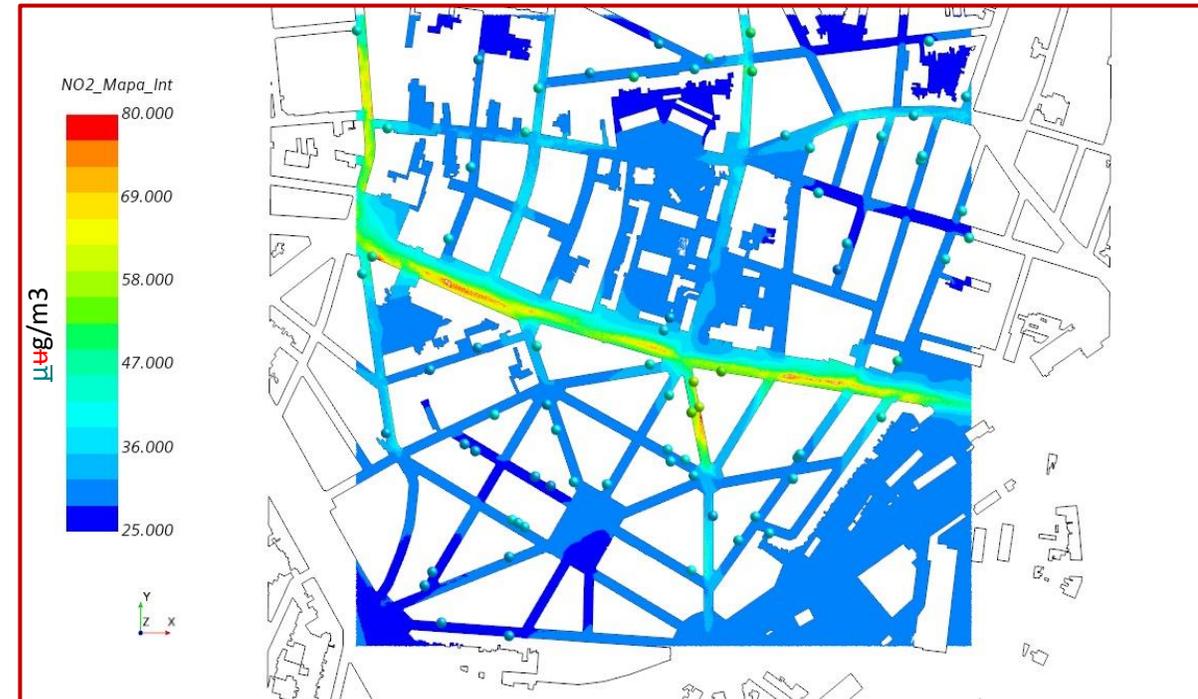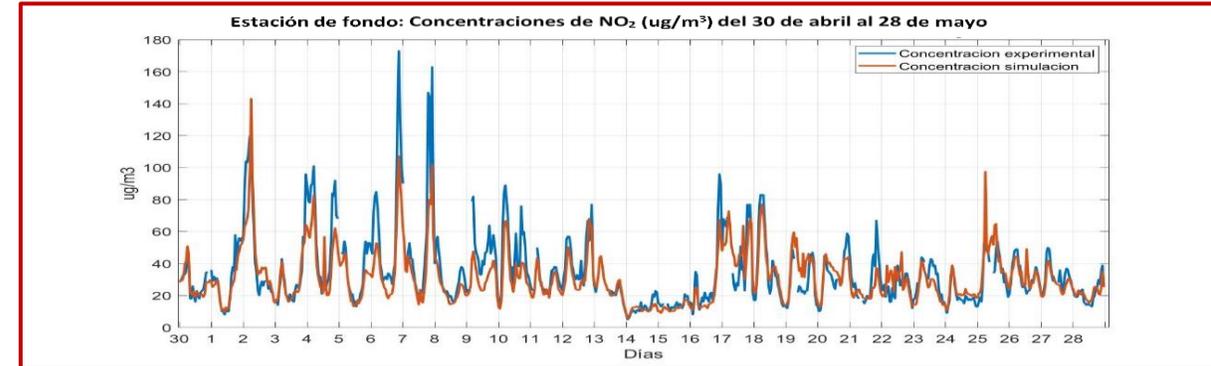# CT4 Intercomparison exercise. Step 2.1

To compute averages (concentration maps) for the complete campaign period (April 30 – May 28) applying the methodologies of each group.

1. *Comparison with passive samplers' data and AQ station data*
2. *Intercomparison among models results.*

Estación de fondo: Concentraciones de NO₂ (ug/m³) del 30 de abril al 28 de mayo

Step 2.1. Sampler series CT4 Tool
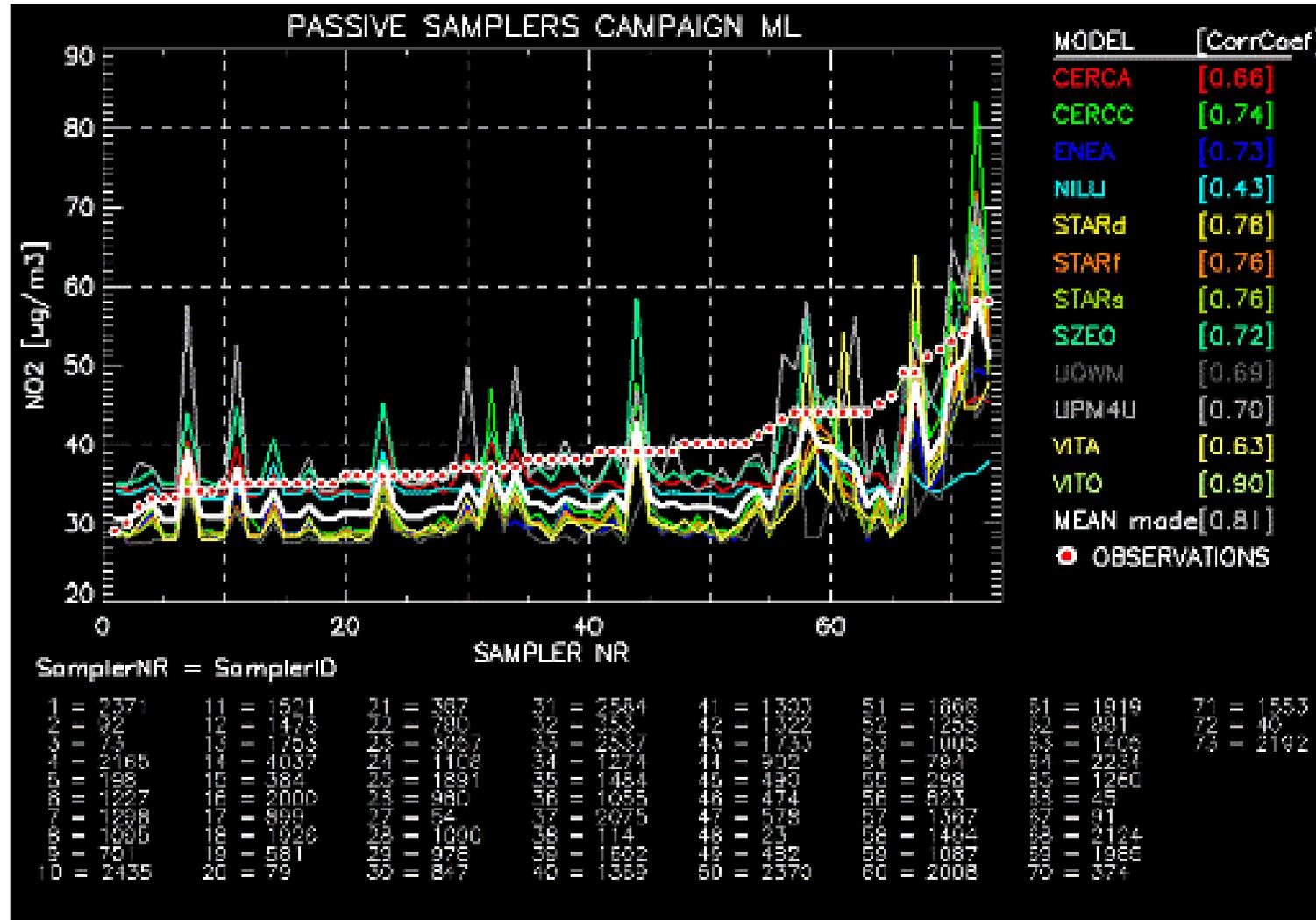
Step 2.1. Statistics - Concentrations

model	MEAN OBS	MEAN-MOD	DEVOBS	DEVMOD	Correl	Bias	NMbias	MFB	RMS	RMSN	MFE	TARGET	FAC2
SZE	39,4	39,5	6,0	7,0	0,72	0,1	0,00	0,00	4,9	0,12	0,08	0,82	1
UPM-PALM4U	39,4	40,5	6,0	8,5	0,70	1,1	0,03	0,02	6,2	0,16	0,10	1,02	1
ENEA-PMSS	39,4	32,0	6,0	5,1	0,73	-7,5	-0,19	-0,21	8,5	0,21	0,22	1,42	1
CERC-CIEMAT	39,4	34,5	6,0	9,5	0,74	-4,9	-0,13	-0,15	8,1	0,19	0,19	1,34	1
CERC-ADMS	39,4	36,7	6,0	4,2	0,66	-2,7	-0,07	-0,07	5,3	0,12	0,11	0,87	1
CIEMAT-SIMPLE	39,4	31,9	6,0	6,1	0,76	-7,5	-0,19	-0,22	8,7	0,21	0,22	1,43	1
CIEMAT-WINDFACTOR	39,4	32,7	6,0	7,3	0,76	-6,7	-0,17	-0,19	8,2	0,20	0,21	1,36	1
CIEMAT-DETAILED	39,4	32,3	6,0	6,7	0,76	-7,1	-0,18	-0,20	8,4	0,20	0,21	1,39	1
UOWM	39,4	31,1	6,0	6,1	0,69	-8,4	-0,21	-0,24	9,6	0,23	0,25	1,60	1
VITO-OPENFOAM	39,4	35,0	6,0	9,7	0,69	-4,4	-0,11	-0,14	8,3	0,20	0,19	1,38	1
VITO-ATMOSTREET	39,4	32,7	6,0	7,1	0,63	-6,8	-0,17	-0,20	8,8	0,21	0,22	1,47	1
NILU-EPISODE	39,4	34,5	6,0	1,4	0,43	-4,9	-0,13	-0,12	7,4	0,16	0,14	1,23	1

- $R^2 \geq 0.70$ ➔ SZE, ENEA, CERC-CIEMAT, CIEMAT (SIMPLE, WINDFACTOR, DETAILED)
- $0.60 \leq R^2 < 0.70$ ➔ CERC-ADMS, UOWM, VITO-OPENFOAM, VITO-ATMOSTREET
- $R^2 < 0.60$ ➔ NILU
- Most of the models underpredict (MFB between -0.07 and -0.24). UPM overpredicts very slightly and SZE has MFB =0.
- All models have FAC2 = 1.
- MFE (0.08, 0.25) lower than in case of STEP 1.0.
- Target < 1 (SZE and CERC-ADMS), Target >1.4 (ENEA, CIEMAT-SIMPLE, UOWM, VITO-ATMOSTREET)
- Standard deviation (SD) of the predictions is very low for NILU (less than 25% of the observed SD). The CERC-ADMS SD is lower than observed one (by 30%), the SD of most of the models is ± 20% the observed SD, but two models (CERC-CIEMAT and VITO-OPENFOAM) exceed the observed SD by more than 50%.

Step 2.1. Scatter-Plots - Concentrations
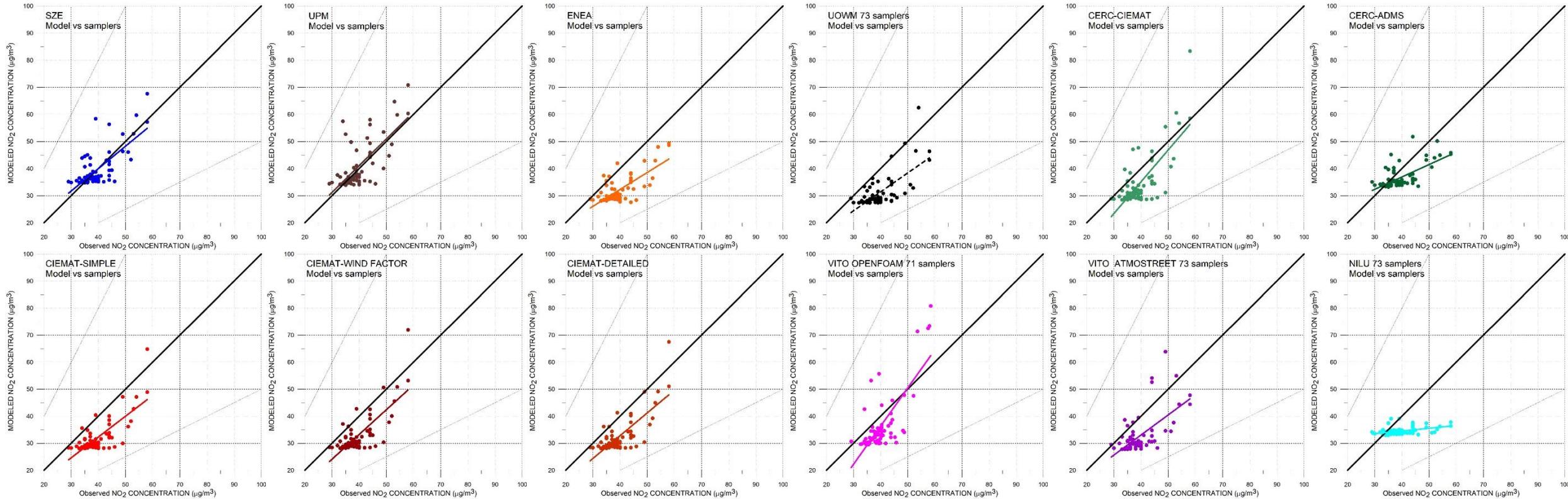
- Taking into account the statistics and scatter plots, most of the models (especially the CFD models) seem to predict fairly good the monthly-averaged concentrations.
- NILU models seems to provide worse results with very low spatial variability in the predicted concentrations.
- In most scatter plots, there points with similar modelled concentrations but different measured concentrations. This issue can be related with the streets where the traffic emissions are neglected in the simulations.

Step 2.1. Statistics – Concentration Difference

model	MEAN OBS	MEAN-MOD	DEVOBS	DEVMOD	Correl	Bias	NMbias	MFB	RMS	MFE	TARGET	FAC2
SZE	6,35	6,37	5,70	7,52	0,62	0,02	0,00	-0,22	5,98	0,94	1,05	0,42
UPM-PALM4U	6,35	8,32	5,70	8,75	0,60	1,97	0,31	0,04	7,27	0,89	1,28	0,45
ENEA-PMSS	6,35	4,98	5,70	5,31	0,66	-1,37	-0,22	-0,30	4,76	0,91	0,84	0,43
CERC-CIEMAT	6,35	8,20	5,70	10,69	0,67	1,85	0,29	-0,04	8,26	0,91	1,45	0,44
CERC-ADMS	6,35	3,96	5,70	4,37	0,54	-2,39	-0,38	-0,48	5,50	1,03	0,96	0,34
CIEMAT-SIMPLE	6,35	5,20	5,70	6,97	0,69	-1,15	-0,18	-0,35	5,27	0,93	0,93	0,44
CIEMAT-WINDFACTOR	6,35	6,18	5,70	8,28	0,69	-0,17	-0,03	-0,23	6,02	0,91	1,06	0,45
CIEMAT-DETAILED	6,35	5,70	5,70	7,55	0,69	-0,65	-0,10	-0,29	5,52	0,92	0,97	0,45
UOWM	6,35	5,04	5,70	7,00	0,59	-1,31	-0,21	-0,41	6,04	1,02	1,06	0,35
VITO-OPENFOAM	6,35	8,39	5,70	10,93	0,63	2,04	0,32	0,02	8,81	0,88	1,55	0,45
VITO-ATMOSTREET	6,35	6,18	5,70	7,92	0,49	-0,17	-0,03	-0,23	7,13	0,95	1,25	0,37
NILU-EPISODE	6,35	1,42	5,70	1,40	0,25	-4,94	-0,78	-0,98	7,40	1,31	1,30	0,17

- $R^2 > 0.60$ for most of the models, $R^2 < 0.60$ for UOWM (0.59), CERC-ADMS (0.54), VITO-ATMOSTREET (0.49) and NILU (0.25)
- Most of the models underpredict slightly (but NILU strongly), and few models overpredict (SZE (very slightly), UPM, CERC-CIEMAT and VITO-OPENFOAM)
- MFE values are between 0.88 and 1.31.
- FAC2 values between 0.40 and 0.45 except to CERC-ADMS, UOWM, VITO-ATMOSTREET (all of these > 0.30) and NILU (0.17)
- Target between (0.84 and 1.55)

Step 2.1. Statistics – Concentration Difference

Columna1	OBSERVED	SZE	UPM	ENEA	CERCCIE	CERCADM	CIEMATSI	CIEMATWF	CIEMATDE	UOWM	VITOFOAM	VITOATMOS	NILU
Number of values	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628
Sum	16690	16740,3	21861	13083,3	21558,8	10409	13664,2	16237,8	14988,5	13243,2	22052,2	16236,5	3719,7
Minimum	0	0	0	0	0	0	0	0	0	0	0	0	0
Maximum	29	32,9	37	21,8	54,9	18,6	36,8	43,8	39,4	35,1	46,4	36,1	6,1
Mean	6,35	6,37	8,32	4,98	8,20	3,96	5,20	6,18	5,70	5,04	8,39	6,18	1,42
Median	5	2,9	4,3	3,1	3,7	1,8	2,4	2,9	2,6	2	4	2,7	0,9
First quartile	2	0,9	1,4	0,8	1,2	0,7	0,8	0,9	0,8	0,7	1,7	1,2	0,4
Third quartile	9	9	14	7,5	11,7	6,3	6,9	8,2	7,7	6,2	10,3	7,7	2,1
Standard deviation	5,7	7,5	8,8	5,3	10,7	4,4	7,0	8,3	7,6	7,0	10,9	7,9	1,4
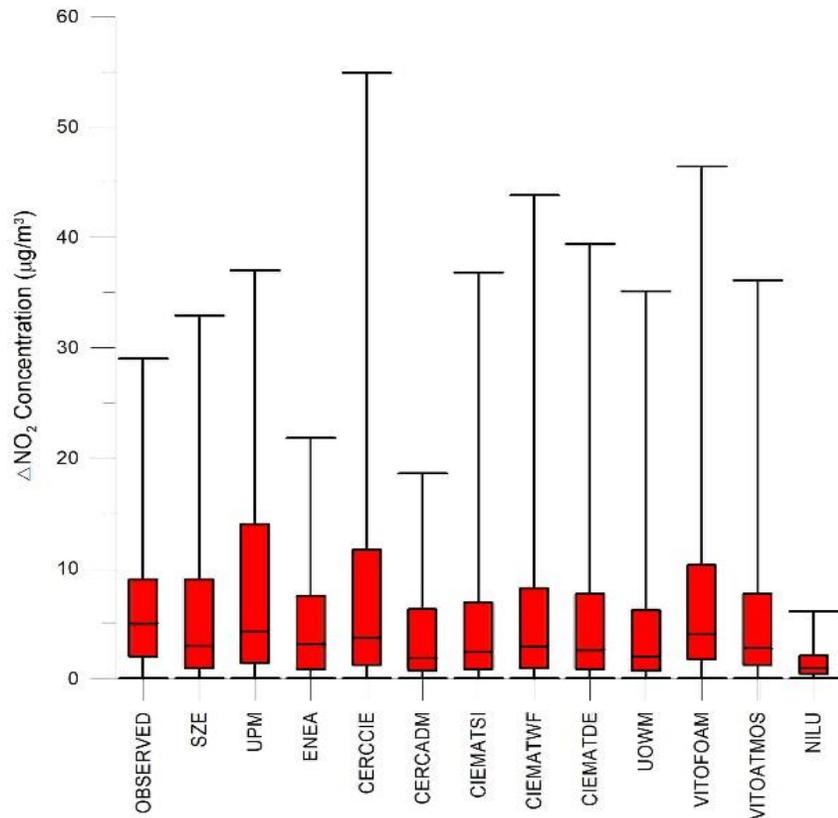
- The observed maximum ΔC is 29 µg/m^3 with a mean value close to 6 µg/m3 and a median value of 5 µg/m^3.
- ΔC median of models is lower than observed, between 0.9 µg/m^3 (NILU) and 4.3 µg/m^3 (UPM).
- Mean of predictions higher than observed (UPM, CERC-CIEMAT, VITO-OPENFOAM). Other clearly smaller (ENEA, CERC-ADMS, CIEMAT-SIMPLE, CIEMAT-DETAILED, UOWM and especially NILU).
- Some models (SZE, CIEMAT-WINDFACTOR, and VITO-ATMOS) have a mean concentration similar to the observed ΔC.
- Maximum ΔC of the models is higher in almost all cases (except ENEA, CERC-ADMS and especially NILU with a maximum of just 6 µg/m^3). In some cases, exceeding 40 µg/m^3 (CERC-CIEMAT, CIEMAT-WINDFACTOR and VITO-OPENFOAM).

Step 2.1. Histograms - Concentration Difference
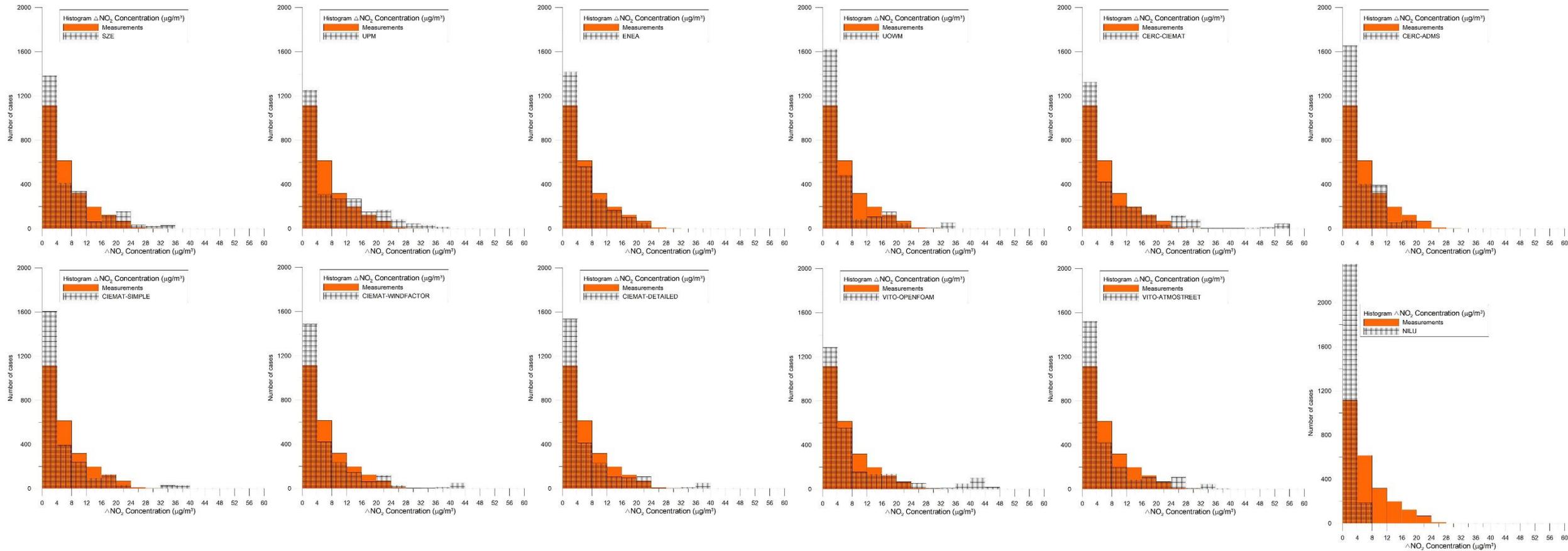
- NILU is the case that differs most from the rest of the models and the observations,
- ENEA distribution is the one that most resembles the observed one.
- There is a general tendency to have more cases of ΔC<4, less in the intermediate ranges and more in the higher ones.

Step 2.1. Statistics – Concentration Gradient

model	MEANOBS	MEANMOD	DEVOBS	DEVMOD	Correl	Bias	NMbias	MFB	RMS	MFE	TARGET	FAC2
SZE	23,97	23,29	36,41	44,21	0,75	-0,68	-0,03	-0,21	29,44	0,94	0,81	0,41
UPM	23,97	31,11	36,41	53,13	0,73	7,14	0,30	0,04	37,10	0,90	1,02	0,44
ENEA	23,97	18,25	36,41	30,10	0,75	-5,72	-0,24	-0,30	24,85	0,91	0,68	0,42
CERC-CIEMAT	23,97	31,51	36,41	75,55	0,69	7,54	0,32	-0,04	57,32	0,92	1,57	0,43
CERC-ADMS	23,97	13,77	36,41	24,54	0,63	-10,20	-0,43	-0,48	30,20	1,03	0,83	0,33
CIEMAT-SIMPLE	23,97	20,08	36,41	49,93	0,70	-3,89	-0,16	-0,34	35,94	0,94	0,99	0,43
CIEMAT-WINDFACTOR	23,97	23,87	36,41	59,42	0,70	-0,10	0,00	-0,23	42,79	0,91	1,18	0,44
CIEMAT-DETAILED	23,97	21,94	36,41	53,32	0,71	-2,03	-0,09	-0,28	37,72	0,93	1,04	0,43
UOWM	23,97	19,87	36,41	50,53	0,60	-4,10	-0,17	-0,40	41,19	1,03	1,13	0,34
VITO-OPENFOAM	23,97	33,35	36,41	74,30	0,72	9,39	0,39	0,03	54,94	0,88	1,51	0,44
VITO-ATMOSTREET	23,97	22,06	36,41	42,83	0,63	-1,91	-0,08	-0,22	34,67	0.95	0,95	0.36
NILU	23,97	4,85	36,41	6,40	0,47	-19,12	-0,80	-0,98	38,92	1,32	1,07	0,16

- R^2 are significantly higher for ∇C than for ΔC for all models.
- Some models have a very little bias (SZE, CIEMAT-WINDFACTOR), others have strong negative BIAS (underprediction) (CERC-ADMS, NILU), while ENEA, CIEMAT-SIMPLE, CIEMAT-DETAILED, UOWM and VITO-ATMOSTREET have lower negative Bias (slight underprediction). UPM, CERC-CIEMAT and VITO-OPENFOAM overpredict significantly.
- MFE values are between 0.88 and 1.32.
- FAC2 values between 0.40 and 0.45 except to CERC-ADMS, UOWM, VITO-ATMOSTREET (all of these > 0.30) and NILU (0.16)
- Target between (0.68 ENEA and 1.51)

Step 2.1. Statistics – Concentration Gradient

| Columna1	OBSERVED	SZE	UPM	ENEA	CERCCIE	CERCADM	CIEMATSI	CIEMATWF	CIEMATDE	UOWM	VITOFOAM	VITOATMOS	NILU
Number of values	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628	2628
Sum	62987,5	61204,7	81754,2	47963,5	82799,3	36175,6	52768	62736,8	57661,3	52208,9	87654,5	57972,5	12736
Minimum	0	0	0	0	0	0	0	0	0	0	0	0	0
Maximum	404,9	625.3	845,2	378,1	2042,4	514,3	1355,2	1615,2	1406,6	1480,2	1296,9	985,5	131,6
Mean	24,0	23,3	31,1	18,3	31,5	13,8	20,1	23,9	21,9	19,9	33,4	22,1	4,8
Median	12,4	9,1	13,5	8	10,9	4,9	7	8,3	7,6	5,2	10,6	7,7	2,7
First quartile	5,4	2,6	3,7	2,4	3,6	2,1	2,3	2,8	2,5	1,8	4,0	2,9	0,9
Third quartile	27,1	25,6	34,1	21,7	29,6	16,4	18,8	22,5	20,8	16,8	30,6	21,6	6,5
Standard deviation	36,4	44,2	53,1	30,1	75,6	24,5	49,9	59,4	53,3	50,5	74,3	42,8	6,4
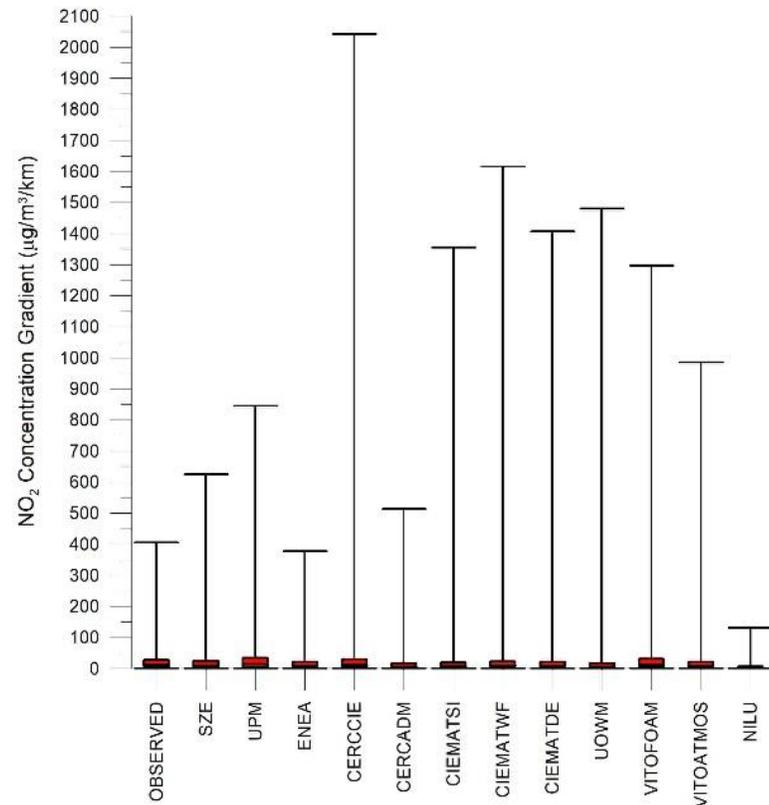
- The SD of ∇C is greater than the SD observed in almost all models except ENEA and especially NILU (15% of the observed SD). The SD of CERC-CIEMAT and VITO-OPENFOAM double that observed and the rest of the models have an SD between 17 and 60% greater than the observed SD.
- Only the mean of VITO-OPENFOAM is higher than observed mean.
- Maximum ∇C of the models is higher in almost all cases (except ENEA, and especially NILU with a maximum of just 30% of what was observed). CERC-CIEMAT predicts maximum ∇C 5 times higher than the observed, while other models (CIEMAT, UPM, UOWM, VITO-OPENFOAM) over-predict it by a factor of 2 to 4.

# Step 2.1. Histograms - Concentration Gradient
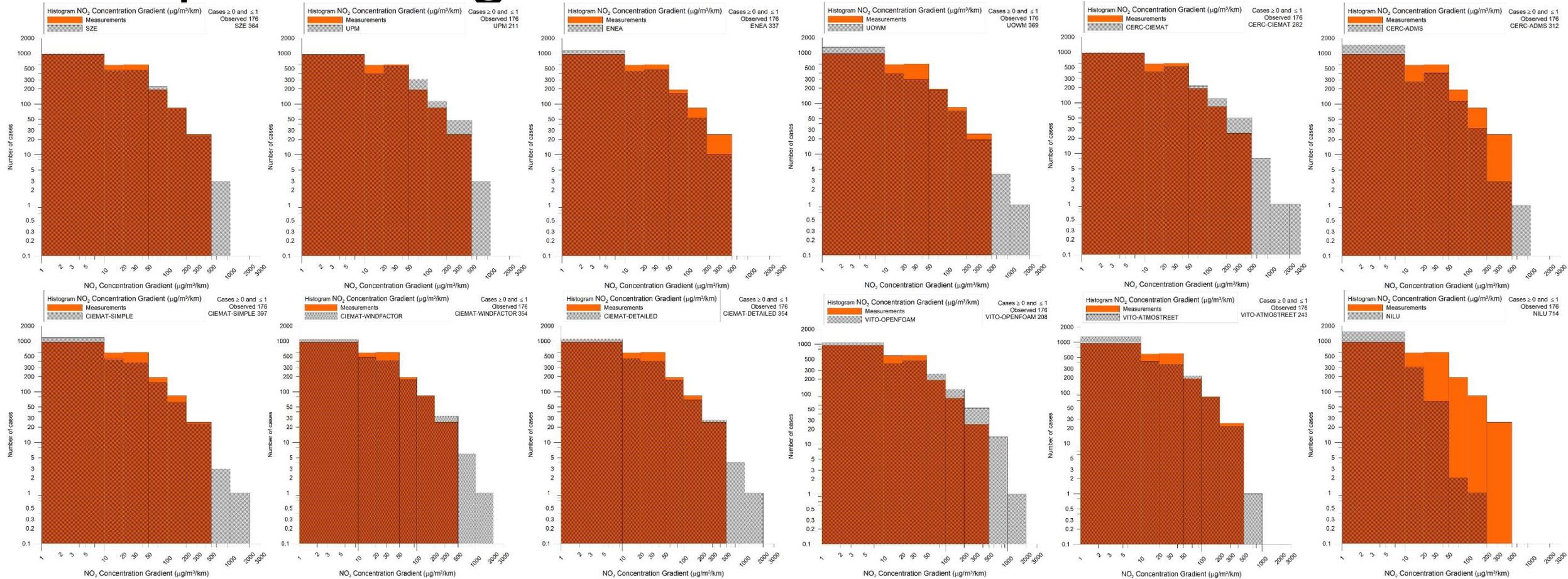
- CFD models relative to the observed ∇C tend to have fewer cases of low ∇C and more of high ∇C, but in many cases this difference is not large.
- Non-CFD models tend to have more cases than the observed ones of low ∇C and less of high ∇C, this is very evident in the case of NILU.
- ENEA seems to be the model than fits better the observed histogram of ∇C.

Step 2.1. Variogram
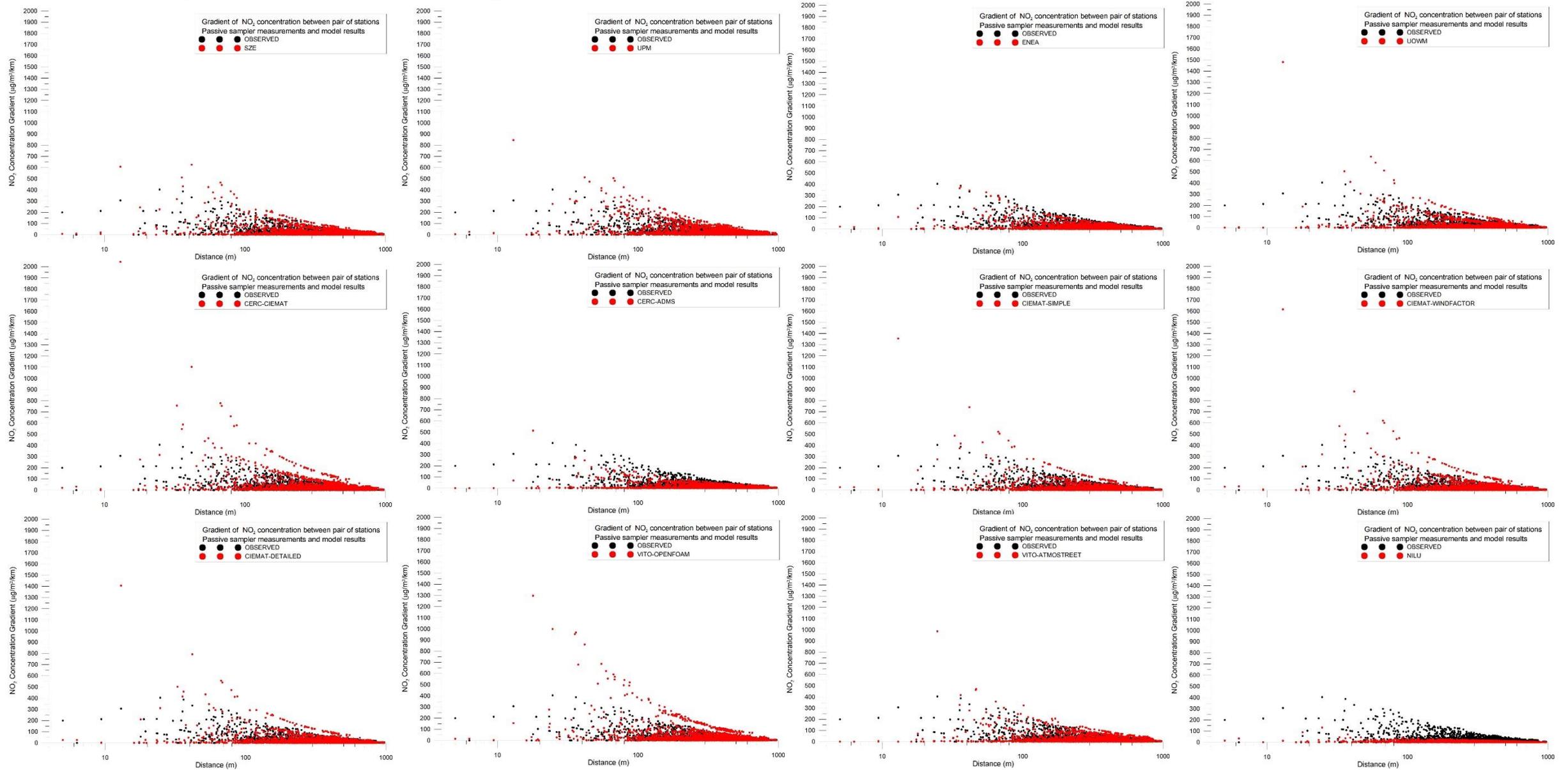
Step 2.1. Scatter-Plots – Concentration Gradient
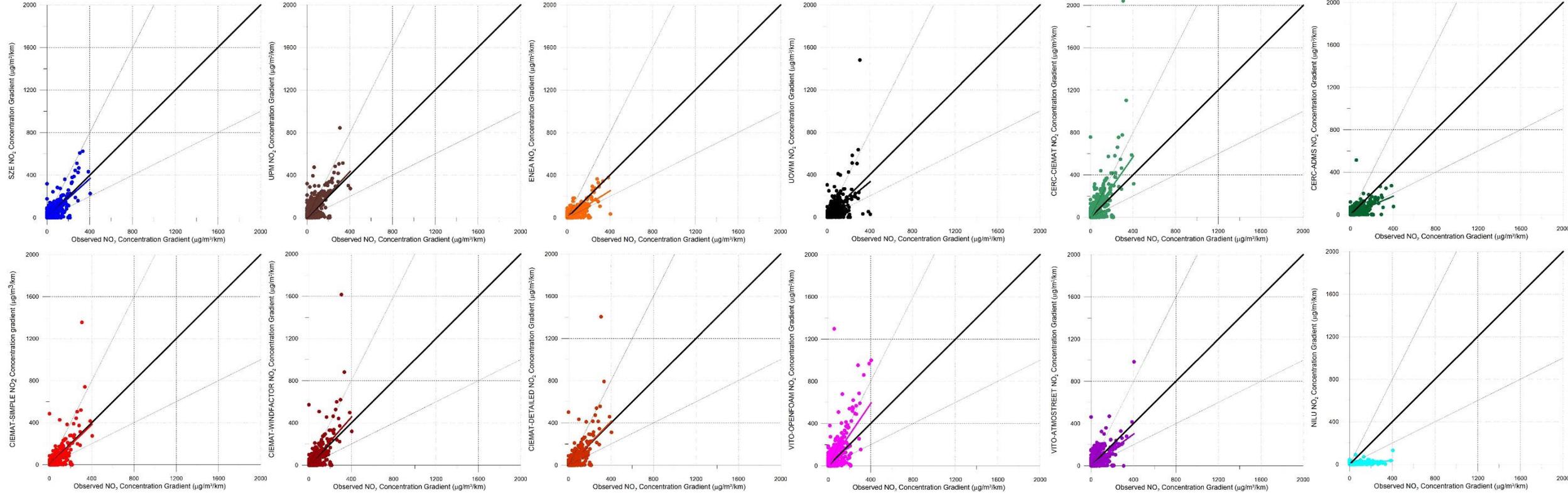
- Taking into account the statistics and scatter plots, most of the models (especially the CFD models) seem to predict ∇C fairly well.
- NILU models seems to provide worse results with very low spatial variability in the predicted concentrations.

Step 2.1. Comments

- Most of the models (especially the CFD models) seem to predict fairly good the monthly-averaged concentrations.

- Most of the models (mainly CFD) seem to predict ∇C pretty well.

- Most of models (except NILU-EPISODE and ENEA-PMSS) predict higher ∇C than the maxima observed ∇C.

- In general, the CFD models seem to simulate better the spatial distribution of the monthly averaged concentrations than other simpler approaches.