
IRSN	0.51	-0.25	75	1.21	3	7	73	70	0.51 (0)	2.61	3.54	0.53
NOAA-ARL-3	0.55	0.03	65	1.16	2	31	69	80	0.55(0)	2.63	3.32	0.75
CTBTO1-2	0.41	-0.01	77	1.73	4	17	76	79	0.41(0)	2.69	3.52	0.84
JAEAI	0.61	-0.23	86	1.37	2	23	72	61	0.61 (0)	2.83	3.60	0.71
CMC-2	0.60	-0.14	81	1.12	2	7	81	64	0.60(0)	2.91	3.84	0.72
Average over all institutions	0.34	0.23	64	2.38	4	29	67	172	0.34(-1)	2.23	2.93	0.46
Median over all institutions	0.41	0.33	66	1.71	3	30	66	116	0.42(0)	2.31	3.09	0.46
Maximum over all institutions	0.61	1.02	86	9.03	13	61	75	903	0.61(1)	2.83	3.60	0.74
Minimum over all institutions	-0.13	-0.71	34	1.19	2	7	57	61	-0.08 (-2)	1.51	1.90	0.16





A detailed look on the scores: SEX63

Table 4: Average statistics and individual statistics for station SEX63 per institution over all run-IDs and for individual run-IDs ordered by Rank

Institution	\mathbf{R}	\mathbf{FB}	F5 [%]	RMSE	NMSE	KS [%]	ACC [%]	NAAD [%]	$\operatorname{CRmax}(\hat{t})$	Rank	Rank KS	\mathbf{SS}
AWE-1	0.17	-1.63	19	2.22	63	61	38	91	0.17 (0)	0.78	1.17	0.03
AWE	0.12	-0.90	41	2.26	35	35	51	95	0.17(0)	1.48	2.14	0.31
LLNL	0.19	-0.88	65	2.14	15	40	60	76	0.19(0)	1.84	2.44	0.15
CTBTO	0.50	-0.89	61	0.93	4	42	51	73	0.60(1)	1.93	2.51	0.29
FOI	0.17	-0.74	66	2.16	13	34	65	78	0.17(0)	1.97	2.63	0.21
PNNL	0.17	-0.63	65	2.17	12	32	64	78	0.17(0)	2.00	2.68	0.25
ARPANSA	0.19	-0.67	73	2.17	12	31	65	77	0.19(0)	2.09	2.78	0.26
ZAMG	0.21	-0.57	72	2.17	11	30	66	75	0.21(0)	2.14	2.84	0.31
JAEA	0.38	-0.44	63	0.99	3	27	59	80	0.38(0)	2.15	2.88	0.49
AWE-2	0.08	-0.16	62	2.31	8	8	64	98	0.17(1)	2.18	3.10	0.59
VINATOM	0.21	0.13	64	2.91	10	18	68	120	0.21(0)	2.30	3.12	0.72
BOKU	0.17	-0.26	73	2.30	9	19	71	89	0.17(2)	2.34	3.15	0.54
NOAA-ARL-1	0.22	-0.45	78	2.07	9	15	78	68	0.22(0)	2.38	3.23	0.22
IRSN	0.22	-0.49	80	2.14	10	20	78	69	0.22(0)	2.38	3.18	0.32
NOAA-ARL-3	0.23	-0.56	84	2.08	10	21	78	67	0.23(0)	2.40	3.19	0.21
NOAA-ARL	0.21	-0.50	82	2.10	9	18	78	68	0.21(-2)	2.40	3.22	0.24
NOAA-ARL-2	0.18	-0.48	83	2.14	10	18	79	70	0.19(-4)	2.41	3.23	0.29
CMC-2	0.25	-0.44	81	2.06	9	16	77	66	0.25(0)	2.43	3.27	0.30
CMC-3	0.24	-0.33	78	2.09	8	14	78	69	0.24(0)	2.46	3.32	0.41
CMC	0.25	-0.35	80	2.08	8	14	78	68	0.25(0)	2.46	3.31	0.39
CMC-1	0.25	-0.29	79	2.09	8	13	78	69	0.25(0)	2.49	3.36	0.44
JAEA1	0.49	-0.45	79	0.89	2	19	69	65	0.49(0)	2.49	3.30	0.50
CTBTO1	0.16	0.26	79	3.82	15	8	82	104	0.20(-1)	2.50	3.42	0.52
KAERI-7	0.18	-0.01	74	2.42	8	11	75	93	0.18(0)	2.52	3.41	0.78
KAERI-8	0.18	-0.02	75	2.42	8	13	76	93	0.18(0)	2.53	3.40	0.78
KAERI-5	0.19	-0.01	75	2.36	7	12	76	92	0.19(0)	2.54	3.42	0.77
KAERI-6	0.18	0.01	75	2.42	8	10	77	93	0.18(0)	2.55	3.45	0.78
KAERI	0.19	0.01	77	2.33	7	10	79	89	0.19(0)	2.59	3.49	0.76
KAERI-1	0.20	0.03	78	2.25	6	7	82	86	0.20(0)	2.63	3.56	0.74
KAERI-3	0.19	0.02	79	2.25	6	7	82	85	0.19(0)	2.64	3.57	0.74
KAERI-4	0.19	0.03	79	2.26	6	8	82	86	0.19(0)	2.64	3 56	0.74
KAERI-2	0.20	0.03	80	2.24	6	8	83	85	0.20(0)	2.65	3.57	> 0.74
Average over all institutions	0.24	-0.46	70	2.10	11	25	68	82	0.25(0)	2.19	2.94	0.39
Median over all institutions	0.20	-0.49	73	2.16	10	24	67	77	0.21(0)	2.23	3.00	0.32
Maximum over all institutions	0.50	0.26	82	3.82	35	42	82	120	0.60 (2)	2.59	3.49	0.76
Minimum over all institutions	0.12	-0.90	41	0.89	2	8	51	65	0.17 (-2)	1.48	2.14	0.15





A detailed look on the scores: USX75

Table 5: Average statistics and individual statistics for station USX75 per institution over all run-IDs and for individual run-IDs ordered by Rank

Institution	\mathbf{R}	\mathbf{FB}	F5 [%]	RMSE	NMSE	KS [%]	ACC [%]	NAAD [%]	$\operatorname{CRmax}(\hat{t})$	\mathbf{Rank}	Rank KS	\mathbf{SS}
AWE-1	0.21	-1.39	21	11.60	71	50	48	95	0.21(-1)	< 1.04	1.54	0.09
AWE	0.22	-1.19	40	11.53	54	34	61	94	0.22(-1)	1.46	2.12	0.10
AWE-2	0.23	-0.99	58	11.45	37	18	73	93	0.23(0)	1.87	2.69	0.12
JAEA	0.36	0.64	55	8.98	13	28	69	167	0.36(0)	2.05	2.77	0.22
ARPANSA	0.45	-0.58	56	10.54	19	32	65	83	0.55(-4)	2.12	2.80	0.39
CTBTO	0.54	-0.52	49	2.96	5	37	60	78	0.54(0)	2.13	2.76	0.51
NOAA-ARL-2	0.43	-0.58	62	10.55	19	28	69	80	0.59(-4)	2.21	2.93	0.32
NOAA-ARL-3	0.51	-0.71	63	10.26	21	28	69	74	0.57(-4)	2.22	2.94	0.22
LLNL	0.66	-0.72	52	9.28	17	32	64	78	0.66(0)	2.24	2.92	0.29
PNNL	0.52	-0.34	52	9.96	13	35	64	84	0.52(0)	2.26	2.91	0.53
NOAA-ARL	0.40	-0.38	62	10.81	17	25	72	91	0.48(-2)	2.27	3.02	0.39
BOKU	0.42	-0.43	61	10.75	17	22	71	94	0.42(0)	2.28	3.06	0.46
FOI	0.60	-0.43	54	9.28	13	31	65	72	0.63(-1)	2.35	3.04	0.49
JAEA1	0.56	0.91	67	7.16	6	22	84	193	0.61(1)	2.37	3.15	0.25
NOAA-ARL-1	0.26	0.15	62	11.62	11	20	77	120	0.28(2)	2.38	3.18	0.62
VINATOM	0.67	0.75	59	32.17	45	12	73	195	0.67(0)	2.39	3.27	0.20
KAERI-8	0.44	-0.11	59	11.52	14	27	67	96	0.57(-1)	2.41	3.14	0.80
ZAMG	0.67	-0.49	56	8.72	12	32	66	70	0.67(0)	2.42	3.10	0.47
CTBTO1	0.67	-0.58	57	8.96	14	28	70	69	0.67(0)	2.42	3.14	0.38
KAERI-7	0.45	-0.05	62	11.56	13	27	69	98	0.55(-2)	2.49	3.22	0.84
KAERI-5	0.45	-0.04	62	11.62	13	27	69	99	0.55(-2)	2.50	3.23	0.85
KAERI-6	0.45	-0.04	62	11.40	13	25	71	98	0.53(-1)	2.52	3.27	0.85
CMC-2	0.56	-0.40	72	9.88	14	20	77	74	0.56(0)	2.60	3.40	0.36
KAERI	0.54	-0.13	70	10.30	12	21	74	86	0.59(-1)	2.67	3.46	0.73
IRSN	0.76	-0.48	71	8.56	11	24	73	64	0.76(0)	2.78	3.54	0.37
CMC	0.64	-0.32	76	9.26	11	19	78	71	0.64(0)	2.79	3.61	0.46
KAERI-4	0.65	-0.27	78	9.04	10	16	78	72	0.65(0)	2.84	3.68	0.54
KAERI-3	0.63	-0.20	79	9.08	10	16	78	74	0.63(0)	2.86	3.70	0.63
KAERI-1	0.63	-0.20	79	9.09	10	16	78	74	0.63(0)	2.86	3.70	0.63
KAERI-2	0.63	-0.16	79	9.09	9	15	78	74	0.63(0)	2.88	3.73	0.68
CMC-3	0.67	-0.29	78	8.98	10	18	79	69	0.67(0)	2.88	3.70	0.50
CMC-1	0.68	-0.26	77	8.92	10	18	79	70	0.68(0)	(2.90)	3.72	0.53
Average over all institutions	0.54	-0.27	58	10.58	17	27	69	99	0.56(-1)	2.31	3.04	0.39
Median over all institutions	0.55	-0.43	57	9.28	13	28	69	84	0.60(0)	2.31	3.05	0.39
Maximum over all institutions	0.76	0.91	76	32.17	54	37	84	195	0.76(1)	2.79	3.61	0.73
Minimum over all institutions	0.22	-1.19	40	2.96	5	12	60	64	0.22 (-4)	1.46	2.12	0.10





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Ensemble optimisation based on RMSE and Pearson's correlation coefficient (PCC)



Analysis valid for the period 20140601 to 20141201. Number of involved members N reduced to 16 (one per participating institution) due to computational limitations. Given N members, there are G=N!/(r!(N-r)!) possible groups of r elements!





Details on statistical metrics

Given N predictions P_j and measurements M_i at times t_j and t_i with mean values \overline{P} and \overline{M} as well as minimum detectable concentrations MDC_j and MDC_i the statistical scores in subsection 2.8 are formally defined as:

$$FB = 2\frac{(\overline{P} - \overline{M})}{(\overline{P} + \overline{M})}$$
(A.1)

$$R = \frac{\sum (M_i - M)(P_i - P)}{\sqrt{(M_i - \overline{M})^2 (P_i - \overline{P})^2}}$$
(A.2)

Let T denote the number of fractions satisfying:

$$0.2 \le \frac{P_i}{M_{i|M_i > 0.0}} \le 5.0 \tag{A.7}$$

and Q the number of pairs with $P_{i|P_i \ge MDC_i}$ and/or $M_{i|M_i \ge MDC_i}$ then F5 is defined as:

$$F5 = \frac{T}{Q}100$$
(A.8)

Given the number of correctly forecasted above MDC values *A* (true positives) and below MDC values *B* (true negatives) as well as the number of not correctly forecasted above MDC values (false positives) *C* and below MDC values *D* (false negatives), the Accuracy is given as:

$$ACC = \frac{A+B}{A+B+C+D} 100$$

(9)





Details on statistical metrics

The Kolmogorov-Smirnov parameter (KSP) is defined as:

 $KSP = Max|D(M_k) - D(O_k)| * 100\%$ (A.7)

where *D* is the cumulative distribution of the predicted and measured (or other predicted) concentrations over the range of k values such that D is the probability that the concentration will not exceed M_k or O_k . The score measures the ability of the model to reproduce the measured (or another predicted) concentration distribution regardless of space and time. The maximum difference between any two distributions cannot be more than 100%.

Further visual evaluations in Kioutsioukis and Galmarini [19] are based on comparing *Cumulative* Density Functions (cdf) of the models and the observations or on showing Taylor diagrams (i.e, a combination of correlation coefficient, root mean square error and standard deviation, Figure 2). The distance between the reference (black point in Figure 2) and model points in a Taylor diagram is then the BC_RMSE . According to Taylor [42] model standard deviation, BC_RMSE and Rcan be combined into a single skill score S_r .

$$S_r = 2(1+R)\left(\frac{\sigma_m}{\sigma_o} + \frac{\sigma_o}{\sigma_m}\right)^{-2} \tag{20}$$

with σ_m and σ_o being the standard deviations of predictions and observations.

The correlation contribution becomes important for large values of BC_RMSE . If one wants to include also the relative bias FB into the skill score, Seibert [34] suggests:

$$S_b = \frac{1}{1 + bFB^2} \tag{21}$$



Details on statistical metrics

A value of b = 10 appears to give a relationship fulfilling Seibert's [34] subjective idea about such a skill score. Finally, both skill scores can be combined into a total skill score S:

$$S = \alpha S_r + (1 - \alpha)S_b \tag{22}$$

The value of α is rather arbitrary and would depend on the application. $\alpha = 0.5$ might be acceptable. An additive and not multiplicative combination of the two scores is suggested because a model that has skill either in reproducing the mean or in reproducing the patterns should be attributed some total skill; the product of the two scores would be zero with one of the factors being zero. In any case, data sets with strongly non-normal distributions might better be transformed before applying any of the measures.