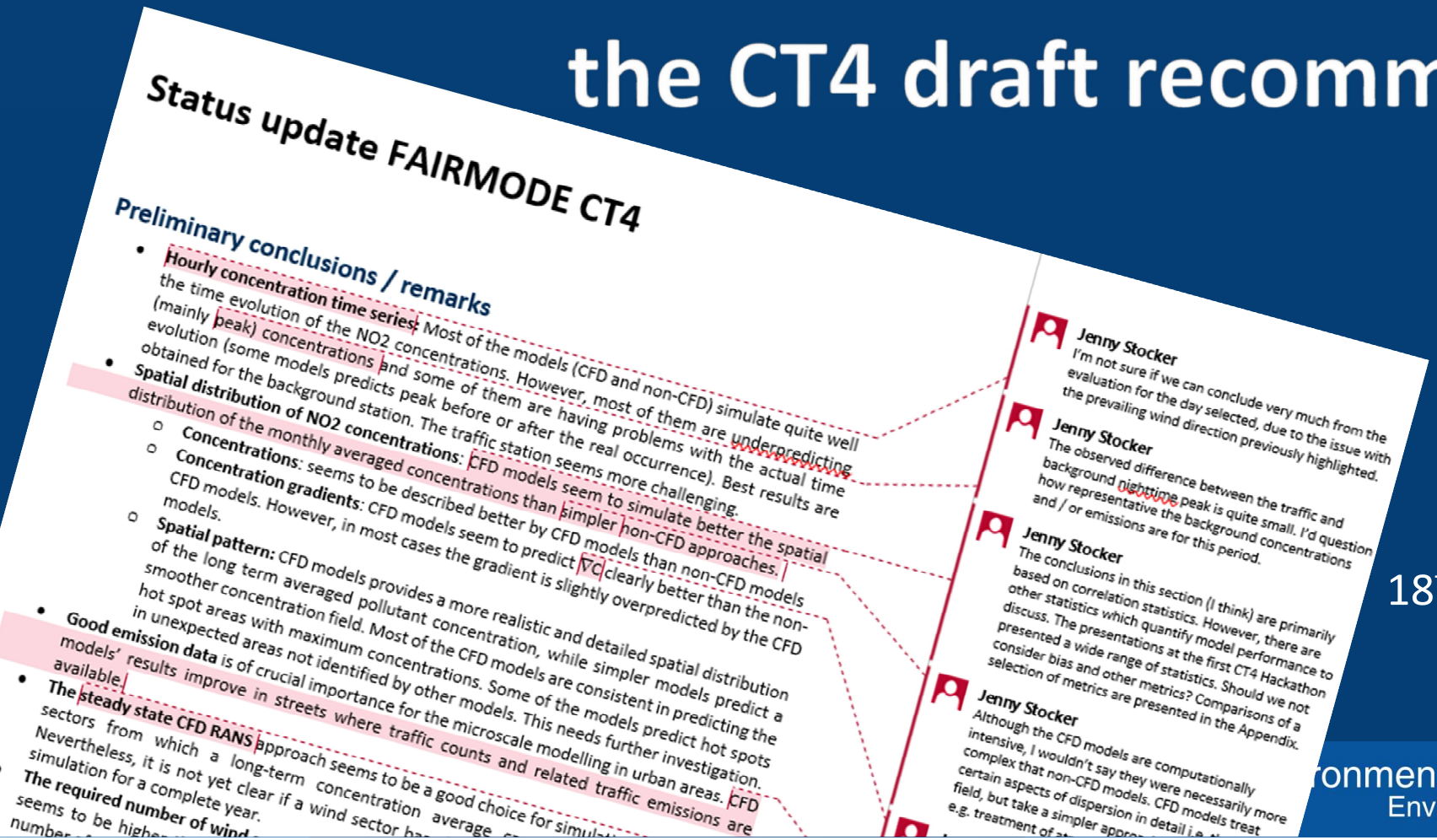
A Gaussian modeller's comments on the CT4 draft recommendations



Status update FAIRMODE CT4

Preliminary conclusions / remarks

- **Hourly concentration time series:** Most of the models (CFD and non-CFD) simulate quite well the time evolution of the NO2 concentrations. However, most of them are underpredicting (mainly peak) concentrations and some of them are having problems with the actual time evolution (some models predicts peak before or after the real occurrence). Best results are obtained for the background station. The traffic station seems more challenging.
- **Spatial distribution of NO2 concentrations**: CFD models seem to simulate better the spatial distribution of the monthly averaged concentrations than simpler non-CFD approaches.
  - **Concentrations**: seems to be described better by CFD models than non-CFD models
  - **Concentration gradients**: CFD models seem to predict VC clearly better than the non-CFD models. However, in most cases the gradient is slightly overpredicted by the CFD models.
  - **Spatial pattern:** CFD models provides a more realistic and detailed spatial distribution of the long term averaged pollutant concentration, while simpler models predict a smoother concentration field. Most of the CFD models are consistent in predicting the hot spot areas with maximum concentrations. Some of the models predict hot spots in unexpected areas not identified by other models. This needs further investigation.
- **Good emission data** is of crucial importance for the microscale modelling in urban areas. CFD models' results improve in streets where traffic counts and related traffic emissions are available.
- **The steady state CFD RANS** approach seems to be a good choice for simul
- **The required number of wind** sectors from which a long-term concentration average Nevertheless, it is not yet clear if a wind sector ba simulation for a complete year. seems to be higher

Jenny Stocker
I'm not sure if we can conclude very much from the evaluation for the day selected, due to the issue with the prevailing wind direction previously highlighted.

Jenny Stocker
The observed difference between the traffic and background nighttime peak is quite small. I'd question how representative the background concentrations and / or emissions are for this period.

Jenny Stocker
The conclusions in this section (I think) are primarily based on correlation statistics. However, there are other statistics which quantify model performance to discuss. The presentations at the first CT4 Hackathon presented a wide range of statistics. Should we not consider bias and other metrics? Comparisons of a selection of metrics are presented in the Appendix.

Jenny Stocker
Although the CFD models are computationally intensive, I wouldn't say they were necessarily more complex that non-CFD models. CFD models treat certain aspects of dispersion in detail i.e. field, but take a simpler appro e.g. treatment of

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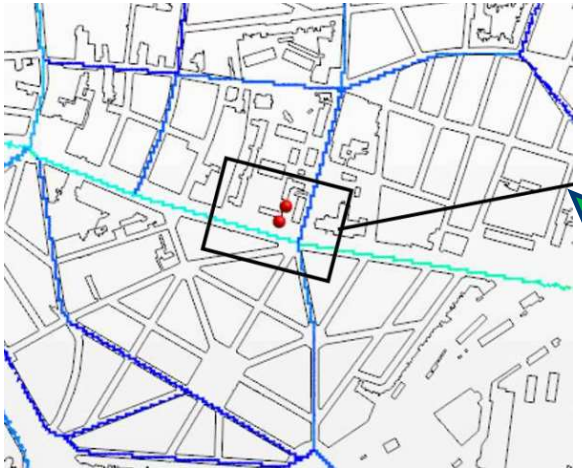
@ FAIRMODE
18th – 20th October 2022

ronmental Research Consultants
Environmental Software and Services

Comments on the 'conclusions' from Task 1

I'm not sure if we can conclude very much from the evaluation for the day selected, due to the issue with the prevailing wind direction previously highlighted i.e. the wind blows from the urban background monitor to the roadside monitor



- **Hourly concentration time series**: Most of the models (CFD and non-CFD) simulate quite well the time evolution of the NO2 concentrations. However, most of them are underpredicting (mainly peak) concentrations and some of them are having problems with the actual time evolution (some m ls predicts peak before or after the real occurrence). Best results are obtained for the b nd station. The traffic station seems more challenging.

The observed difference between the traffic and background nighttime peak is quite small. I'd question how representative the background concentrations and / or emissions are for this period.

Could we have selected a 'better' hourly time series to model?

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Comments on the 'conclusions' from Task 2

The conclusions in this section (I think) are primarily based on correlation statistics. However, there are other statistics which quantify model performance to discuss. The presentations at the first CT4 Hackathon presented a wide range of statistics. Should we not consider bias and other metrics? Comparisons of a selection of metrics are presented in the [in the following slides].

- **Spatial distribution of NO2 concentrations**: CFD models seem to simulate better the spatial distribution of the monthly averaged concentrations than simpler non-CFD approaches.

Although the CFD models are computationally intensive, I wouldn't say they were necessarily more complex that non-CFD models. CFD models treat certain aspects of dispersion in detail i.e. the flow field, but take a simpler approach to other aspects e.g. treatment of atmospheric stability and chemistry.

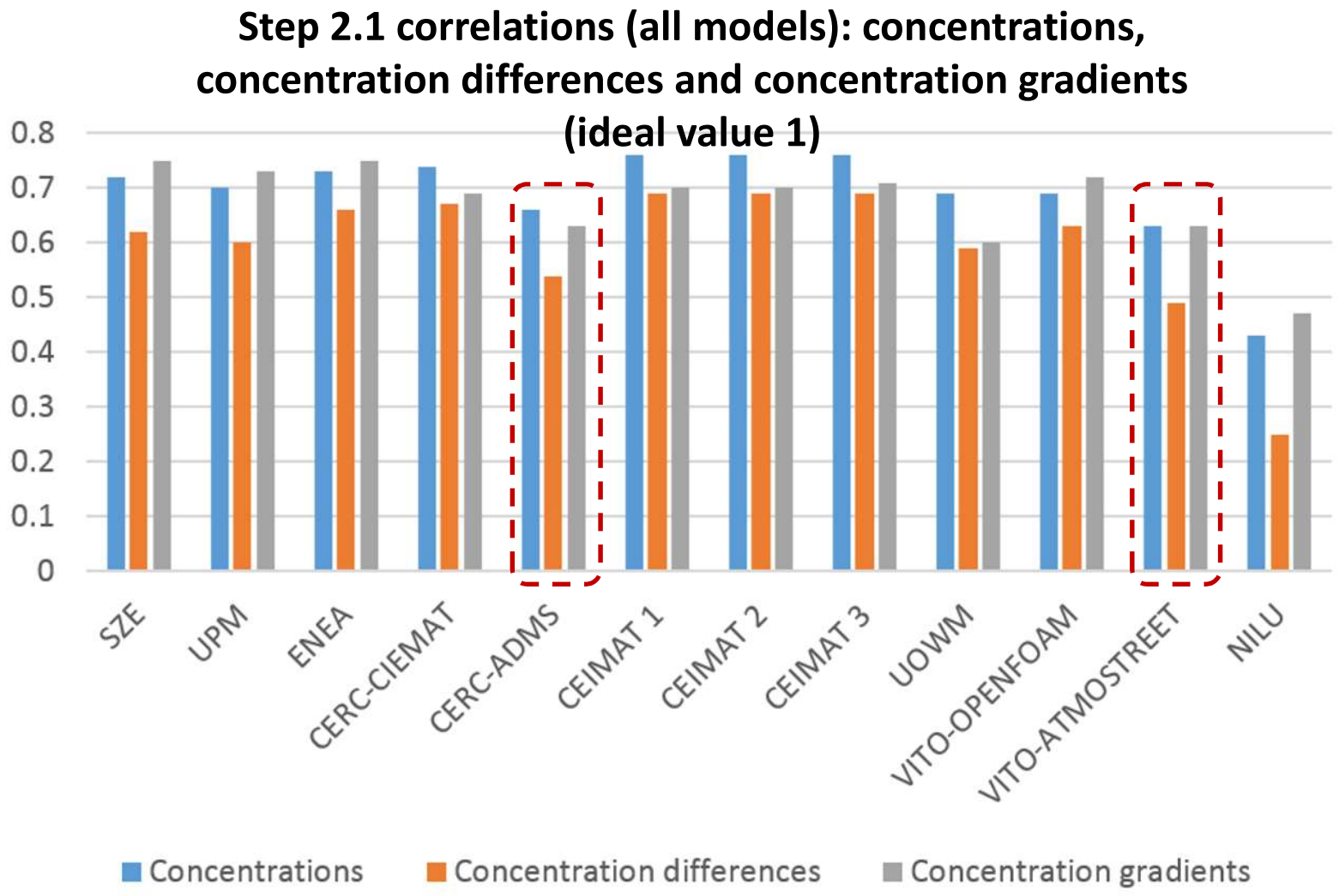
Need to define ∇C

CFD models seem to predict ∇C clearly better

CERC

Additional analysis of Step 2.1 statistics

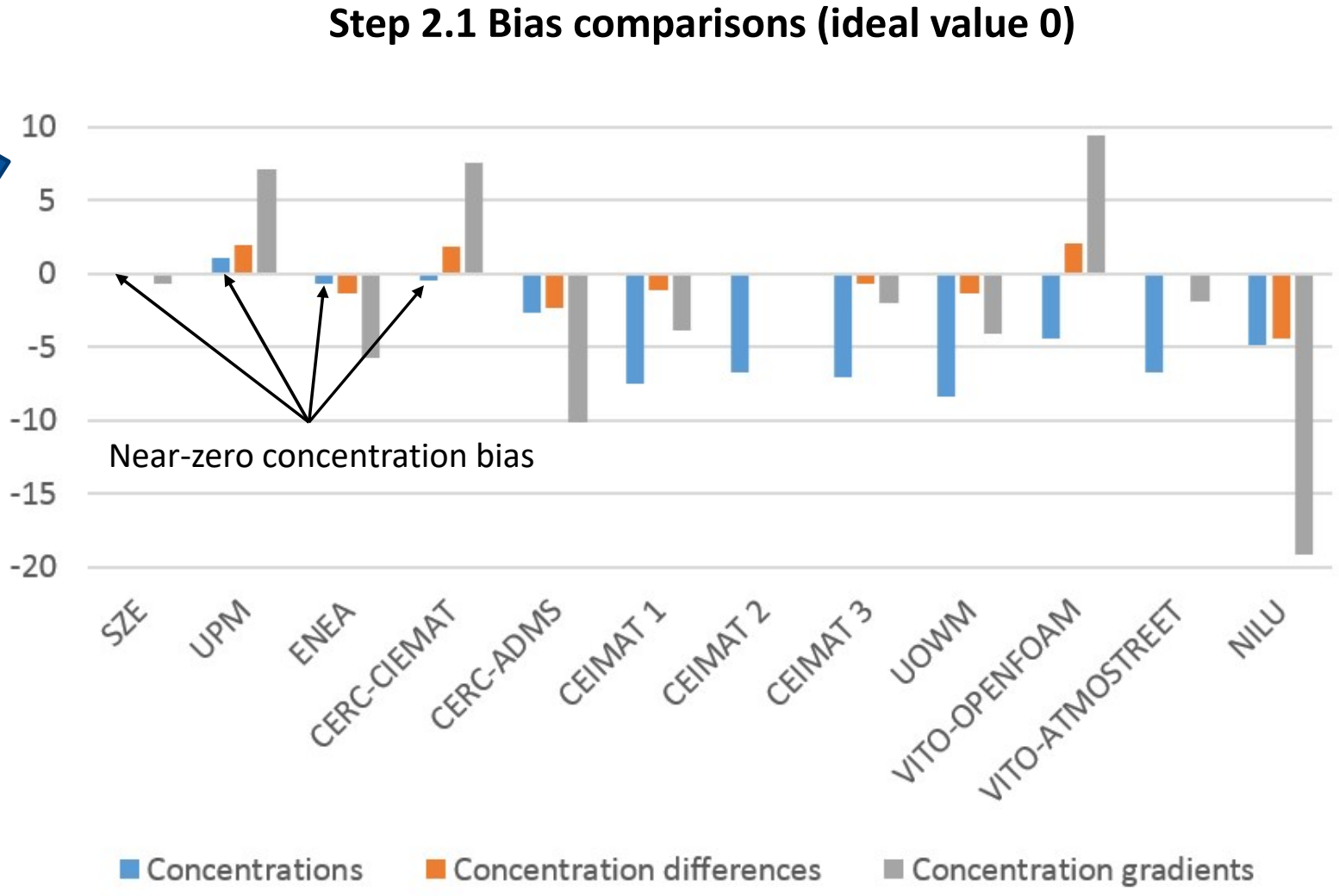
Correlations indicate that the CFD consistently predict better spatial spreads of NO2 than the 'simpler' models, but the difference between CFD and the better 'simpler' models isn't large e.g. CERC-ADMS, VITO-ATMOSTREET



CERC

Additional analysis of Step 2.1 statistics

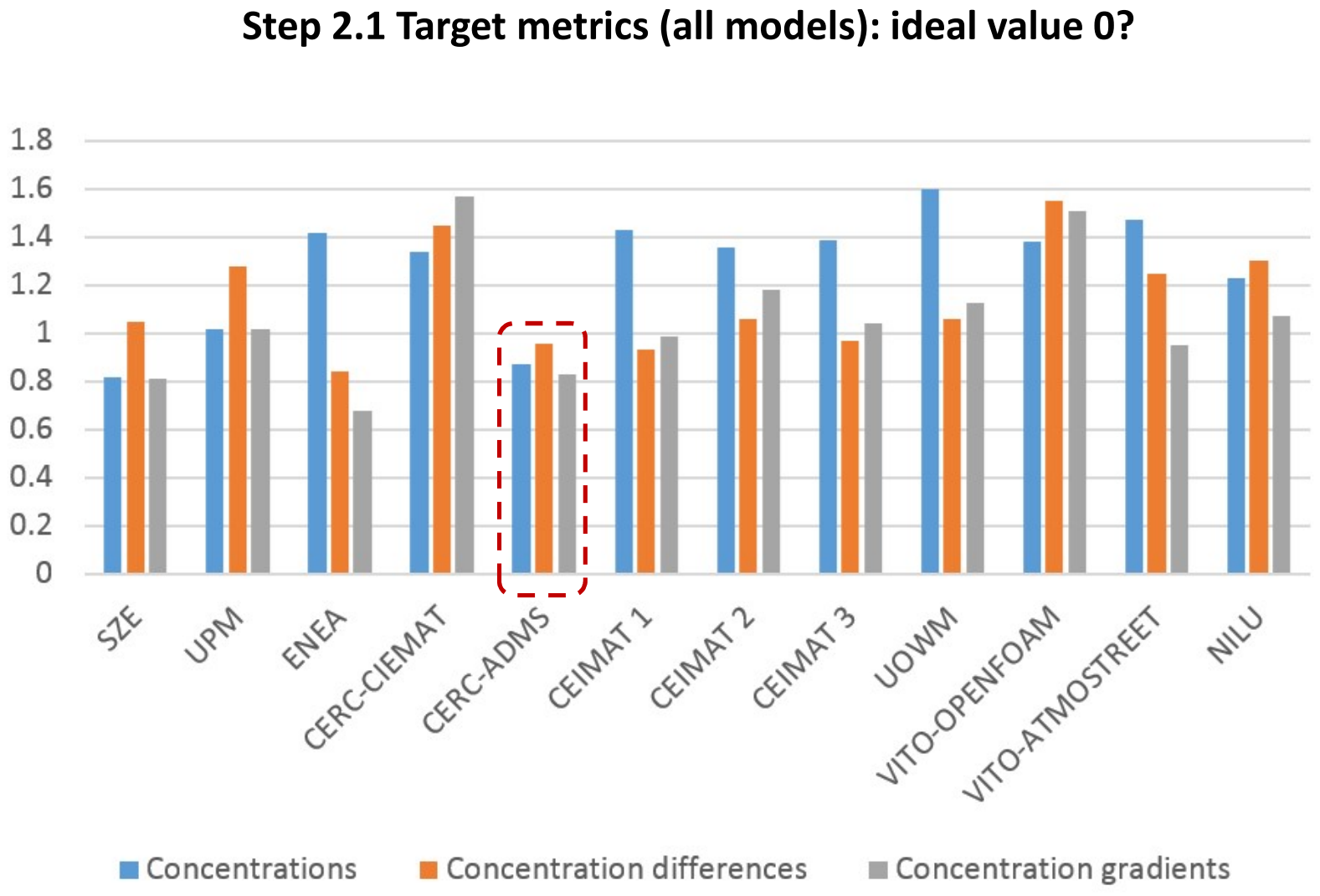
The bias plot suggests (to me) that some of the results are calibrated. This is definitely the case for CERC-CEIMAT, where the concentration bias is close to zero. Is this also true for SZE? And any of the other models? Do any of the calibrations have a spatial component?



CERC

Additional analysis of Step 2.1 statistics

The comparisons of the Target metrics (Figure 3) show that the 'simpler' ADMS model performs well and consistently. However, I'm not sure what the Target metric is for this dataset - and I'm assuming the ideal value is 0?



CERC

A Gaussian modeller's comments on the CT4 draft recommendations

Comments on the 'conclusions' from Task 2

- **Good emission data** is of crucial importance for the microscale modelling in urban areas. CFD models' results improve in streets where traffic counts and related traffic emissions are available.

I'd be more forceful about this. Modelled concentrations in the vicinity of roads not included in the emissions inventory are likely to be poor. For detailed AQ modelling studies such as those involving CFD simulations, emissions inventories should include emissions estimates from as many roads as possible, because the influence of flow field on dispersion may amplify the concentrations to generate hotspots even on low trafficked roads.

- Simulated wind sectors with only **one reference wind speed** could be sufficient for computing long-term average concentrations. The 1/v dependency of concentrations is a fair approach

I may have missed it but have we done a comparison of a study where more than one reference wind speed is used, and compared the results to a one wind speed case?
PRESENTED YESTERDAY

Maybe that any guidance note needs a summary of CFD model types.

- **The steady state CFD RANS** approach seems to be a good choice

CERC

Comments on the Pending questions

- Are the data recorded at a limited number of AQ monitoring stations sufficient to evaluate the methodology performance at microscale?

For this study, the passive sampler network seems to have generated the majority of the evaluation results. Certainly, the analyses of the spatial spread of concentrations has been informative. For this study, it may be that comparison at continuous monitors (Task 1) could have been extended to cover a longer time period. But for subsequent studies, if data from a higher density of continuous monitors or sensor were available then the spatial analyses (Task 2.1) could be done for multiple instances, for example each wind direction modelled.

- Are the investigated models/methodologies good enough to compute other indicators besides average concentrations, that is: maxima/peak concentrations or high percentiles? FAIRMODE MQO could be used for such an evaluation.

How does this relate to the Target statistics presented in Step 2.1?