Валидация WRF-Chem моделирования антропогенного вклада Санкт-Петербурга в содержание CO_2

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Photo by Margarita Sedeeva

Why the monitoring of CO_2 urban emissions is important today?

1. CO_2 – the main anthropogenic greenhouse gas (GHG) - influences the radiation balance of the Earth leading to an increase in tropospheric air temperature

2. CO_2 content in the atmosphere keeps rising due to man-made activity

3. Megacities have essentially determined (~70%) the anthropogenic CO_2 emissions in the last few decades

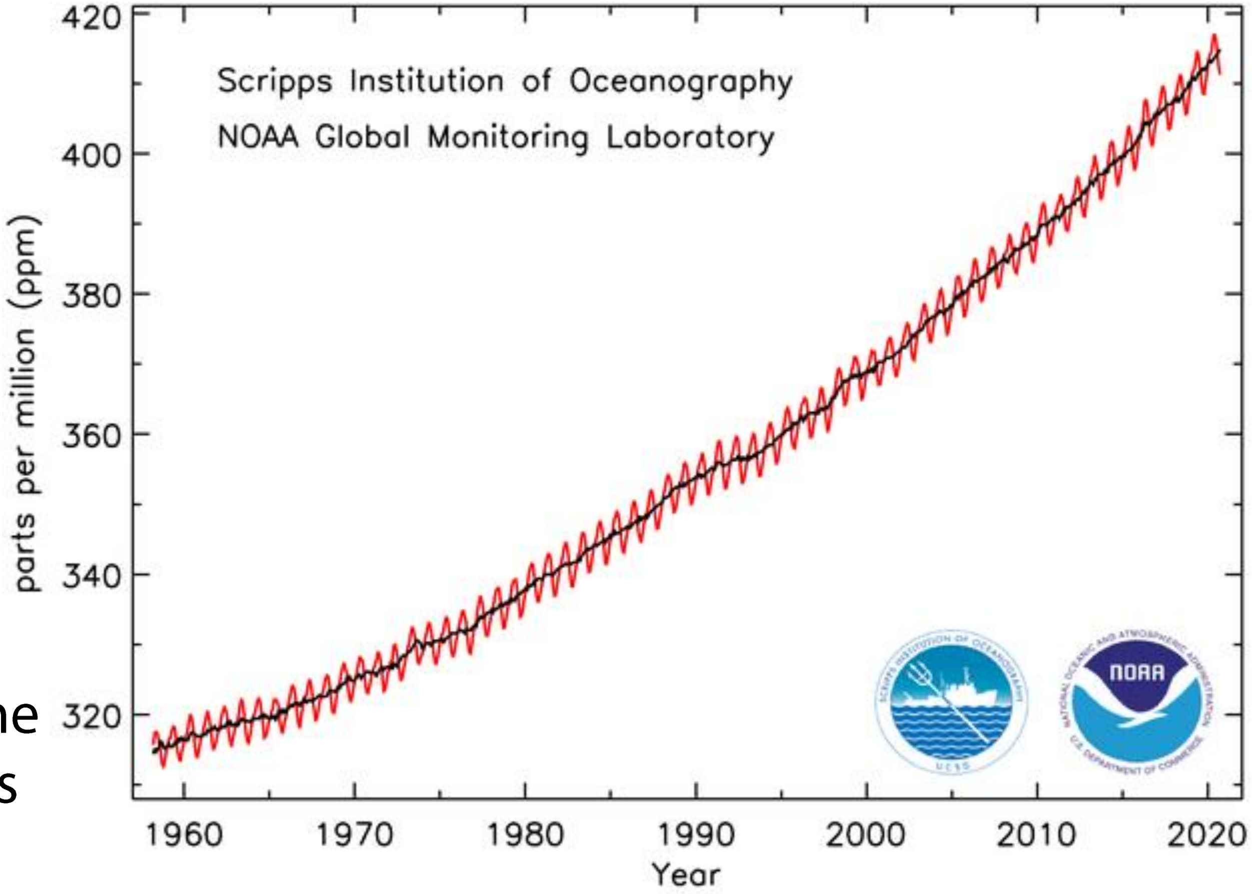


Fig.1 Trend of near-surface atmospheric CO_2 mixing ratio for the period 1958-2020 at Mauna Loa Observatory, Hawaii, USA

Original from https://www.esrl.noaa.gov/gmd/ccgg/trends/

How can we estimate CO_2 urban emissions?

1. GHGs Inventories (Bottom-up)

- Based on documented data of potential CO_2 sources (amount of fossil fuel used, number of active cement manufactures, etc.)

Inaccuracies can reach 50% and more![1]

[1] Bergamaschi et al., 2015
Locatelli et al., 2013
Basu et al., 2018

2. Inverse modelling (Top-down)

Observation data

- In-situ
- Remote

+

Modelling of CO_2 transport in the atmosphere

- 3-D numerical chemistry transport models;
- Lagrangian dispersion models;
- Box models;
- Others

+

A priori information

- CO_2 sources/sinks
- Initial and boundary conditions

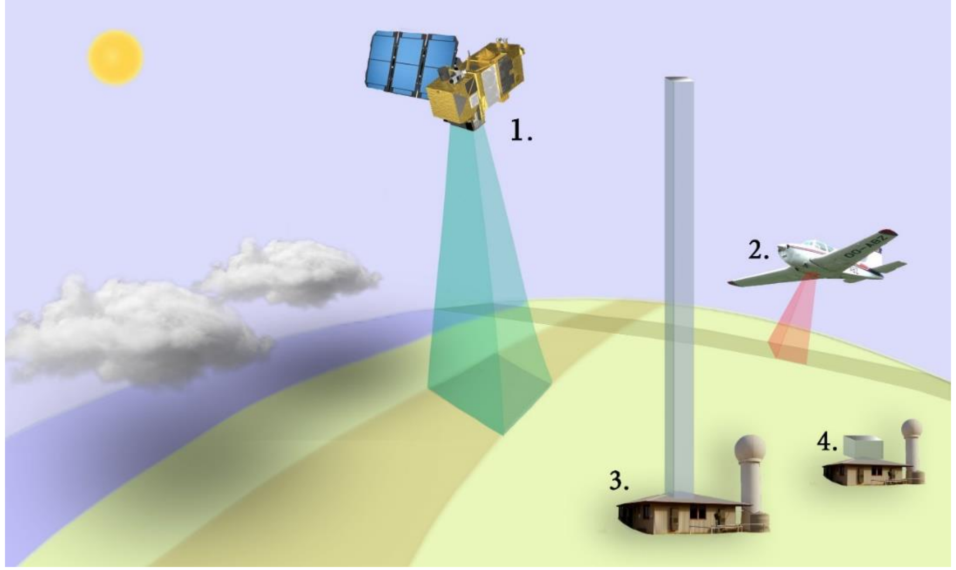


Fig.2 Main methods of atmospheric observations (1 – satellite, 2 – airplane, 3 – remote ground-based, 4- in-situ)

Relevance of the stady:

- Since numerical modelling of CO_2 transport significantly determine accuracy of emission estimates, the models used in solving of inverse problem have to be validated

Aims:

- It the current research we validate capability of high resolution numerical chemistry transport model WRF-Chem to simulate atmospheric transport of CO_2 on the territory of megacity Saint-Petersburg (Russia)

- On the basis of this study we will try to understand whether it is profitable to implement the model to the estimations of anthropogenic CO_2 emissios from the territory of Saint-Petersburg.

Methods: CO_2 in-situ observations in Peterhof and Helsinki (extra data)

Instruments:

Peterhof[1]

- Los Gatos Research Greenhouse Gas Analyzer (LGR GGA-24-r-EP)

Helsinki[2]

- Picarro G1301 Methane/Carbon Dioxide Analyzer

Station and observation data:

Peterhof[1]

- Position - SPbU Faculty of Physics, Peterhof;
- Height – ~ 6 m AGL
- Suburb of Saint-Petersburg, located in green area with limited roadway network
- Measurement error - 50-150 ppb depending on accumulation time (100-5 s respectively).

Helsinki[2]

- Position - Finnish Meteorological Institute (FMI, Helsinki)
- Height – ~ 30 m AGL
- Semi-urban site with commercial buildings, residential and green zones
- Measurement error - ~ 20 ppb for 1 minute averaged measurements.

[1] Foka et al., 2019

[2] Kilkki J. et al., 2014

Methods: wind observations in Peterhof and Helsinki

Peterhof

Helsinki[1]

Instruments:

- Weather station WXT536

- Data from FIM data service - https://www.ilmatieteenlaitos.fi

Station and observation data:

- Position - SPbU Faculty of Physics, Peterhof
- Height – ~ 18-20 m AGL
- Suburb of Saint-Petersburg, located in green area with limited roadway network
- Measurement error – wind speed 3%, wind direction 3° (at 10 m/s).

- Position – Kumpula, FMI (Helsinki)
- Height – ~ 24 m AGL
- Semi-urban site with commercial buildings, residential and green zones

Methods: CO_2 ground-based remote and satellite observations in Peterhof and Saint-Petersburg

1. Stationary measurements in Peterhof[1]

2. Emission Monitoring Mobile Experiment[2] (EMME)

Instruments:

- Fourier spectrometer Bruker 125HR at SPbU Faculty of Physics.

- Couple of mobile Bruker EM27/SUN Fourier transform infrared (FTIR) spectrometers

Observation data:

- Data type: XCO_2
- Position - SPbU Faculty of Physics, Peterhof
- Measurement error – 2-3%
- Temporal coverage – 3-6 h per day, 54 days in 2019

- Data type: $dTCCO_2$ between two parallel measurements and XCO_2
- Positions - 7 unique sites around St.-Petersburg
- Measurement error – 0.025%
- Temporal coverage – 3-4 h per day, 9 (EMME) and 81 (stand-alone EM27/SUN) days in 2019

[1] Timofeyev et al., 2019
[2] Makarova et al., 2021

Methods: CO_2 ground-based remote and satellite observations in Peterhof and Saint-Petersburg

1. OCO-2 (Orbiting Carbon Observatory) satellite measurements[1]

Instruments:

- Three spectrometers - O_2 A-band (0.757– 0.775 µm), a weak CO_2 band (1.594–1.627 µm) and a strong CO_2 band (2.043–2.087 µm)
- Measure solar radiation reflected by the Earth
- Orbit – Sun-synchronous

Observation data:

- Data type: XCO_2
- Spatial resolution - < 3 km^2
- Temporal coverage – 1 h per day (for Saint-Petersburg)
- Measurement error – 0.2-0.3% (relatively to 415 ppm).

[1] Frankenberg et al., 2015

Methods: numerical modelling of CO$_2$ atmospheric transport

Weather **R**esearch and **F**orecasting – **Chem**istry (WRF-Chem)

- Numerical weather prediction and atmospheric chemistry transport model on regional scale;
- Spatial resolution – from tens to ~ 1 km;
- Ability to consider time-varying fluxes of gases.

WRF-Chem first simulation:
focus on CO_2 near-surface mixing ratio

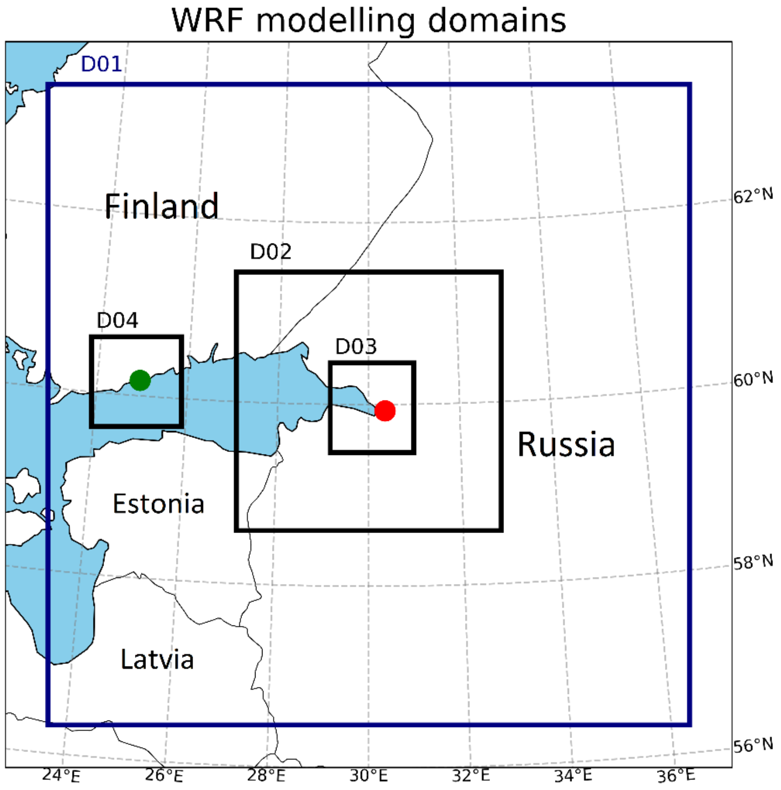


Fig. 3 Modelling domains;
Red circle – Saint-Petersburg, green circle – Helsinki.

Table 4. The main characteristics of the WRF-Chem runs

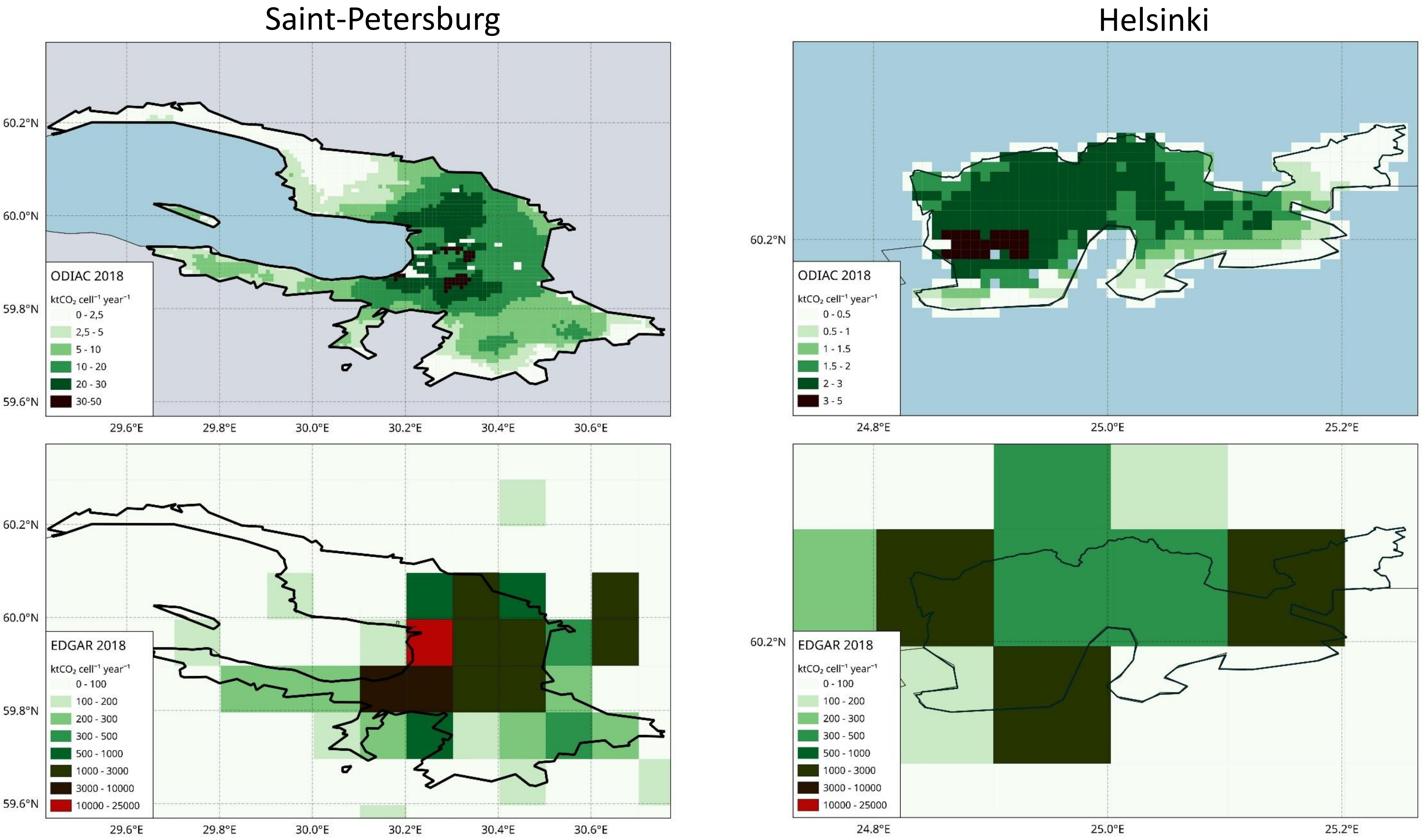
No of WRF-Chem Model Run		1	2	3
Horizontal resolution		D01 – 8 km, D02 – 4 km D03, D04 – 2 km		
Vertical resolution		25 hybrid vertical layers (up to 50 hPa)		
Initial and boundary conditions	**Meteorology**	GFS ANL (0.5°, 6 h)	ERA5 analysis (0.25°, 6 h)	
	Atmospheric CO_2 mixing ratio	CarbonTracker NRT analysis of CO_2 (2x3°, 6 h)		
Length of simulation		9 days of March and April 2019 (at least 2 model days for one day to be analyzed)		
CO_2 sources and sinks	**Anthropogenic emissions (1a, 1b)**	**ODIAC 2018**		**EDGARv6.0 2018**
	Biogenic fluxes (2)	VPRM Online (WRF-Chem module)		

1a. **ODIAC** (**O**pen-source **D**ata **I**nventory for **A**nthropogenic **C**O_2) –spatial resolution ~1 km

1b. **EDGAR** (**E**missions **D**atabase for **G**lobal **A**tmospheric **R**esearch) – spatial resolution ~10 km.

2. **V**egetation **P**hotosynthesis and **R**espiration **M**odel (**VPRM**) – model of CO_2 biogenic fluxes (*Mahadevan et al., 2008*).

WRF-Chem first simulation: apriori anthropogenic emissions of CO$_2$



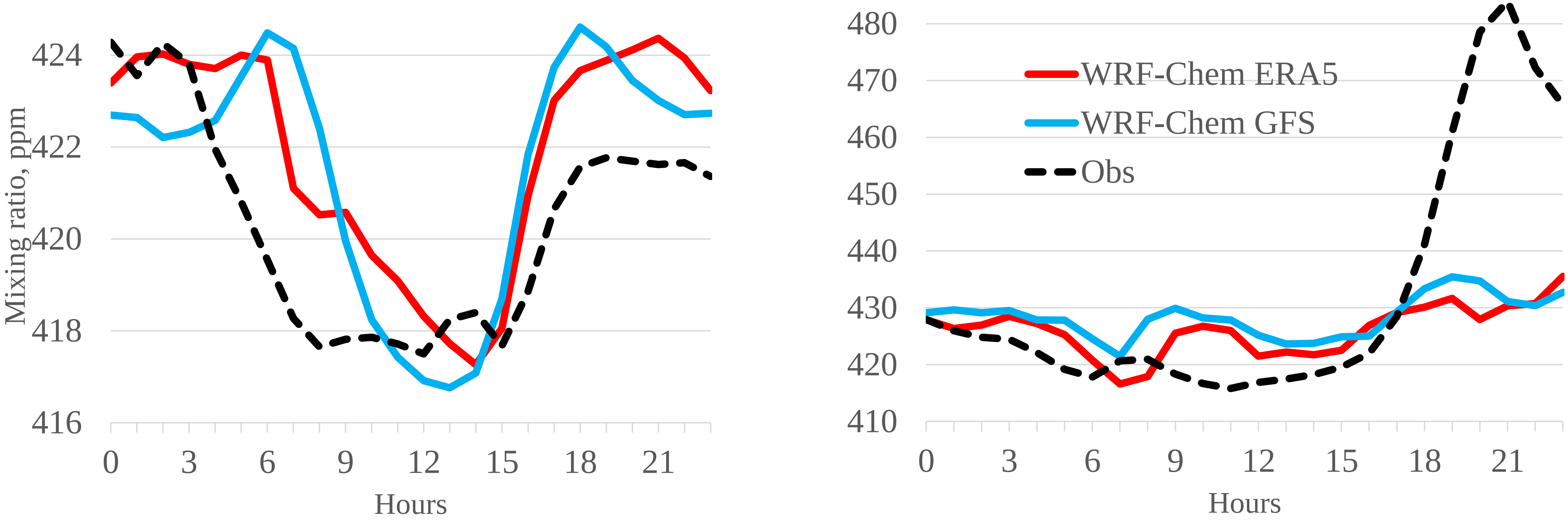
ODIAC 2018
space.res. ~ **1km^2**

EDGAR 2018
space.res. ~ **10km^2**

Fig. 4 Apriori anthropogenic CO$_2$ emissions according to ODIAC 2018 and EDGAR 2018 data for Saint-Petersburg and Helsinki

WRF-Chem vs <u>in-situ</u> measurements of <u>near-surface</u> CO_2 in Peterhof: two sets of meteo boundary conditions (GFS vs ERA5)

R – 0.72 (ERA5, GFS)
Bias – 3.1-3.3 ppm (ERA5,GFS)
RMSD – 13.5 ppm (ERA5,GFS)

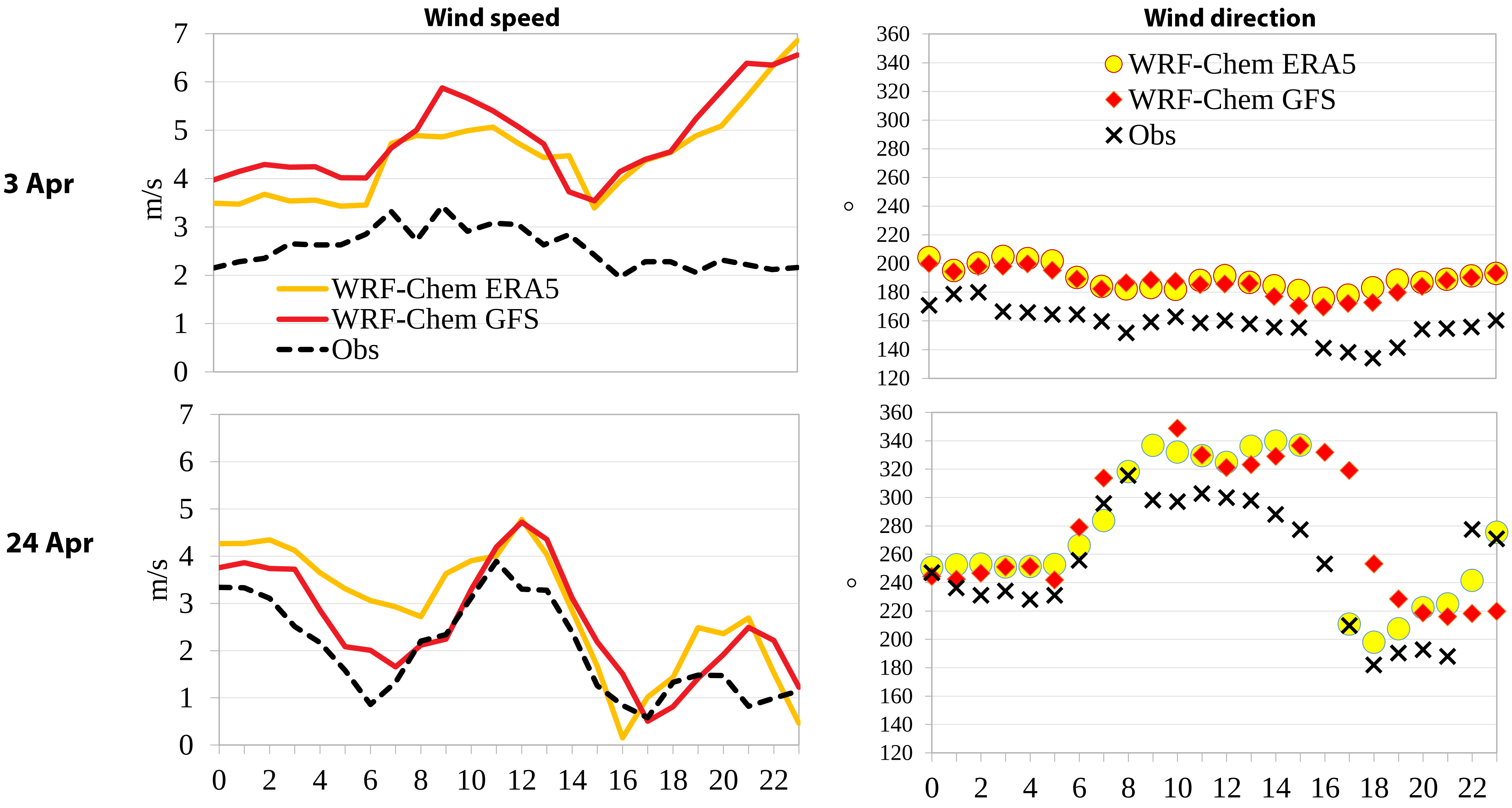


3 Apr (the best fit)

24 Apr (the worst fit)

Fig. 5 Modelled and observed near-surface CO_2 mixing ratio <u>with different meteo boundary conditions</u> in Peterhof during 3 and 24 April 2019

WRF-Chem vs in-situ near-surface wind measurements in Peterhof: two sets of boundary conditions (GFS vs ERA5)



R – 0.7 (ERA5, GFS)
Bias – -1.4 (ERA5), -1.1 (GFS) m/s
RMSD – 1.8 (ERA5), 1.6 (GFS) m/s

R – 0.76 (ERA5), 0.61 (GFS)
Bias – 13.9 (ERA5), -8.1 (GFS) °
RMSD – 45.7 (ERA5), 47.5 (GFS) °

Fig. 6 Modelled and observed near-surface wind speed with different meteo boundary conditions in Peterhof during 3 and 24 April 2019

WRF-Chem vs in-situ measurements of near-surface CO_2 in Helsinki: two sets of boundary conditions (GFS vs ERA5)

R – 0.46-0.38 (ERA5, GFS)
Bias - -1.2 - -1.1 ppm (ERA5, GFS)
RMSD – 5.7-6.1 ppm (ERA5,GFS)

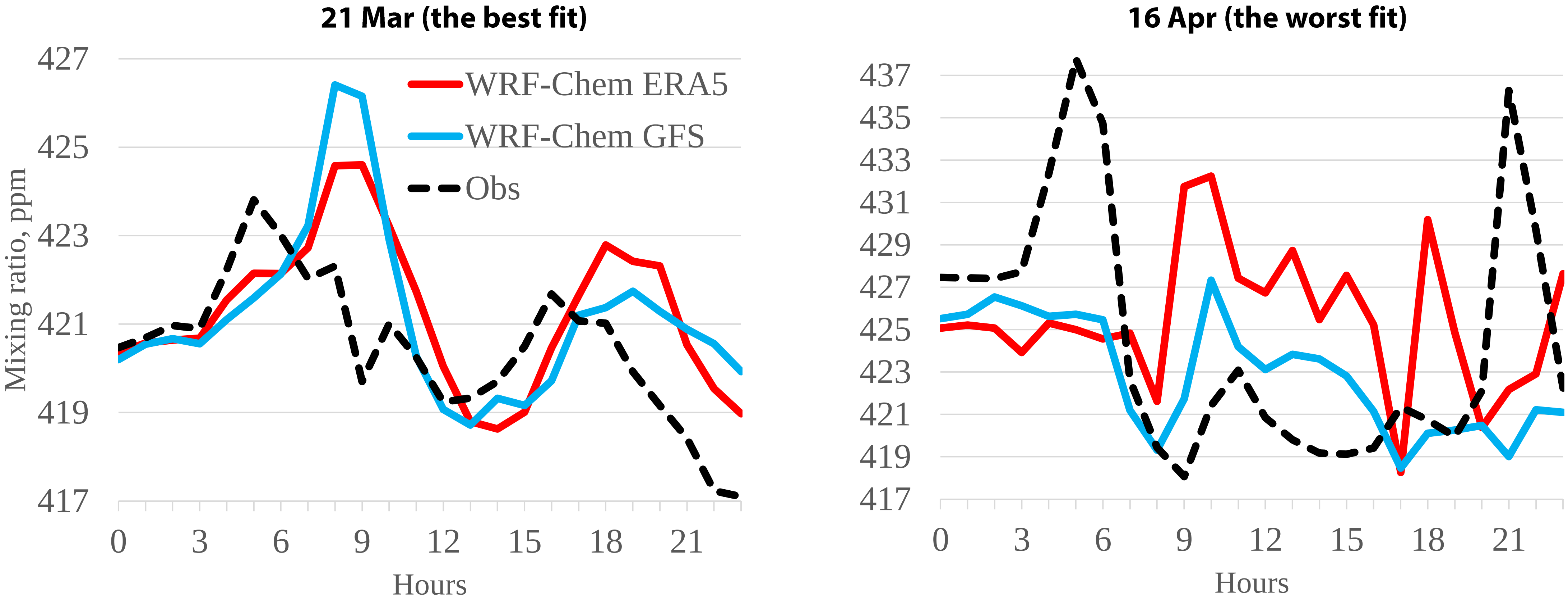
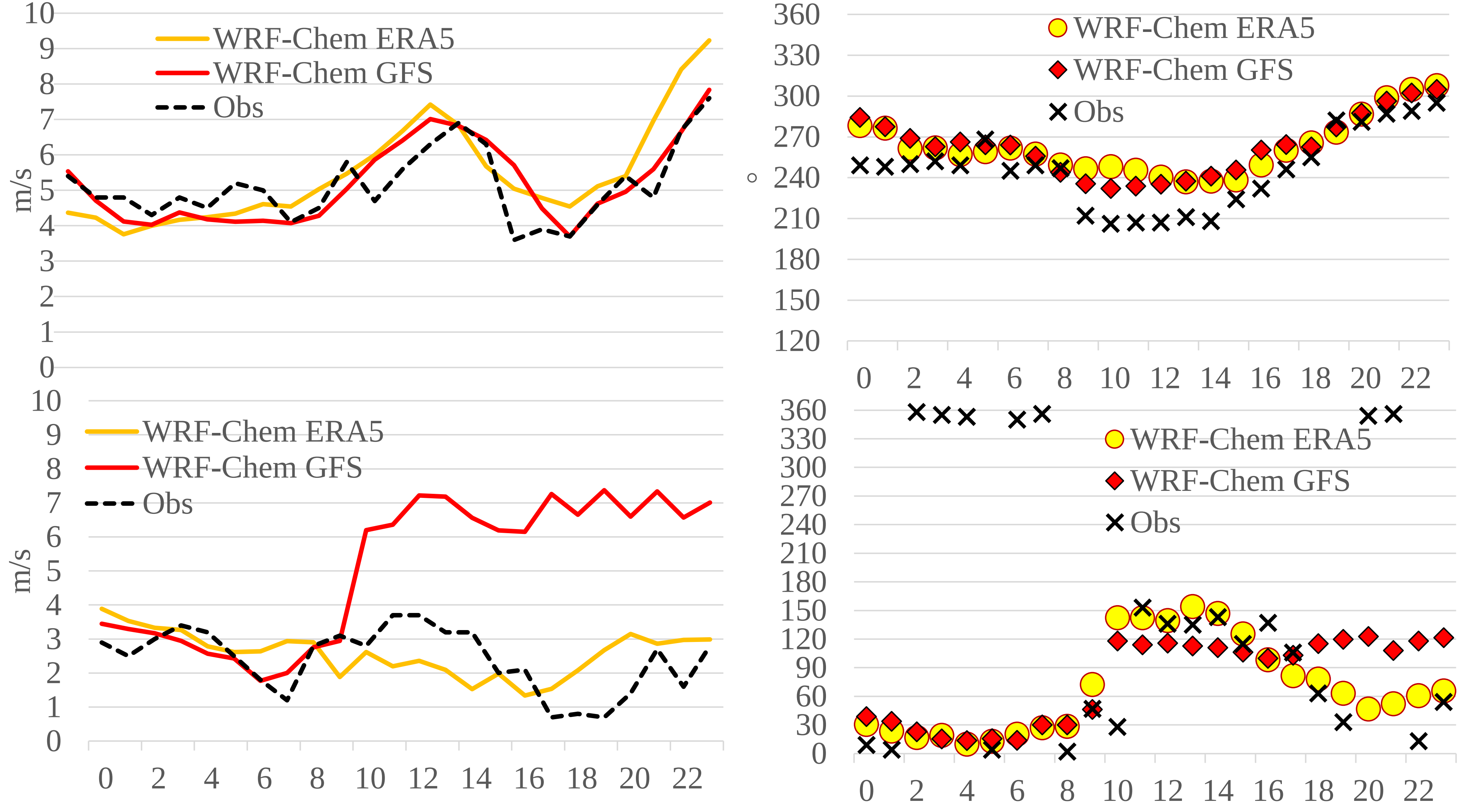


Fig. 7 Modelled and observed near-surface CO_2 mixing ratio with different meteo boundary conditions in Peterhof during 21 March and 16 April 2019

WRF-Chem vs in-situ near-surface wind measurements in Helsinki: two sets of boundary conditions (GFS vs ERA5)



Wind speed

Wind direction

21 Mar

16 Apr

R – 0.65-0.49 (ERA5, GFS)
Bias – -0.8 (ERA5), -0.9 (GFS) m/s
RMSD – 1. 5 (ERA5), 1.8 (GFS) m/s

R – 0.62-0.66 (ERA5, GFS)
Bias – 20.3 (ERA5), -17.8 (GFS) °
RMSD – 45.7 (ERA5), 44.3 (GFS) °

Fig. 8 Modelled and observed near-surface wind speed with different meteo boundary conditions in Helsinki during 21 March and 16 April 2019

WRF-Chem vs in-situ measurements of near-surface CO_2 : two sets of anthropogenic emissions (ODIAC vs EDGAR)

R – 0.72 (ODIAC)
0.50 (EDGAR)
RMSD – 13.5 ppm (ODIAC)
34.9 ppm (EDGAR)

R – 0.46 (ODIAC)
0.42 (EDGAR)
RMSD – 5.7 ppm (ODIAC)
11.4 ppm (EDGAR)

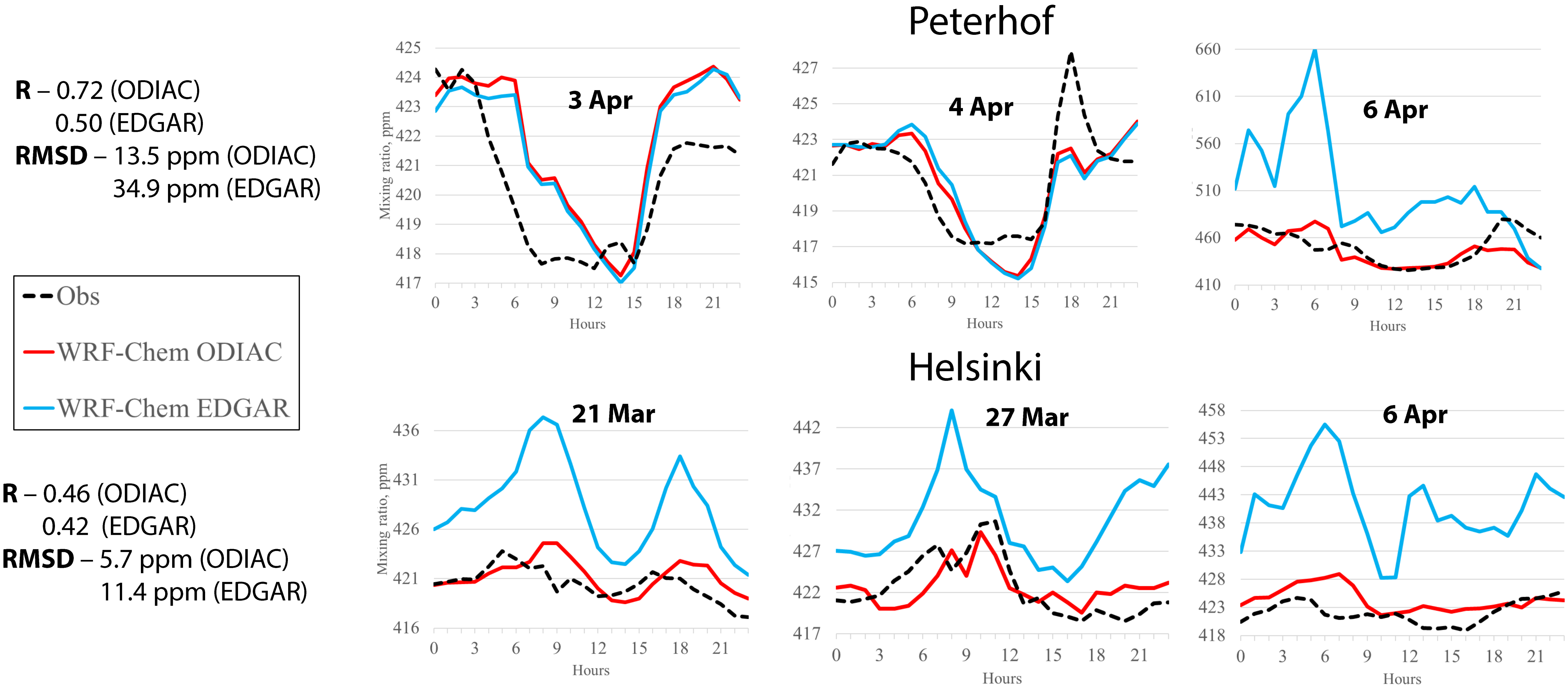
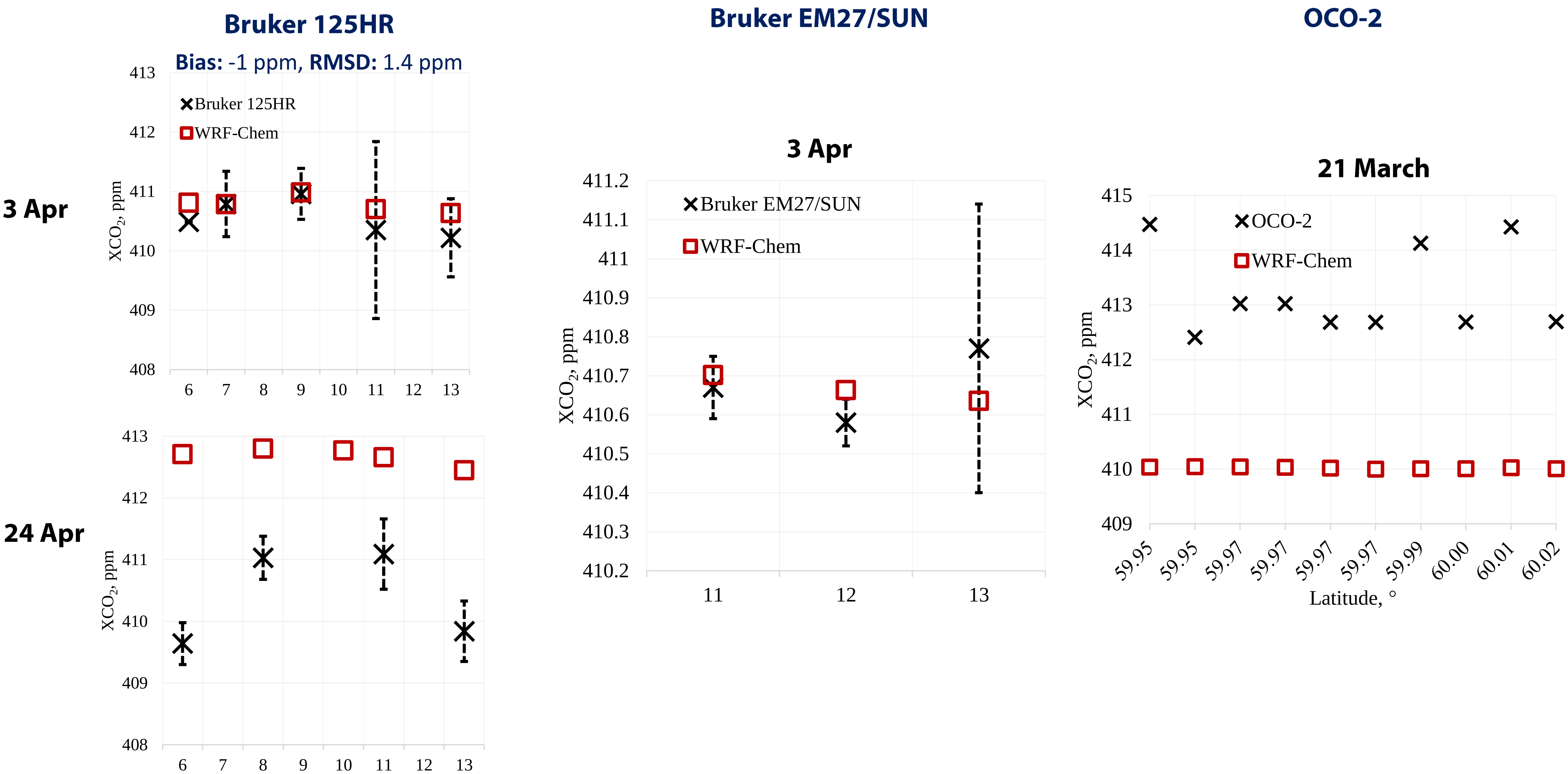


Fig. 9 Best and worst modelled and observed near-surface CO_2 mixing ratio with different anthropogenic emissions in Peterhof and Helsinki during several days of March-April 2019

WRF-Chem vs remote measurements of XCO_2 in Peterhof



Bruker 125HR

Bias: -1 ppm, **RMSD:** 1.4 ppm

Bruker EM27/SUN

OCO-2

Fig. 10 XCO_2 according to ground-based and satellite remote measurements in Peterhof and WRF-Chem simulation data for several days of April 2019

WRF-Chem vs EMME remote measurements of dTCCO$_2$ in Saint-Petersburg

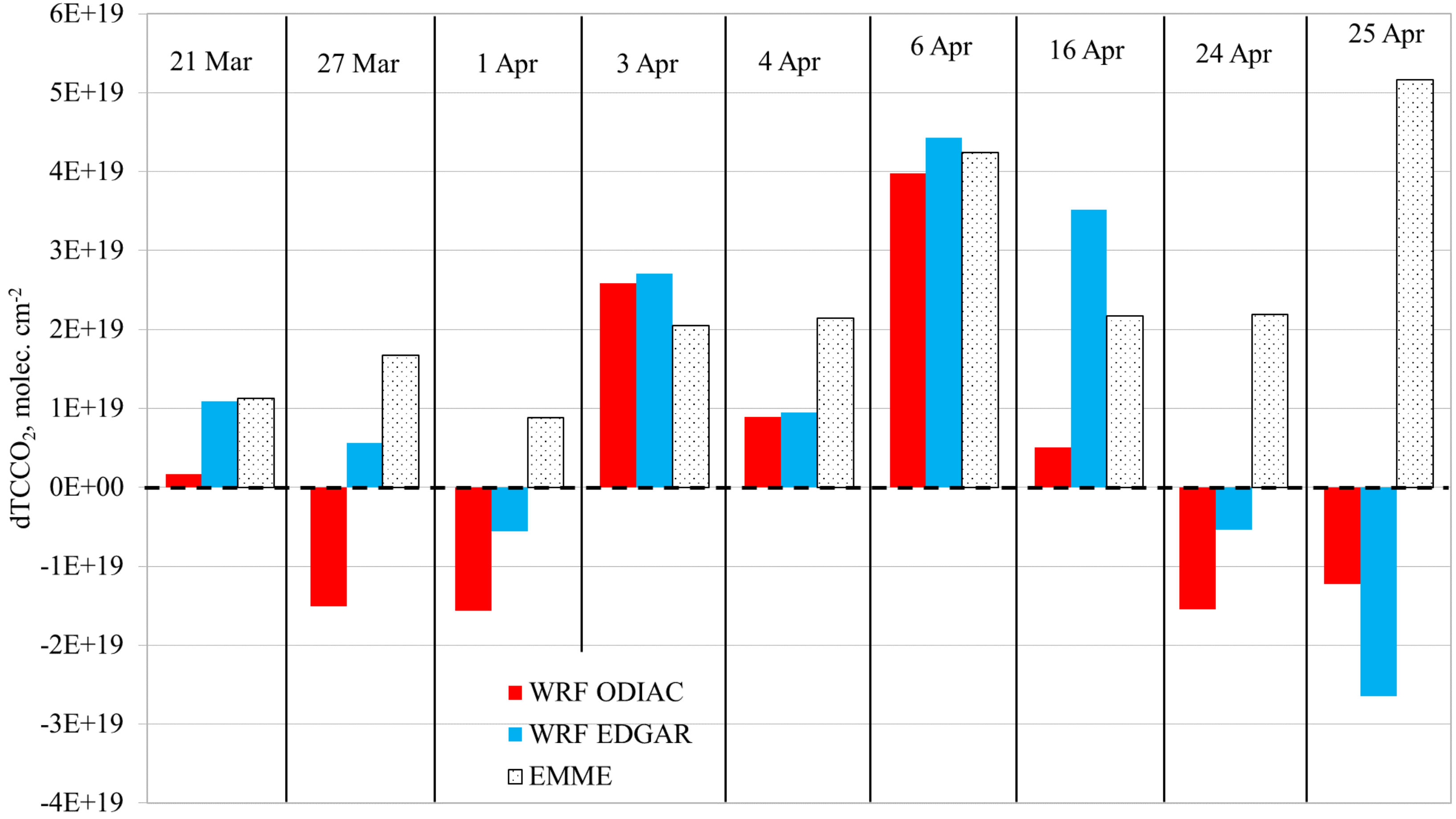


Fig. 11 Daily average dTCCO$_2$ according to EMME measurements around Saint-Petersburg and WRF-Chem simulation data averaged in neighboring model cells for several days of March-April 2019

WRF-Chem vs EMME remote measurements of dTCCO$_2$ in Saint-Petersburg

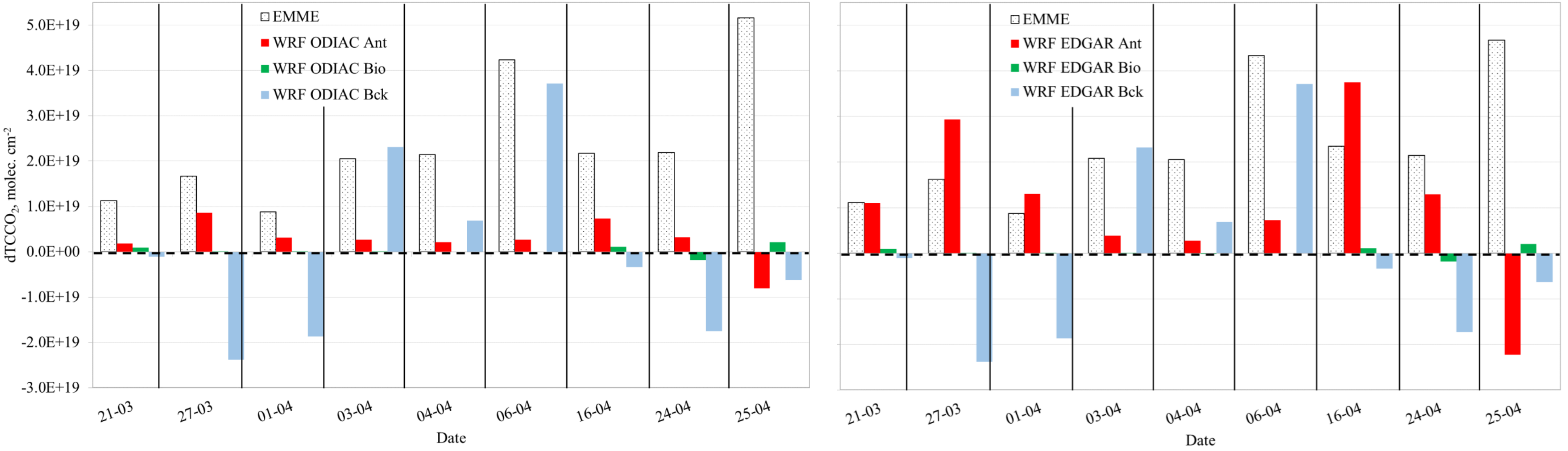


Fig. 12 Daily average dTCCO$_2$ according to EMME measurements around Saint-Petersburg and WRF-Chem simulation data from different sources* for several days of March-April 2019

*__Ant__ – anthropogenic CO$_2$ sources
Bio – biogenic CO$_2$ sources and sinks
Bck – background CO$_2$ or boundary conditions

WRF-Chem second simulation:
focus on CO_2 content in atmospheric column

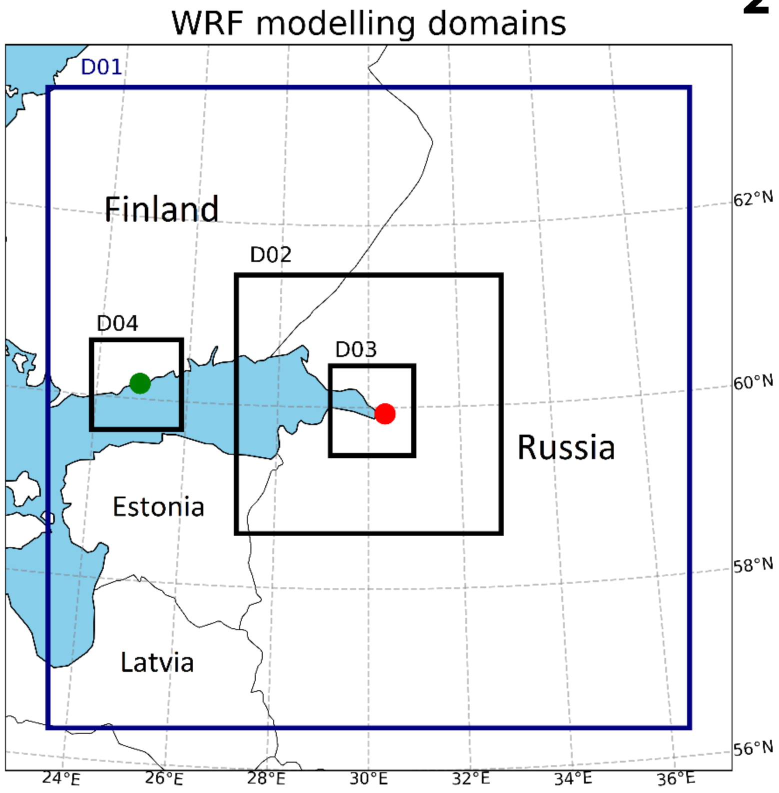


Fig. 13 Modelling domains;
Red circle – Saint-Petersburg, green circle – Helsinki.

Table 5. The main characteristics of the WRF-Chem runs

No of WRF-Chem Model Run		1
Horizontal resolution		D01 – 8 km, D02 – 4 km D03, D04 – 2 km
Vertical resolution		25 hybrid vertical layers (up to 50 hPa)
Initial and boundary conditions	**Meteorology**	ERA5 analysis (0.25°, 6 h)
	Atmospheric CO_2 mixing ratio	CarbonTracker NRT analysis of CO_2 (2x3°, 6 h)
Length of simulation		9 days of March and April 2019 (at least 2 model days for one day to be analyzed)
CO_2 sources and sinks	**Anthropogenic emissions (1)**	**ODIAC 2019**
	Biogenic fluxes (2)	VPRM Online (WRF-Chem module)

1.

ODIAC (**O**pen-source **D**ata **I**nventory for **A**nthropogenic **C**O_2) –spatial resolution ~1 km

2.

Vegetation **P**hotosynthesis and **R**espiration **M**odel (**VPRM**) – model of CO_2 biogenic fluxes (*Mahadevan et al., 2008*).

WRF-Chem second simulation: anthropogenic emissions of CO_2

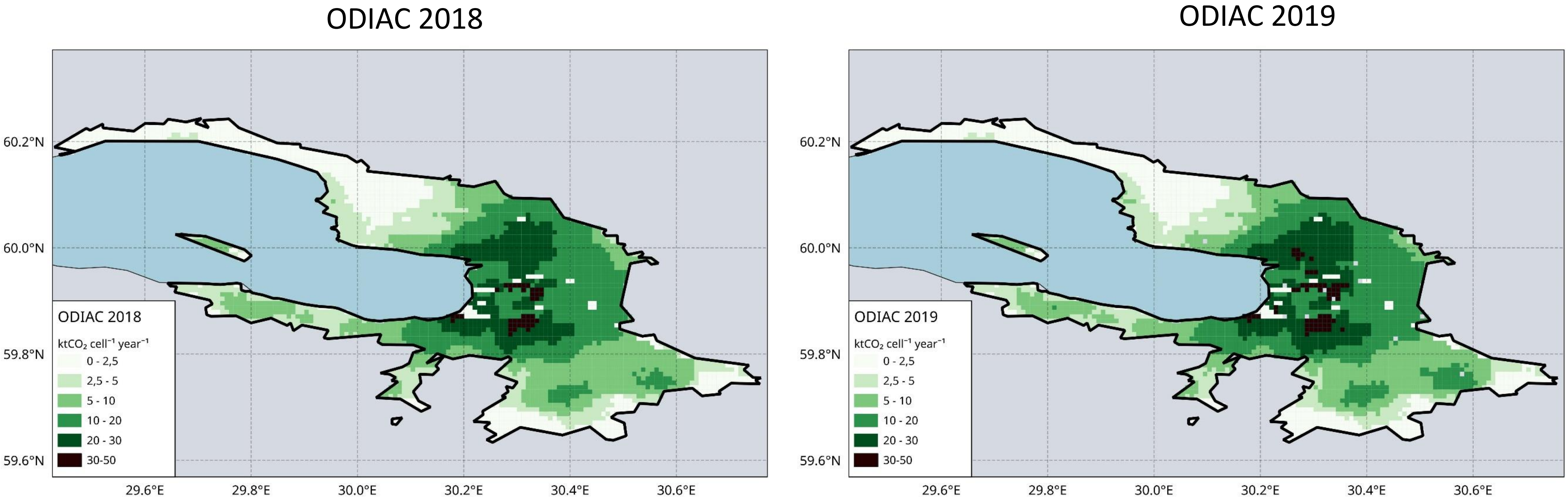


Fig. 14 Apriori anthropogenic CO_2 emissions according to ODIAC 2018 and 2019 data for Saint-Petersburg

Integral anthropogenic CO_2 emissions are higher on ~ 60%

WRF-Chem vs Bruker 125HR and EM27/SUN in Peterhof: specific days of January – May 2019

125HR
Bias: -0.8 ppm
RMSD: 1.5 ppm

EM27/SUN
Bias: 0.6 ppm
RMSD: 1.7 ppm

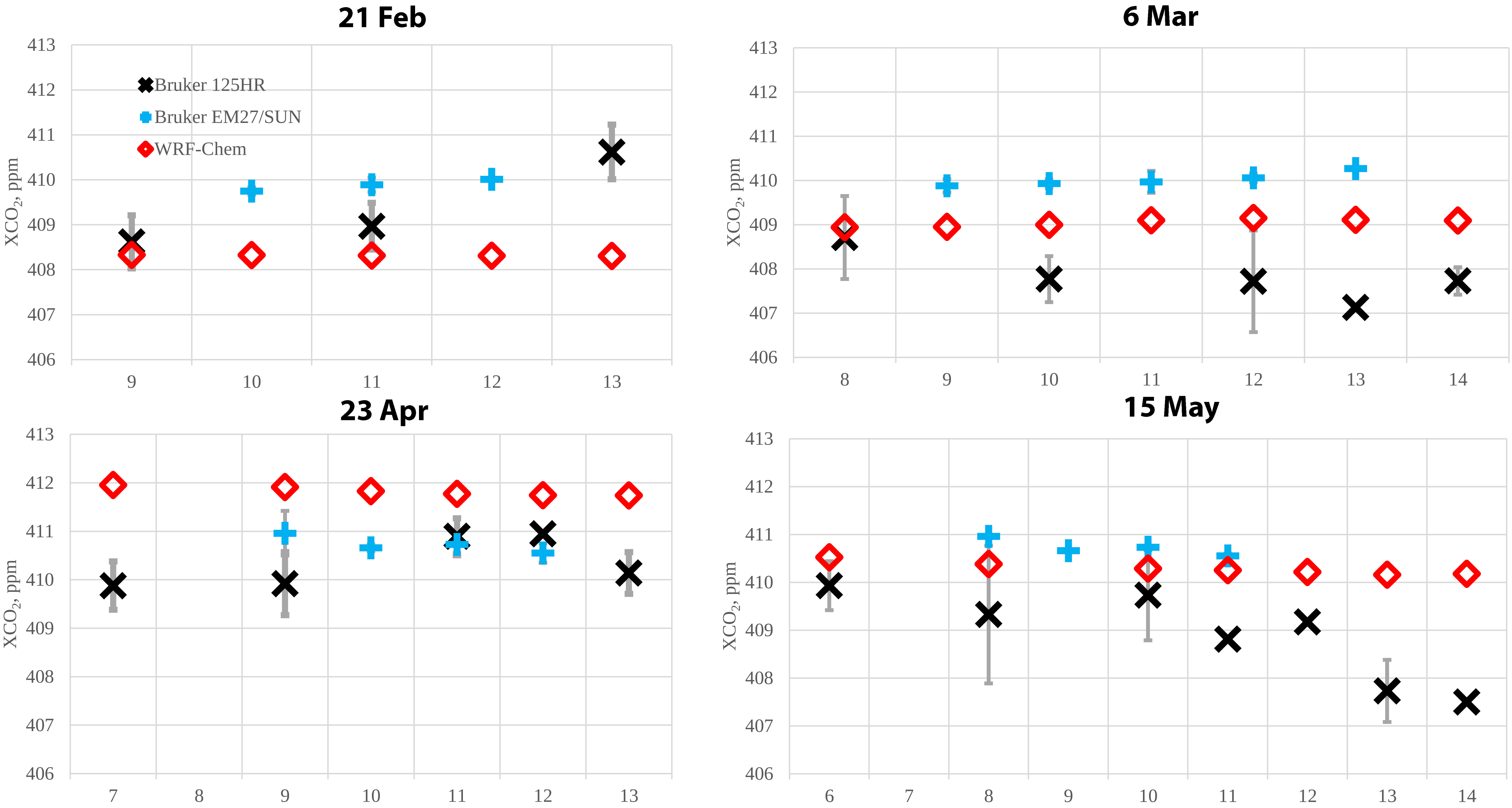
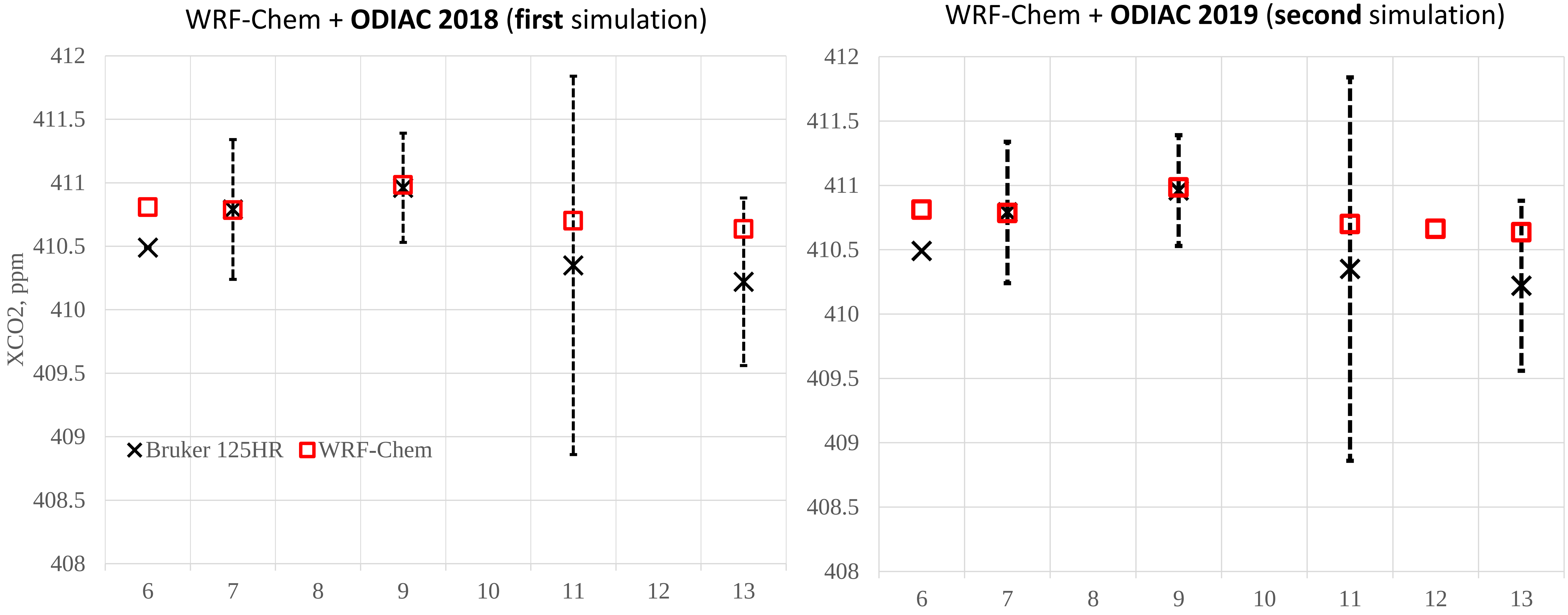


Fig. 15 XCO_2 according to Bruker 125 HR and EM27/SUN measurements in Peterhof and WRF-Chem simulation data for several days of Jan-Feb 2019

WRF-Chem vs Bruker 125HR and EM27/SUN in Peterhof: specific days of January – May 2019



3 Apr

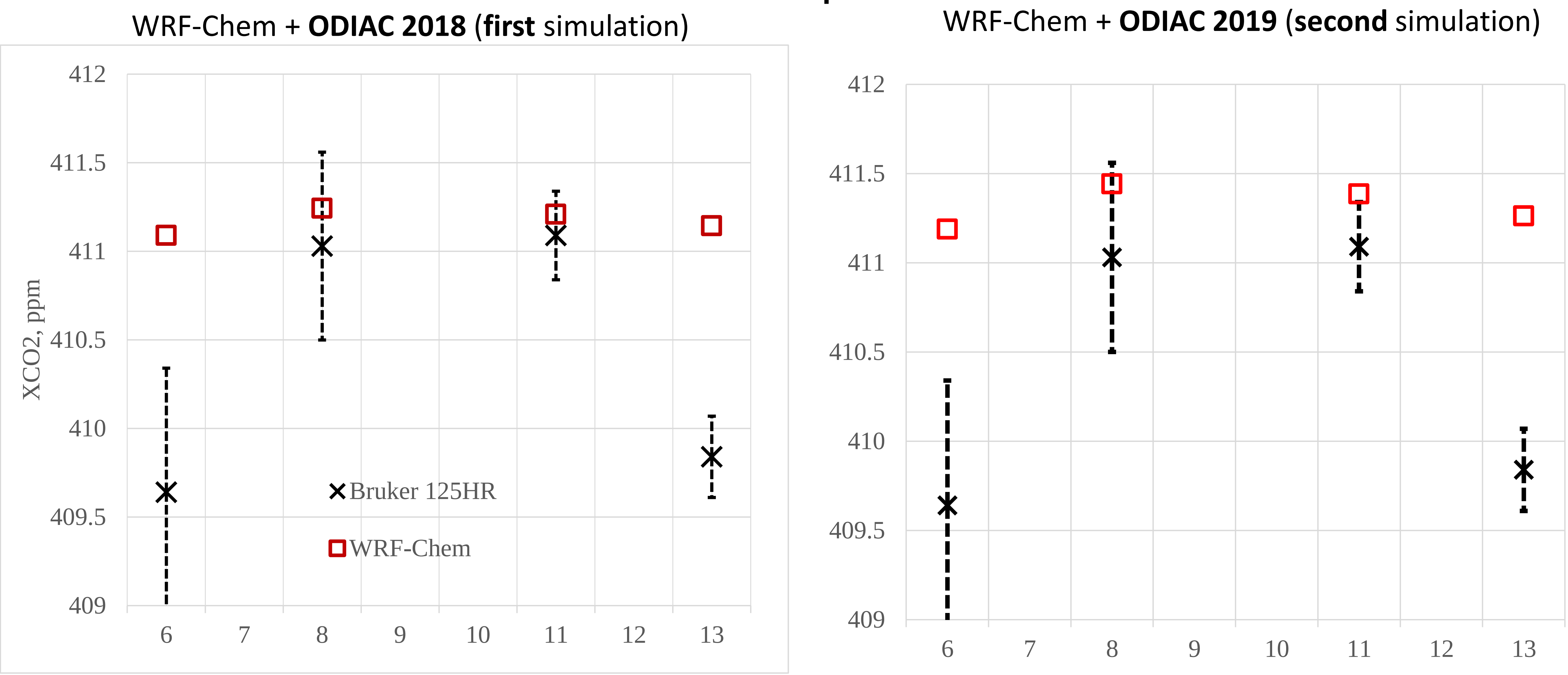
WRF-Chem + **ODIAC 2018** (**first** simulation)

WRF-Chem + **ODIAC 2019** (**second** simulation)

Fig. 16 XCO_2 according to Bruker 125 HR and EM27/SUN measurements in Peterhof and WRF-Chem simulation data with ODIAC 2018 and 2019 for 3 Apr 2019

WRF-Chem vs Bruker 125HR and EM27/SUN in Peterhof: specific days of January – May 2019

16 Apr



WRF-Chem + **ODIAC 2018** (**first** simulation)

WRF-Chem + **ODIAC 2019** (**second** simulation)

Fig. 17 XCO_2 according to Bruker 125 HR and EM27/SUN measurements in Peterhof and WRF-Chem simulation data with ODIAC 2018 and 2019 for 16 Apr 2019

Conclusions

Modelling of the near-surface CO_2 content in Peterhof and Helsinki

1. The WRF-Chem adequately (**R=0.7**) simulated the temporal variation in the near-surface CO_2 mixing ratio on a high spatial resolution in Peterhof (Saint Petersburg, Russia) and notably worse (**R** ~ **0.4-0.5**) in Helsinki (Finland) in March and April 2019;

2. The main discrepancies in near-surface CO_2 modelling were connected to inaccuracies in spatial distribution of CO_2 anthropogenic emissions and probably to complex weather situations during specific days;

3. However modelling of ground-level wind speed and direction using ERA5 data as initial and boundary conditions fit well with weather observations in both cities – Saint-Petersburg and Helsinki – **R** ~ **0.6-0.8, bias** ~ **1 m/s** (WS) and **13-20°** (WD), **RMSD** ~ **2** m/s (WS) and **46°** (WD);

4. WRF-Chem modelled data based on CO_2 anthropogenic emissions inventory EDGAR overestimated the observed near-surface CO_2 content in Peterhof and Helsinki comparing to ODIAC;

Conclusions

Modelling of CO_2 total column content in Peterhof and near Saint-Petersburg

5. WRF-Chem model simulates CO_2 content in a total atmospheric column according to the comparison with Bruker 125HR and EM27/SUN data relatively well with **bias** ~ **0.5-1 ppm** and **RMSD** ~ **1.4-1.7 ppm;**

6. The modelled CO_2 in a total atmospheric column underestimated the OCO-2 measurements;

Conclusions

Modelling of Saint-Petersburg contribution to CO_2 content

7. WRF-Chem is capable to simulate temporal variation of the contribution of Saint-Petersburg to CO_2 content ($dTCCO_2$) during specific weather conditions, but can significantly underestimate (with negative sign) the city`s contribution.

8. Probably the underestimation of Saint-Petersburg`s anthropogenic contribution by WRF-Chem modelling was related to:

- errors in CO_2 anthropogenic emission inventory (wrong spatial distribution and small values)
- errors in CO_2 boundary conditions (high CO_2 content at the domain`s boundaries)
- errors in modelling complex weather situations (e.g. changes of air mass movement direction to the opposite at the city-scale)

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We are grateful to scientific teams of SPbU, Voeikov Main Geophysical Observatory, Karlsruhe Institute of Technology (Karlsruhe, Germany), University of Bremen (Bremen, Germany) for in-situ CO_2, EMME 2019, Bruker EM27/SUN and Bruker 125HR measurements in Peterhof.

Also we would like to thank Russian State Hydrometeorology University`s IT team for providing an access to computing facilities.

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Thank you!

Photo by Margarita Sedeeva