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 undergredicting Hourly concentration time series: Most of the models (CFD and non-CFD) simulate quite with the time evolution of the NO2 concentrations. However, most of them are baving problems are baving problems are baving problems are baving problems with the actual time. the time evolution of the NO2 concentrations. However, most of them are undergregoried (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 (mainly peak) concentrations and some of them are having problems with the actual time obtained for the harkoronind station. The traffic station seems more challenoing. Best results are Jenny Stocker evolution (some models predicts peak before or after the real occurrence). best I'm not sure if we can conclude very much from the 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 kimpler hom cfn annroaches I'm not sure in we can conclude very induct in our same evaluation for the day selected, due to the issue with Spatial distribution of NO2 concentrations: CFD models seem to simulate better the simulate better the simulate better the second batter by CFD models than bimpler hon-CFD approaches in the second batter by CFD models than non-CFD approaches in the second batter by CFD models evaluation in the vary selected, one to the laster interview of the prevailing wind direction previously highlighted. Sution of the monthly averaged concentrations than simpler hon-CFD approaches (Concentrations: seems to be described better by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models coordinated by CFD models than non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (Concentration gradiente: CFD models than the non-CFD models (CFD models than the non-CFD models (CFD models than the non-CFD models than the non-CFD models (CFD models than the non-CFD models than the non-CFD models (CFD models than the non-CFD models than the non-CFD models (CFD models than the non-CFD models than the non-CFD models than the non-CFD models than the non-CFD models (CFD models than the non-CFD models the Jenny Stocker Concentrations: seems to be described better by CFD models than non-CFD models Concentration gradients: CFD models seem to predict VC clearly better than non-CFD models CFD models Linuxeurar in more cases the gradient is clightly outermadicted by the CFD The observed difference between the traffic and hackground Dighting Peak is quite small, I'd question Concentration gradients: CFD models seem to predict VG clearly better than the non-CFD models. However, in most cases the gradient is slightly overpredicted by the CFD model. **Jenny Stocker** background Oleptions peak is quite striam. I is question how representative the background concentrations and / or emissions are for this period. Models. **Spatial pattern:** CFD models provides a more realistic and detailed spatial distribution of the long term averaged nollistant concentration while cimuler models provides a models and detailed spatial distribution @ FAIRMODE Spatial pattern: CFD models provides a more realistic and detailed spatial distribution of the long term averaged pollutant concentration, while simpler models predict a concentration, while simpler models predict a models are concentration prediction to predict a concentration of the cen models are concentration of the centration of Jenny Stocker The conclusions in this section (I think) are primarily 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 concentrations of the models are consistent in predicting the models models models models models models to the models models models are consistent in the models of the models models models models are consistent in the models of the models models models are consistent in the models of the models models models are consistent in the models models are consistent in the models models are consistent in the models are consistent in the models models are consistent in the models are co based on correlation statistics. However, there are Smoother concentration field. Most of the CFD models are consistent in predicting the for spot areas with maximum concentrations. Some of the models predicting the insumarian areas not identified by other models. This needs further investigation <u>18th – 20th October 2022</u> other statistics which quantify model performance to hot spot areas with maximum concentrations. Some of the models predict not spot in unexpected areas not identified by other models. This needs further investigation anticeing data is of criscial importance for the microscale modelling in urban areas in the investigation. in unexpected areas not identified by other models. This needs further investigation and the second discuss. The presentations at the first CT4 Hackathon Discuss, The presentations at the matter that the resentation presented a wide range of statistics. Should we not Good emission data is of crucial importance for the microscale modelling in urban areas. CPU available i Presenteu a vriue range un statistica, unuum vrente Consider bias and other metrics? Comparisons of a consider blas and other metrics : من المعالية من ع selection of metrics are presented in the Appendix. available The steady state CFD RANS Bpproach seems to be a good choice for simulation certains from which a long-term concentration and the statement of the Q Jenny Stocker sectors from which a long-term concentration average Although the CFD models are computationally Nevertheless, it is not yet clear if a wind sector has menough the cromotions are computationally intensive, I wouldn't say they were necessarily more intensive, I wouldn't say they were necessarily mo complex that non-CFD models. CFD models treat simulation for a complete year. certain aspects of dispersion in detail i.e. onmental Research Consultants The required number of wind field, but take a simpler approx seems to be higher **Environmental Software and Services** e.g. treatment of a

.

A Gaussian modeller's comments on the CT4 draft recommendations 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 models predicts peak before or after the real occurrence). Best results are obtained for the base of station. The traffic station seems more challenging.

CERC

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? A Gaussian modeller's comments on the CT4 draft recommendations 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 VC clearly better

CERC

A Gaussian modeller's comments on the CT4 draft recommendations 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**



Step 2.1 correlations (all models): concentrations, concentration differences and concentration gradients

CERC

A Gaussian modeller's comments on the CT4 draft recommendations 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

Step 2.1 Bias comparisons (ideal value 0)



A Gaussian modeller's comments on the CT4 draft recommendations 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

Concentrations
Concentration differences
Concentration gradients

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.

CERC

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

A Gaussian modeller's comments on the CT4 draft recommendations **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?

