Full year simulations vs scenarios simulations in the SZE pollution model

László Környei, Zoltán Horváth, Bence Liszkai
Széchenyi István University,
Győr, Hungary

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Unsteady microscale simulations
Dispersion model in **OpenFOAM**

1. Wind field computation: URANS with k-eps turbulence model for incompressible fluids

$$\nabla\cdot(\rho\mathbf{u}) = 0$$

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = \mathbf{g} + \nabla\cdot\overline{(\tau)} - \nabla\cdot(\rho\mathbf{R})$$

$$\frac{D}{Dt}(\rho k) = \nabla\cdot(\rho D_k \nabla k) + P - \rho\epsilon$$

$$\frac{D}{Dt}(\rho\epsilon) = \nabla\cdot(\rho D_\epsilon \nabla\epsilon) + \frac{C_1\epsilon}{k}\left(P + C_3\frac{2}{3}k\nabla\cdot\mathbf{u}\right) - C_2\rho\frac{\epsilon^2}{k}$$

- Steady simulations are also used (e.g. for the initial state)
- Boundary conditions: inlet conditions based on interpolated, time-dependent ECMWF wind data or generated from logarithmic wind profile, zero-gradient outflow.

2. Dispersion computation:

- s: NOx concentration from emission calculated with scalar transport with volumetric source S_s

$$\frac{\partial}{\partial t}s + \nabla\cdot(\mathbf{u}s) - \nabla\cdot(D_s\nabla s) = S_s$$

- D_s (mixing coeff.): Function of turbulent viscosity (from URANS) and PBL-height (from ECMWF met. sim.):

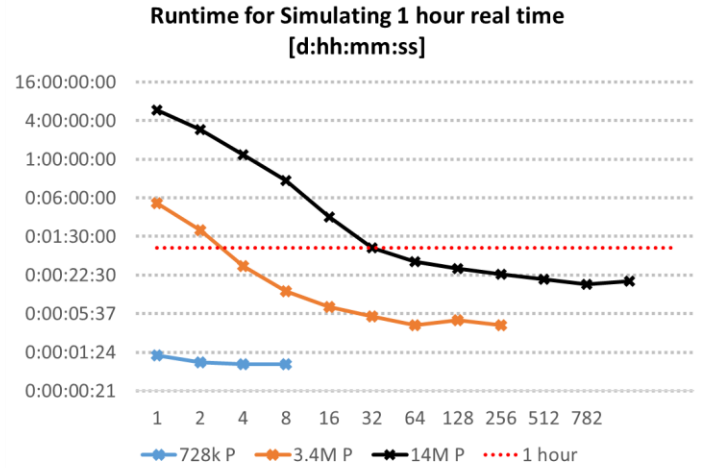
$$D_s = D_0 + b\cdot\nu_t h_{PBL}, \qquad D_0, b \text{ const.}, \ \nu_t = C_\mu\frac{k^2}{\epsilon}$$

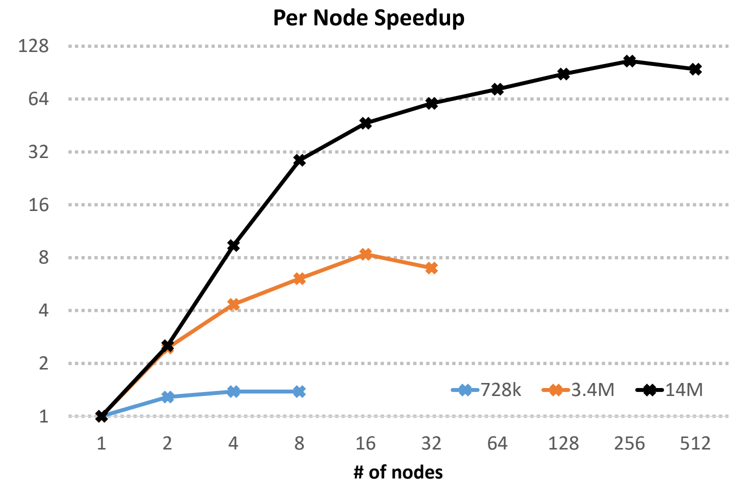
- NOx value = s + background concentrations (which is given by the user or from CAMS CDS data)
- NOx is converted to NO2 by multiplying NOx and reference time series of meas. for the NO2 / NOx ratio

Unsteady microscale simulations
Parallel performance in **OpenFOAM**

Benchmarking for scalability for the NO2 simulation to Győr

- Computer: Hawk, HLRS (5632 x 2 x 64 core AMD Rome 7702), 1 node=128 core
- Mesh sizes 728k, 3.4M, 14M, which mean 4 meter, 2 meter, 1 meter ground level resolution, resp.
- Code is optimized (in collab. with EXCELLERAT CoE): ca.10 times faster than the initial settings





Mesh size | resolution	Time for simulation of 1 physical day	Time for simulation of 1 physical year	Estimated Sim. Cost on Hawk (1 node hour = €1.13)
728k (Gyor) | 4 meter	0.4 hour (on 4 nodes)	5.6 days (on 4 nodes)	€540
3.4M (Gyor) | 2 meter	1.5 hours (on 16 nodes)	22.7 days (on 16 nodes)	€8.800
14M (Gyor) | 1 meter	6.5 hour (on 256 nodes)		

Unsteady microscale simulations
Accuracy and performance characteristics for a **full year**

Participation in the CT4 Antwerp intercomparison exercise with OpenFOAM

The simulation, including evaluations of the indicators

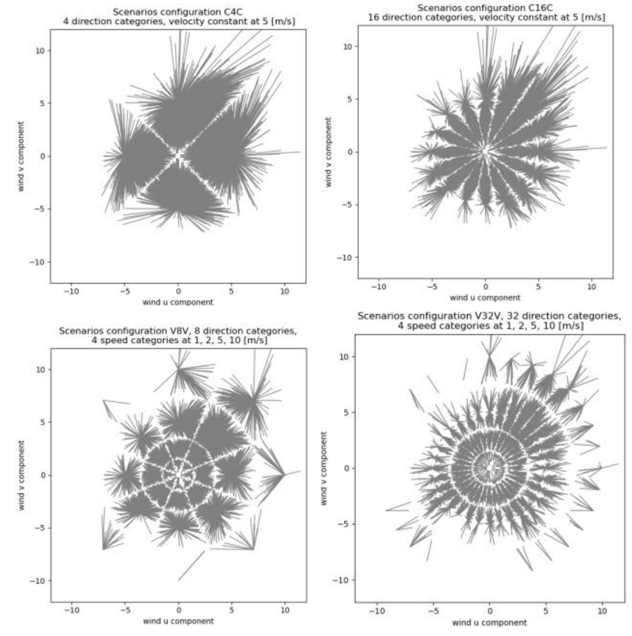
- done consecutively, 12 times one month
- Hardware: Solyom (local cluster in Győr) and on Irene (PRACE cluster in France)
- Simulation time for 1 month: 34.4 hours (on Solyom), 25 hours (on Irene)
- Antwerp, #cells = 3.3M octree, mesh resolution = 2 m (at ground level)
- PBL height from ECMWF (coupled through Polytope API)
- Output data size = 120GB per month, 1.4 TB in total

Simulation re-done mid-October 2022 due to failure in some input data.

- Accuracy from the hourly values of the computations for January 2016: median of the relative errors is 13% (backgr. station) and 30% (street station).

Steady microscale simulations
Scenario setups and simulations

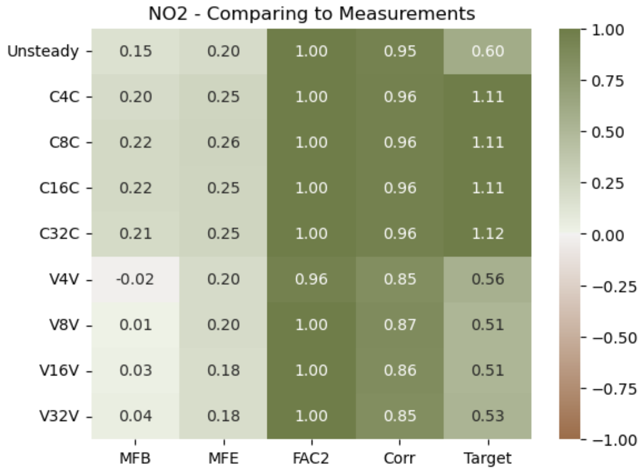
- 128 scenario setup:
  - 32 wind directions, 4 wind speeds: 1, 2, 5, 10
- Two types of scenario setups:
  - Constant velocity scenarios,
    mapped to 5m/s in 4, 8, 16, 32 directional tiling
  - Variable velocity scenarios
    mapped to 1, 2, 5 and 10 m/s with 4, 8, 16 or 32 directions
- Scenario evaluation and NO2 calculation:

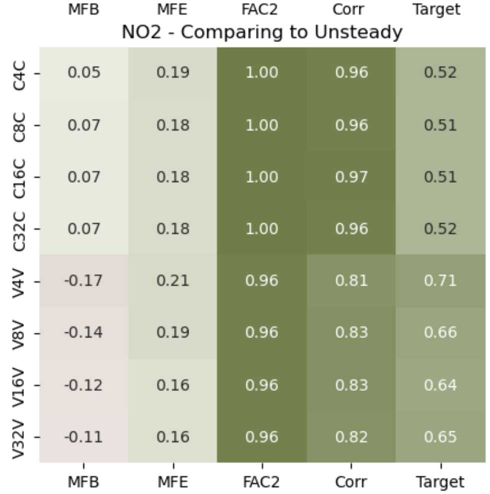


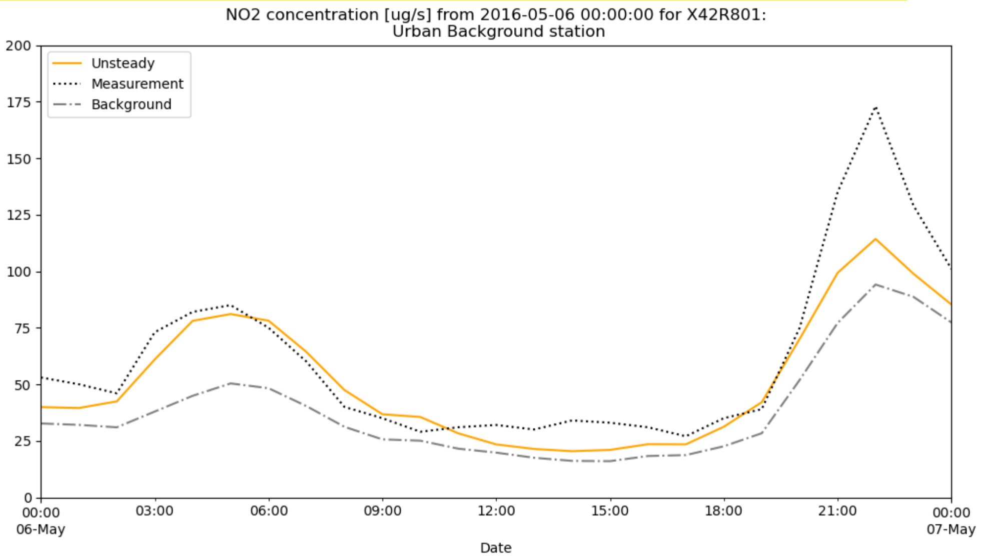
$$NO2_{approx} = F_w(t) \cdot F_m(t) \cdot F_h(t) \cdot NOx_{scenario} \cdot \frac{V_{scenario}}{V(t)} \cdot \frac{NO2_{station}(t)}{NOx_{station}(t)} + BackGroundNO2(t)$$

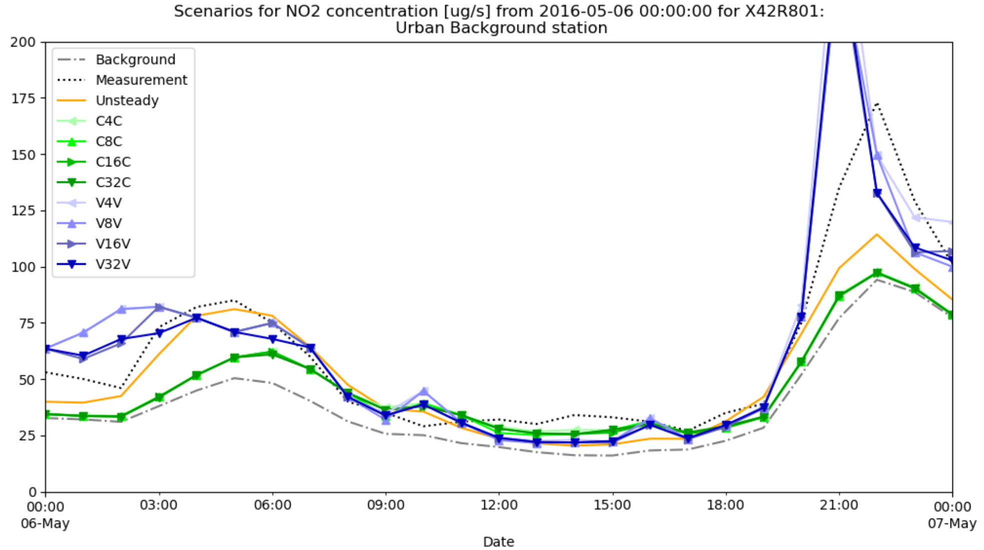
$$AVG(NO2_{approx}) = AVG\left(F_w(t) \cdot F_m(t) \cdot F_h(t) \cdot NOx_{scenario} \cdot \frac{V_{scenario}}{V(t)} \cdot \frac{NO2_{station}(t)}{NOx_{station}(t)}\right) + AVG\left(BackGroundNO2(t)\right)$$

Results – Stage1 – May 6th – Urban Background

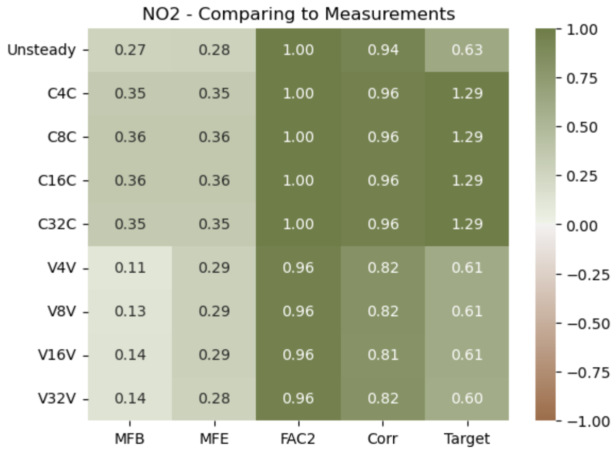


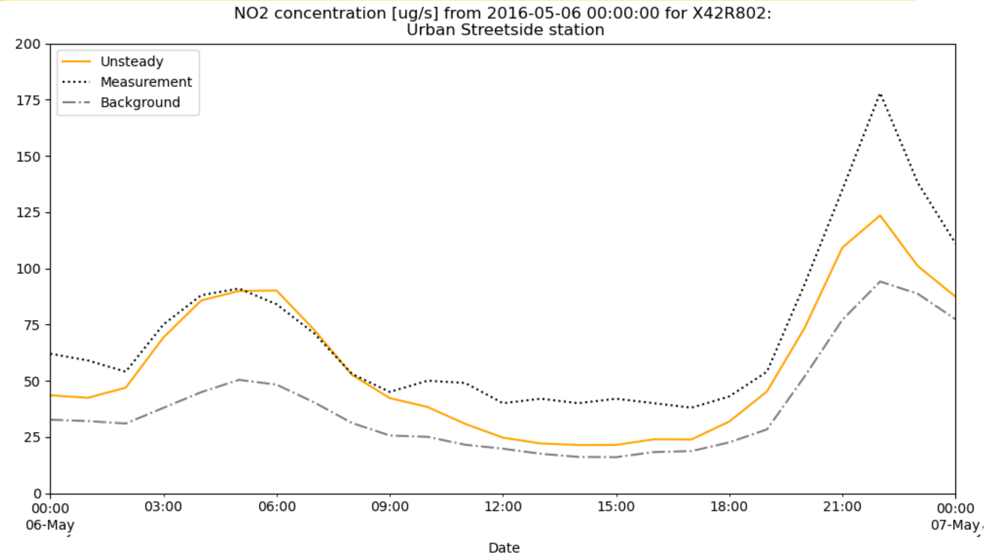


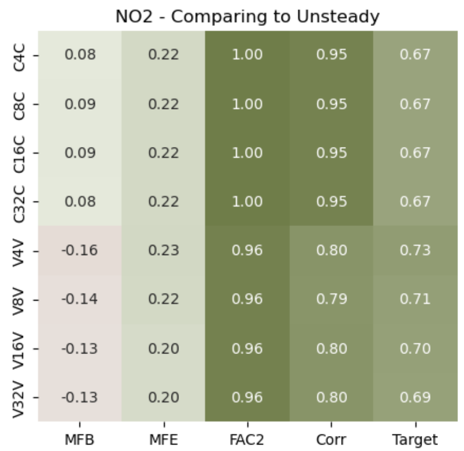


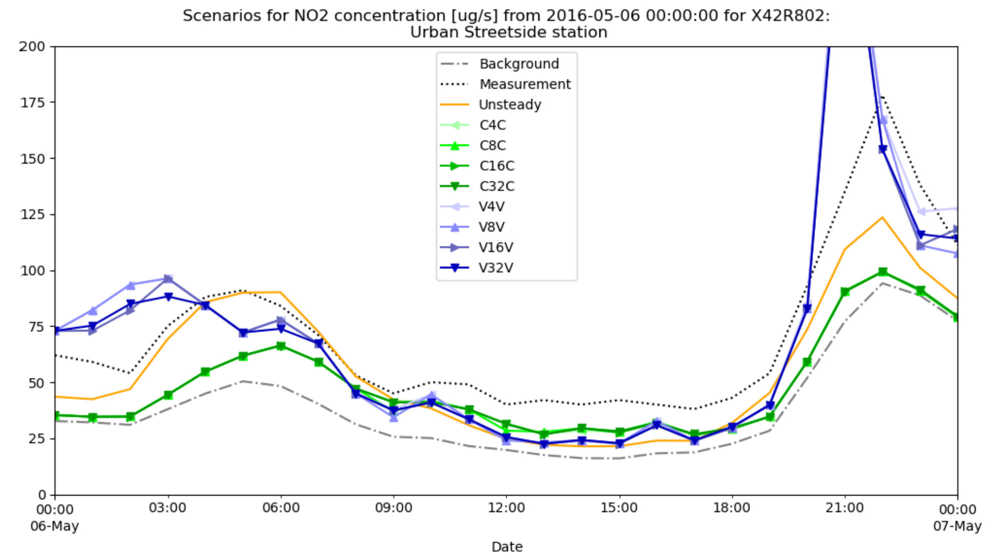


Results – Stage1 – May 6th – Urban Streetside

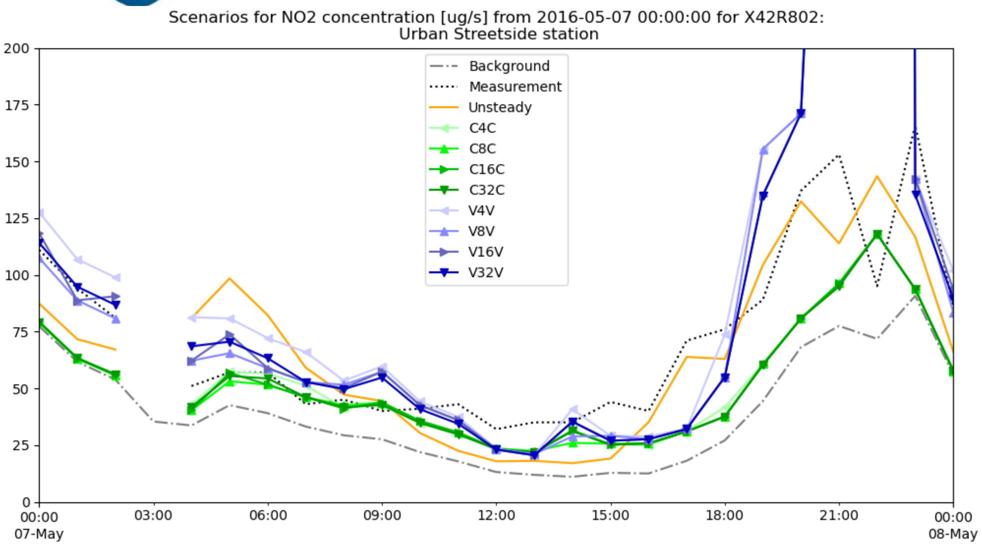






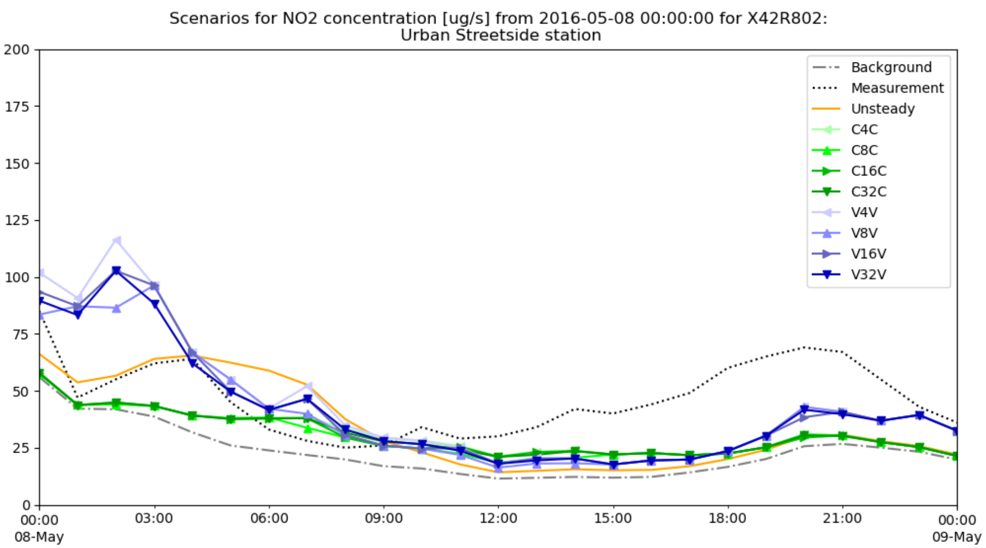


1-day results, 7th and 8th of May
Urban Streetside Station



NO2 - Comparing to Measurements

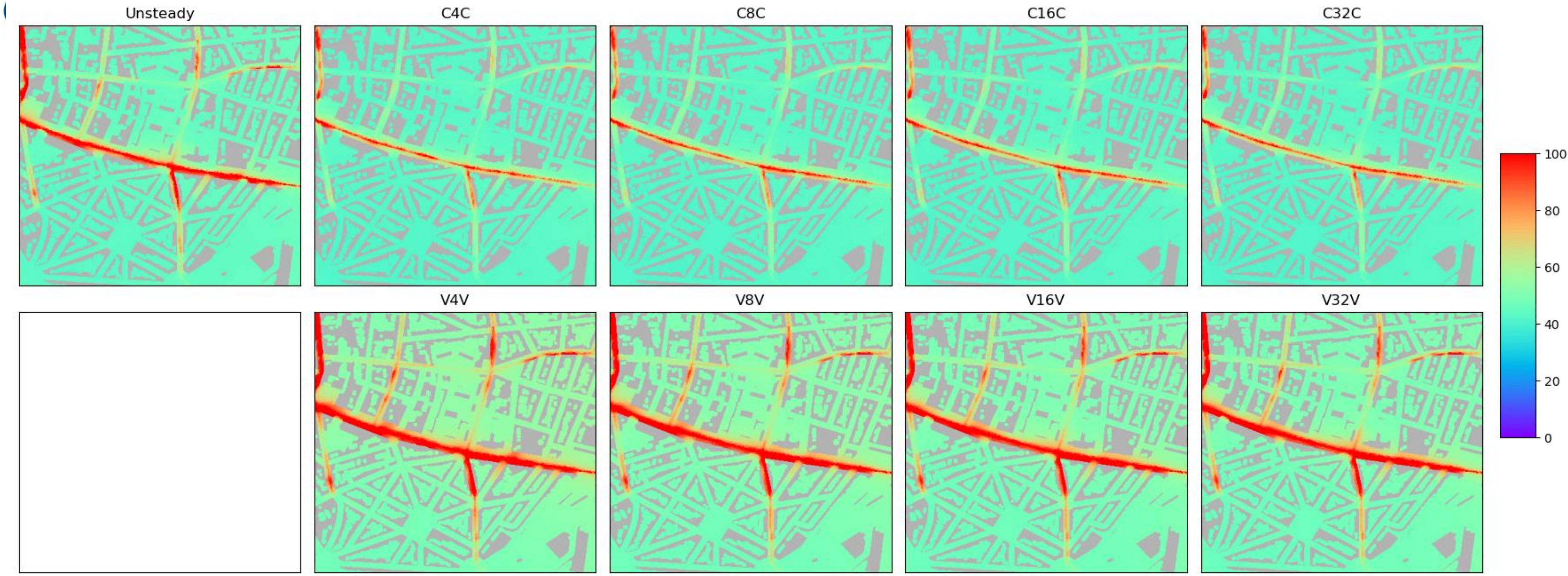
	MFB	MFE	FAC2	Corr	Target
Unsteady	0.14	0.34	0.92	0.80	0.65
C4C	0.29	0.33	0.96	0.83	1.16
C8C	0.31	0.34	0.92	0.84	1.16
C16C	0.30	0.33	0.92	0.84	1.16
C32C	0.30	0.33	0.92	0.84	1.17
V4V	-0.17	0.39	0.88	0.20	1.02
V8V	-0.07	0.34	0.88	0.20	1.02
V16V	-0.08	0.35	0.88	0.20	1.02
V32V	-0.08	0.34	0.88	0.20	1.02



NO2 - Comparing to Measurements

	MFB	MFE	FAC2	Corr	Target
Unsteady	0.37	0.55	0.60	0.35	1.25
C4C	0.37	0.44	0.76	0.43	2.27
C8C	0.42	0.46	0.72	0.52	2.22
C16C	0.39	0.44	0.76	0.48	2.26
C32C	0.39	0.45	0.76	0.46	2.26
V4V	0.16	0.44	0.72	0.49	0.88
V8V	0.23	0.43	0.76	0.53	0.89
V16V	0.20	0.43	0.76	0.52	0.88
V32V	0.20	0.42	0.76	0.51	0.90

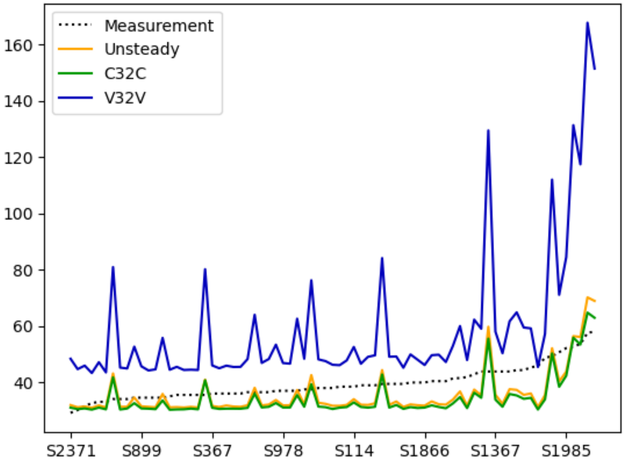
Results – Stage1 – May 6th – AOI

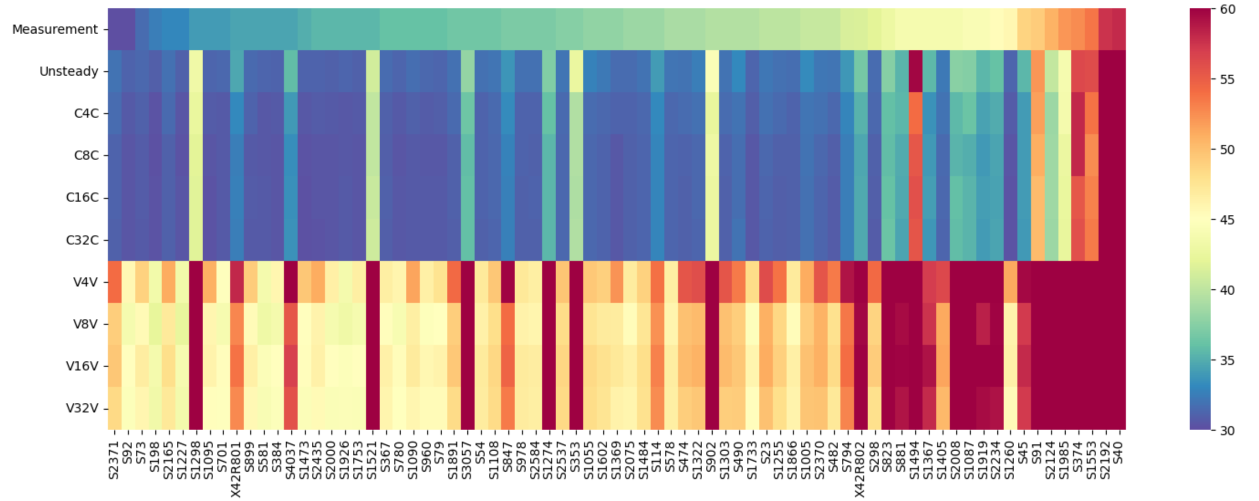


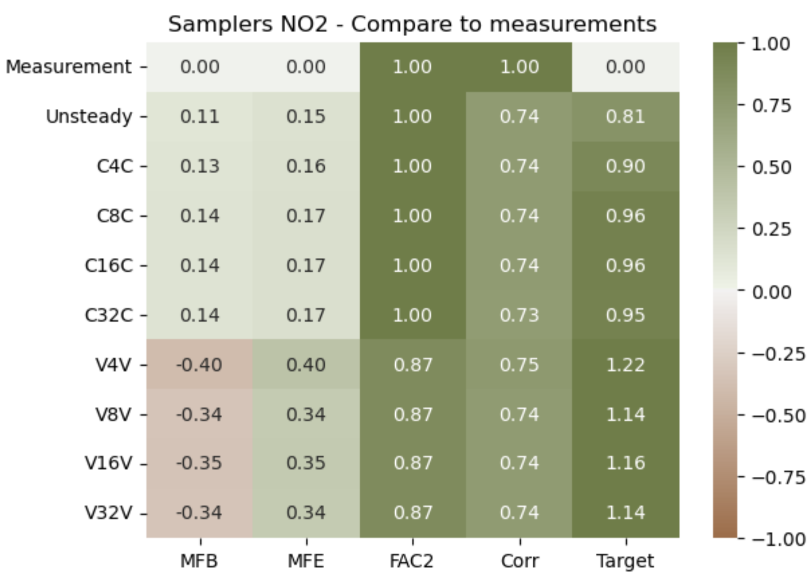
Stage 1 AOI NO2 - compare to measurements

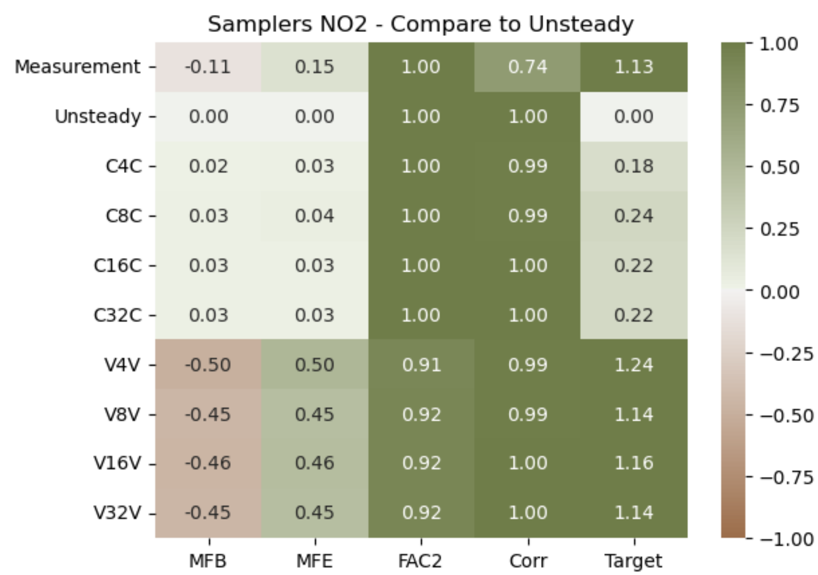
	MFB	MFE	FAC2	Corr	Target
Unsteady	0.00	0.00	1.00	1.00	0.00
C4C	0.09	0.09	1.00	0.98	1.11
C8C	0.10	0.10	1.00	0.99	1.28
C16C	0.10	0.10	1.00	0.99	1.22
C32C	0.10	0.10	1.00	0.99	1.28
V4V	-0.15	0.15	1.00	0.98	0.42
V8V	-0.12	0.12	1.00	0.99	0.35
V16V	-0.09	0.10	1.00	0.99	0.29
V32V	-0.09	0.09	1.00	0.99	0.28

Results – Stage2 – Samplers

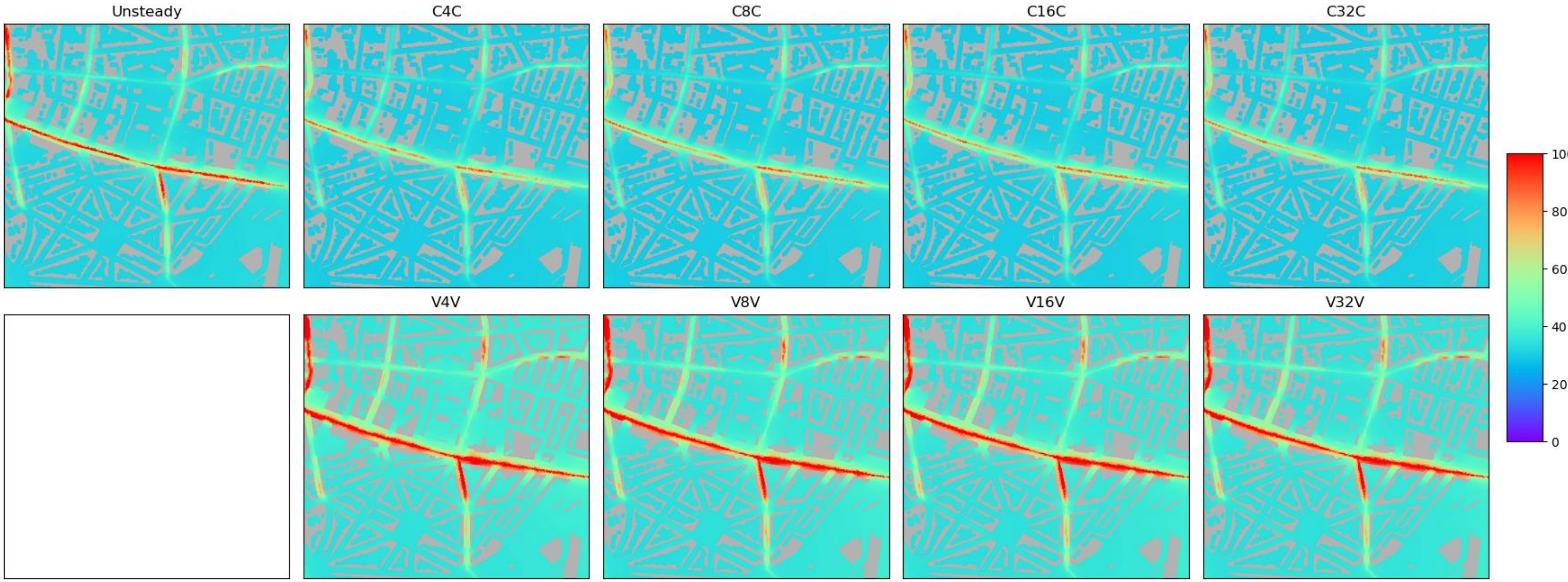








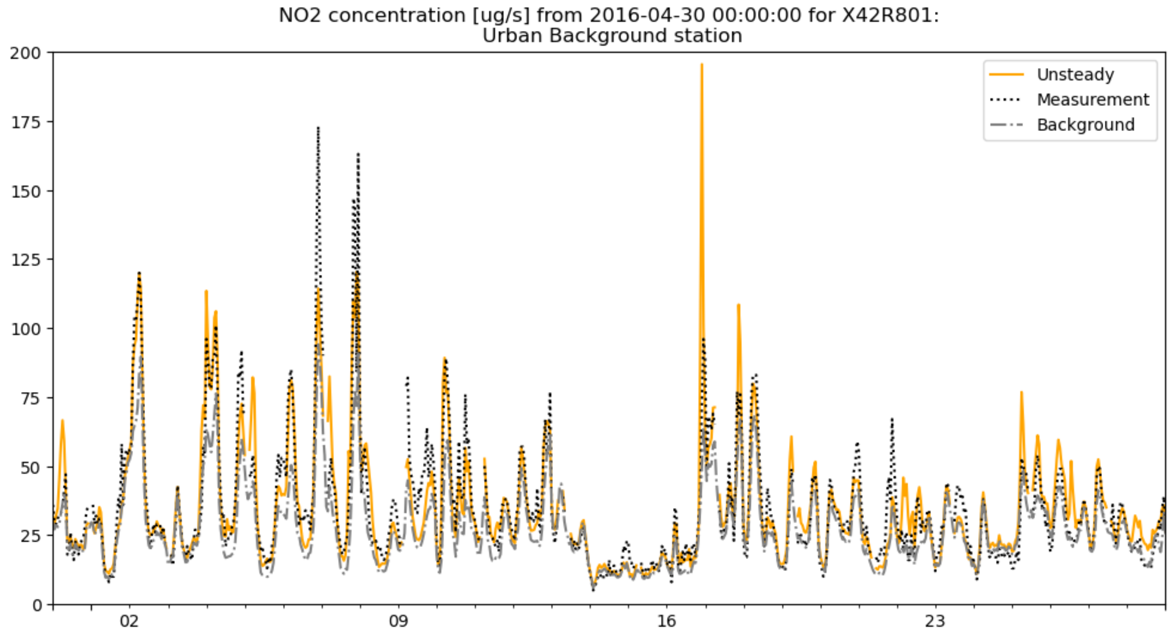
Results – Stage2 – AOI

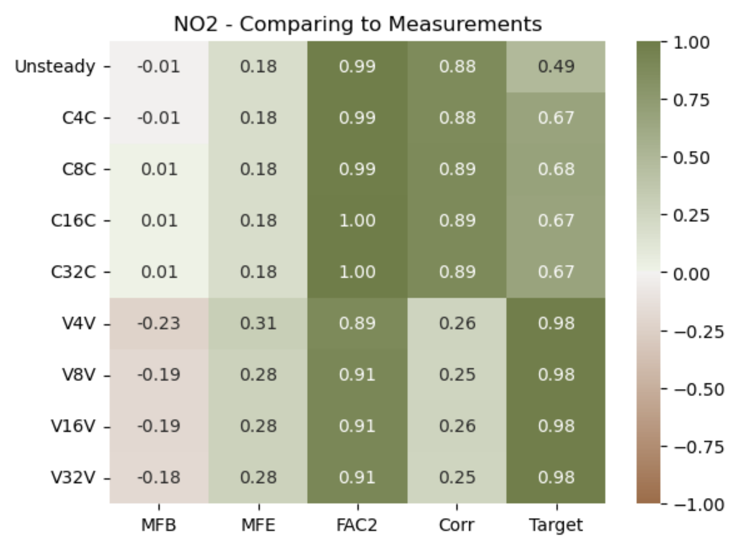


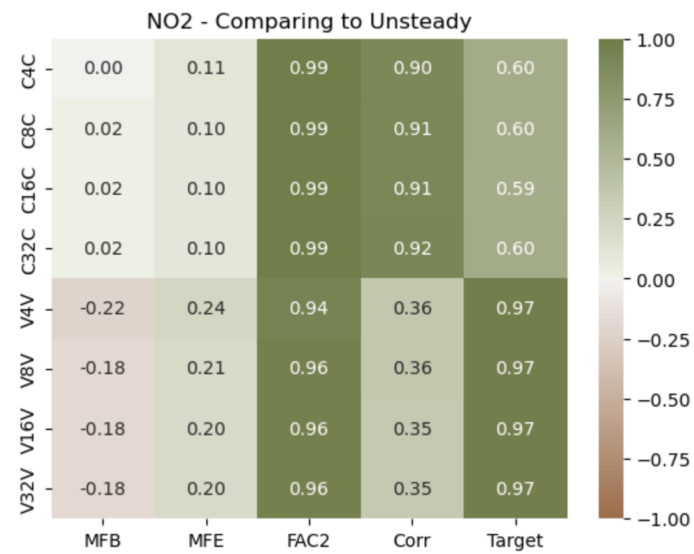
Stage 2 AOI NO2 - compare to measurements

	MFB	MFE	FAC2	Corr	Target
Unsteady	0.00	0.00	1.00	1.00	0.00
C4C	0.08	0.08	1.00	0.98	0.76
C8C	0.09	0.09	1.00	0.99	0.81
C16C	0.09	0.09	1.00	0.99	0.81
C32C	0.09	0.09	1.00	0.99	0.85
V4V	-0.15	0.15	1.00	0.98	0.42
V8V	-0.13	0.13	1.00	0.99	0.34
V16V	-0.12	0.12	1.00	0.99	0.34
V32V	-0.12	0.12	1.00	0.99	0.32

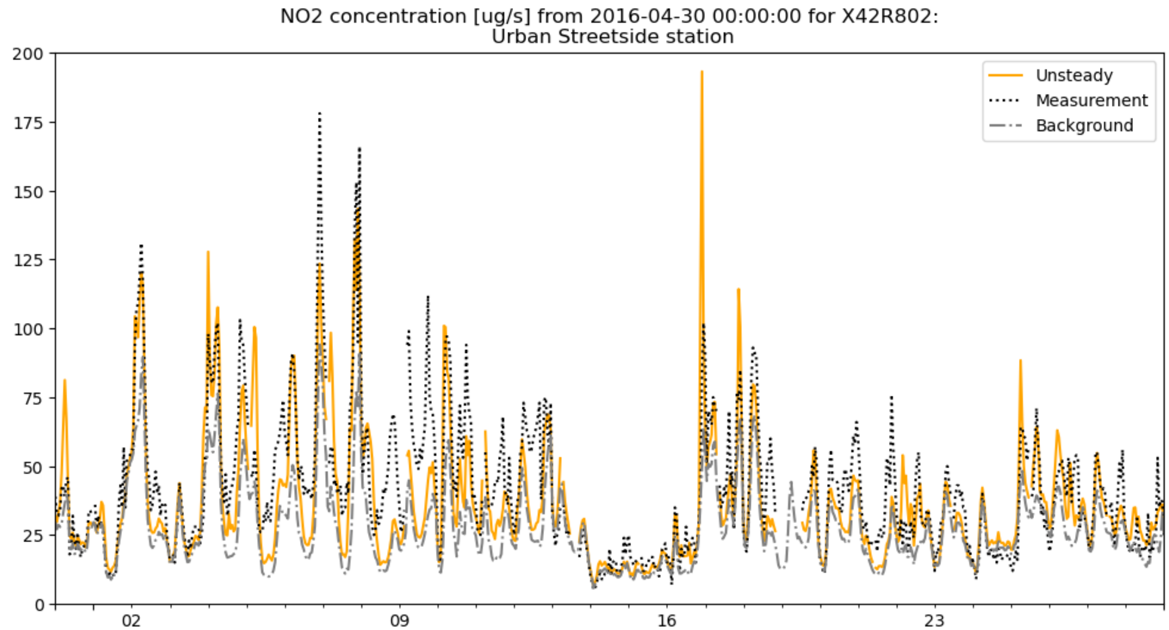
Results – Stage2 – Station 801







Results – Stage2 – Station 802



NO2 - Comparing to Measurements

	MFB	MFE	FAC2	Corr	Target
Unsteady	0.11	0.27	0.94	0.81	0.66
C4C	0.11	0.25	0.98	0.84	0.88
C8C	0.12	0.25	0.97	0.85	0.91
C16C	0.12	0.25	0.97	0.85	0.90
C32C	0.12	0.25	0.98	0.85	0.90
V4V	-0.13	0.36	0.88	0.23	0.99
V8V	-0.10	0.35	0.88	0.23	0.98
V16V	-0.10	0.34	0.88	0.23	0.99
V32V	-0.10	0.34	0.88	0.23	0.98

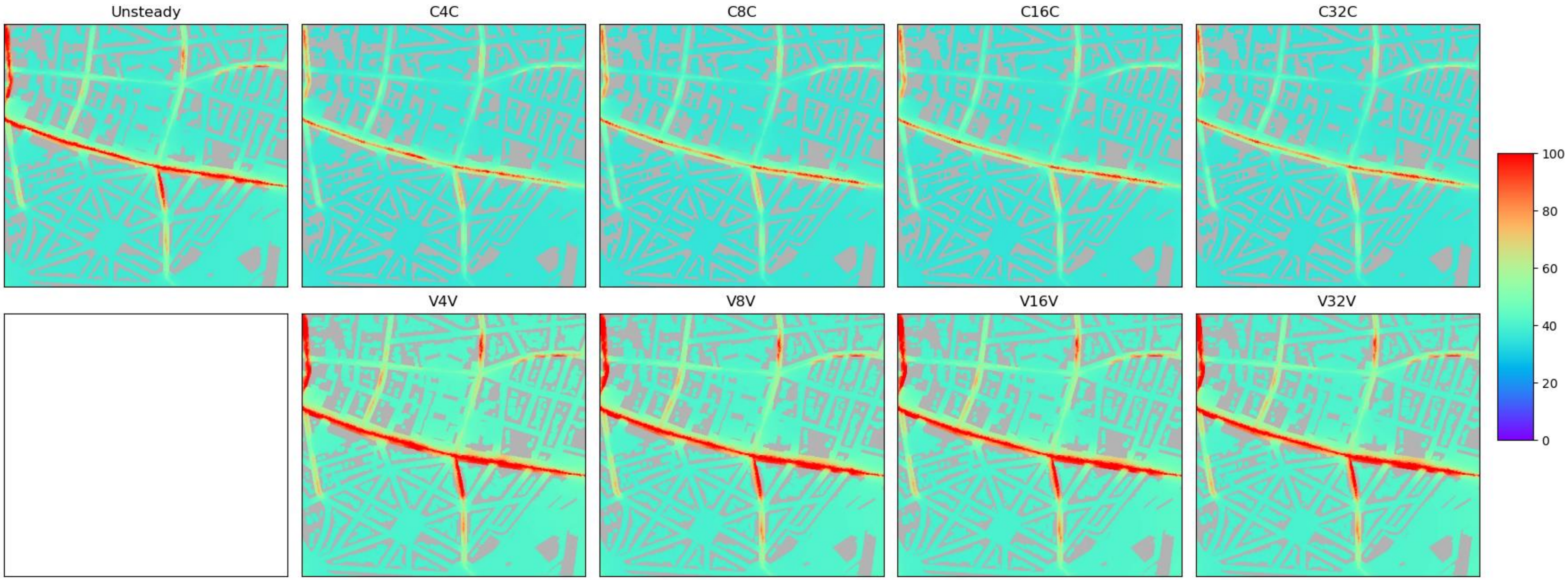
Colour scale: 1.00, 0.75, 0.50, 0.25, 0.00, −0.25, −0.50, −0.75, −1.00

NO2 - Comparing to Unsteady

	MFB	MFE	FAC2	Corr	Target
C4C	-0.00	0.13	0.99	0.88	0.67
C8C	0.01	0.12	0.99	0.89	0.67
C16C	0.01	0.12	0.99	0.89	0.67
C32C	0.01	0.12	0.99	0.89	0.67
V4V	-0.25	0.27	0.92	0.37	0.98
V8V	-0.22	0.25	0.93	0.37	0.97
V16V	-0.22	0.24	0.94	0.37	0.97
V32V	-0.22	0.24	0.94	0.37	0.97

Colour scale: 1.00, 0.75, 0.50, 0.25, 0.00, −0.25, −0.50, −0.75, −1.00

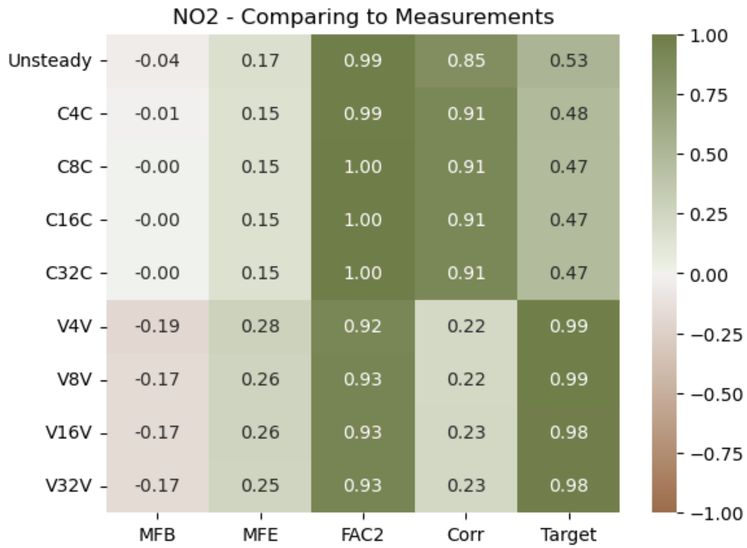
Results – Stage3 – AOI

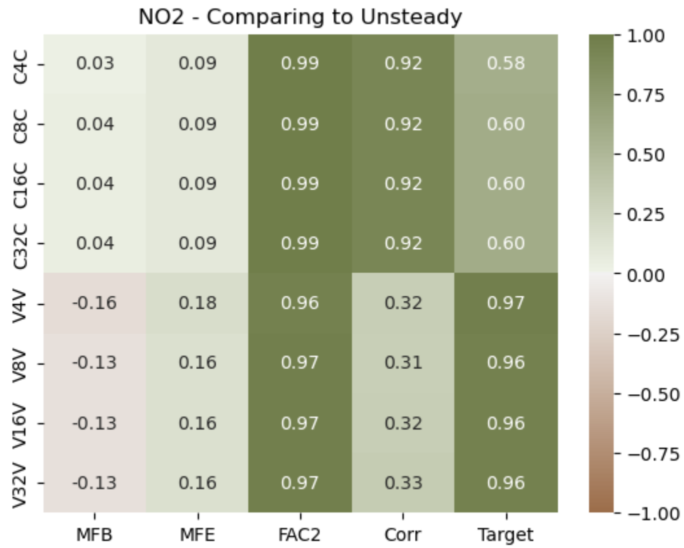


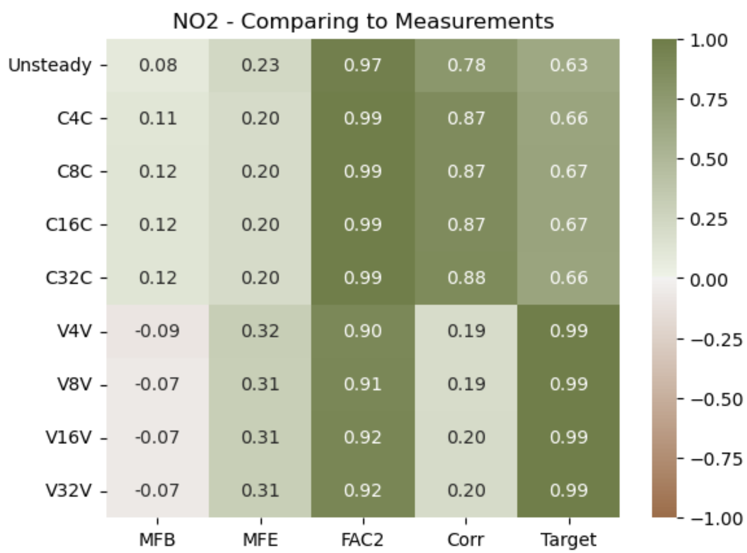
Stage 3 AOI NO2 - compare to measurements

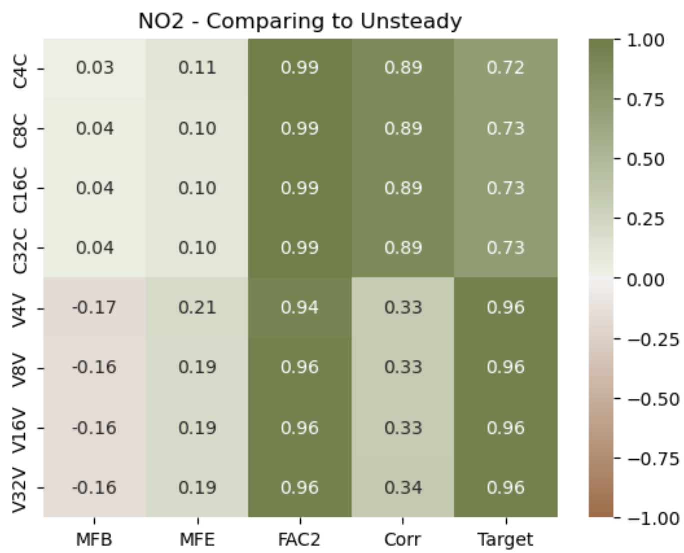
	MFB	MFE	FAC2	Corr	Target
Unsteady	0.00	0.00	1.00	1.00	0.00
C4C	0.09	0.09	1.00	0.97	1.00
C8C	0.10	0.10	1.00	0.98	1.21
C16C	0.10	0.10	1.00	0.99	1.19
C32C	0.10	0.10	1.00	0.99	1.22
V4V	-0.10	0.10	1.00	0.98	0.32
V8V	-0.07	0.08	1.00	0.99	0.25
V16V	-0.08	0.08	1.00	0.99	0.24
V32V	-0.07	0.08	1.00	0.99	0.25

Results – Stage3 – Stations – Statistics only









4. Conclusions

1. We have done unsteady CFD simulation for a full year with OpenFOAM for NO_2 for Antwerp 2m resolution at ground level (3M cells)
    1. Accuracy has been tested in the CT4 intercomparison exercise
    2. Running time: 12*1.5 days on a cluster and 12*1 days on PRACE HPC
    3. Computational time costs on Hawk: €9.000
    4. The code is now 10-20 times faster than at the start of the HiDALGO-project
2. We have compared steady scenario simulations with the full year unsteady simulation and the measurements.
    1. Unsteady produce best results most of the time
    2. Unable to determine which scenario is best with constant wind speed.
    3. More investigation needed for low speed accuracy of scenario modells.

Thank you!

Contact: Zoltán Horváth, horvathz@math.sze.hu
László Környei, laszlo.kornyei@math.sze.hu