

# High-resolution simulations of atmospheric CO<sub>2</sub> over complex terrain – representing the Ochsenkopf mountain tall tower

D. Pillai<sup>1</sup>, C. Gerbig<sup>1</sup>, R. Ahmadov<sup>2,\*</sup>, C. Rödenbeck<sup>1</sup>, R. Kretschmer<sup>1</sup>, T. Koch<sup>1</sup>, R. Thompson<sup>3,1</sup>, B. Neininger<sup>4</sup>, and J. V. Lavrié<sup>1</sup>

<sup>1</sup>Max Planck Institute of Biogeochemistry, Jena, Germany

<sup>2</sup>NOAA Earth System Research Laboratory, Boulder, Colorado, USA

<sup>3</sup>Laboratoire des Sciences du Climat et l'Environnement (LSCE), UMR8212, Gif-sur-Yvette, France

<sup>4</sup>MetAir AG, Flugplatz, 8915 Hausen am Albis, Switzerland

\* also at: Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, USA

Received: 20 December 2010 – Published in Atmos. Chem. Phys. Discuss.: 1 March 2011

Revised: 21 July 2011 – Accepted: 22 July 2011 – Published: 1 August 2011

**Abstract.** Accurate simulation of the spatial and temporal variability of tracer mixing ratios over complex terrain is challenging, but essential in order to utilize measurements made in complex orography (e.g. mountain and coastal sites) in an atmospheric inverse framework to better estimate regional fluxes of these trace gases. This study investigates the ability of high-resolution modeling tools to simulate meteorological and CO<sub>2</sub> fields around Ochsenkopf tall tower, situated in Fichtelgebirge mountain range- Germany (1022 m a.s.l.; 50°1'48" N, 11°48'30" E). We used tower measurements made at different heights for different seasons together with the measurements from an aircraft campaign. Two tracer transport models – WRF (Eulerian based) and STILT (Lagrangian based), both with a 2 km horizontal resolution – are used together with the satellite-based biospheric model VPRM to simulate the distribution of atmospheric CO<sub>2</sub> concentration over Ochsenkopf. The results suggest that the high-resolution models can capture diurnal, seasonal and synoptic variability of observed mixing ratios much better than coarse global models. The effects of mesoscale transports such as mountain-valley circulations and mountain-wave activities on atmospheric CO<sub>2</sub> distributions are reproduced remarkably well in the high-resolution models. With this study, we emphasize the potential of using high-resolution models in the context of inverse modeling frameworks to utilize measurements provided from mountain or complex terrain sites.

## 1 Introduction

It is well known that atmospheric CO<sub>2</sub> is rising due to fossil fuel combustion and deforestation. Being the most important anthropogenic greenhouse gas, accumulation of CO<sub>2</sub> in the atmosphere is reported to be the major cause of global warming (Le Treut et al., 2007). Out of the total emitted CO<sub>2</sub>, about 55 % is taken up by natural reservoirs (the land biosphere and ocean), while the rest, the so-called “airborne fraction”, stays in the atmosphere. However, this fraction exhibits large interannual variability due to the varying source and sinks of CO<sub>2</sub>, mainly over land. Quantifying these sources and sinks is highly demanded in predicting future increases in atmospheric CO<sub>2</sub> to a high degree of certainty. This requires profound understanding of natural process involved in sequestering carbon and their variability. Furthermore, it is essential to understand the feedback mechanisms between the carbon cycle and the global climate system to enable, in the near future, the implementation of emission reduction and sequestration strategies towards mitigating adverse effects of climate change.

Two approaches are currently used to infer the source-sink distribution of CO<sub>2</sub> globally, namely the bottom-up and top-down methods. In the bottom-up approach, the local scale process information, such as that obtained from eddy covariance towers, is scaled-up using diagnostic or process-oriented models in combination with remote sensing measurements to derive net CO<sub>2</sub> exchanges between the land surface and the atmosphere on regional or global scales (e.g. Masek and Collatz, 2006). However, the accuracy of this approach relies on the representativeness of the local flux measurement site, hence one can expect significant uncertainties due to the extrapolation of non-representative eddy



Correspondence to: D. Pillai  
(kdhanya@bgc-jena.mpg.de)

flux tower measurements. On the other hand, in the top-down approach, the variability in atmospheric CO<sub>2</sub> concentrations are observed to better understand the causes of variability in the source/sink distribution by inverting the atmospheric transport matrix (inverse modeling). The scarcity of concentration data and uncertainties in simulating atmospheric transport can introduce large uncertainties in this approach.

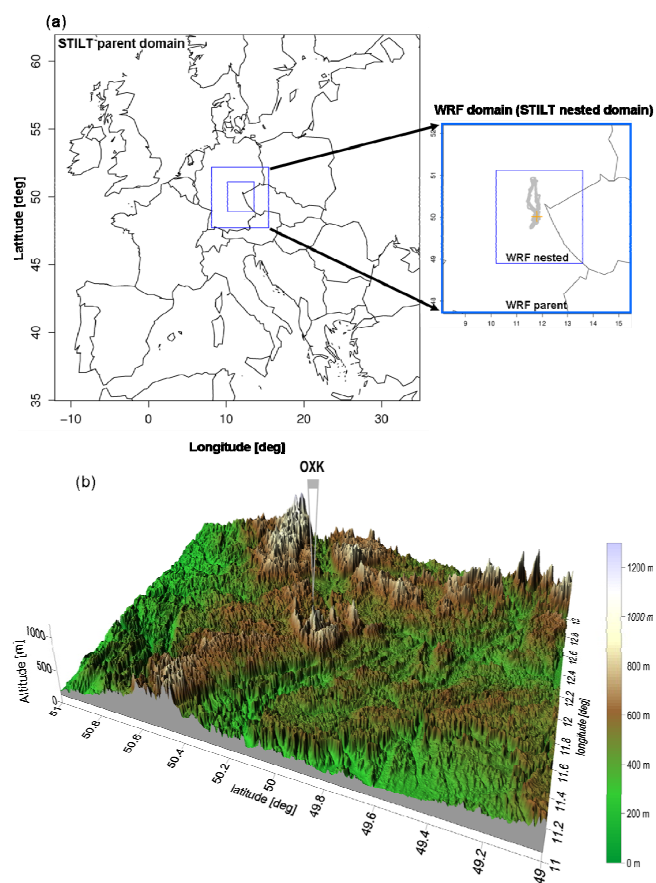
A number of studies used inverse modelling tools at global and regional scales (Enting, 1993; Tans et al., 1990; Jacobson et al., 2007; Rödenbeck et al., 2003; Gurney et al., 2002; Gourdjji et al., 2008; Lauvaux et al., 2008) together with global networks of observations, which also recently include tall tower observatories, to calculate the source-sink distribution of CO<sub>2</sub>. Tall tower observatories sample the lower atmosphere over continents up to altitudes of 200 m or more, and the resulting CO<sub>2</sub> concentration profiles provide information on regional fluxes. In order to better resolve the responses of various vegetation types and the impact of human interventions (land use change and land management) on land-atmosphere fluxes, inversions need to focus on smaller scales and to utilize continental (non-background) measurements of CO<sub>2</sub>. This becomes problematic since the aforementioned in-situ measurements are often influenced by strongly spatially and temporally varying surface fluxes (fossil fuel emissions and biosphere-atmosphere exchange) in the near field and by mesoscale transport phenomena, thus reducing their horizontal scale of representativeness (the scale at which the measurement represents the underlying process) to about 100 km (Gerbig et al., 2009).

Mountain sites, on the other hand, provide measurements with larger scale representativeness compared to measurements made from towers over flat terrain. Moreover, the longest greenhouse gas records are often from mountain sites (e.g. Schauinsland in Germany and Monte Cimone in Italy) (Levin et al., 1995; Reiter et al., 1986), making them a valuable ingredient for assessing longer term variations in carbon budgets. However, the mesoscale atmospheric transports at these sites such as mountain-valley circulations and terrain induced up-down slope circulations are found to have a strong influence on the atmospheric distribution of trace gas mixing ratios (Gangoiti et al., 2001; Pérez-Landa et al., 2007; van der Molen and Dolman, 2007). These significant variations of atmospheric concentrations appear at relatively small scales that are not resolved by current global transport models used in inversions, complicating the interpretation of these measurements. The unresolved variations can introduce significant biases in flux estimates and renders the flux estimation strongly site-selection dependent, sometimes causing the net annual sink strength of a whole continent to change by nearly a factor two (Peters, 2010). A model inter-comparison study over Europe, using various transport models with different horizontal and vertical resolutions, suggested that the fine-scale features are better resolved at increased horizontal resolution (Geels et al., 2007). Moreover, the study of (Geels et al., 2007) discusses the limitations of

using atmospheric concentration data from mountain stations in inversions due to the model's (both global and regional scale models) inability to represent complex terrain and to capture mesoscale flow patterns in mountain sites. Therefore, inversion studies usually tend to exclude the data from mountain or complex terrain sites, impose less statistical weighting (larger uncertainty), or implement temporal data filtering to the measurements (e.g. selection of nighttime only data at mountain sites).

The effect of transport errors on tracer concentrations are investigated in many studies (Lin and Gerbig, 2005; Gerbig et al., 2008; Denning et al., 2008) and the uncertainties for modeled mixing ratios during growing seasons due to the difference in advection and vertical mixing, can be as large as 5.9 ppm (Lin and Gerbig, 2005) and 3.5 ppm (Gerbig et al., 2008) respectively. Thus, it is pertinent to minimize these large and dominant uncertainties in inverse modeling systems. One approach would be to increase the spatial resolution of the models in order to capture the "fine-structures" as well as to use improved boundary layer schemes to better represent the vertical mixing. Furthermore, fluxes in the near-field of the observatories are highly variable, calling for a-priori fluxes to be specified at high spatial resolution. Detailed validations of such high-resolution forward models using networks of atmospheric measurements are needed to assess how well the transport and variability of atmospheric tracers are represented. A number of studies using high-resolution models for resolving mesoscale transport in the atmosphere showed substantial improvements in simulating atmospheric CO<sub>2</sub> concentrations under various mesoscale flow conditions (Ahmadov et al., 2009; Sarrat et al., 2007; van der Molen and Dolman, 2007; Tolk et al., 2008).

This paper uses high-resolution modeling tools together with airborne campaign measurements to address the representativeness of greenhouse gas measurements at one particular mountain site, the Ochsenkopf station (Fig. 1). The site has complex terrain with valleys and mountains (Fig. 1b), where terrain slopes influence atmospheric transport and consequently the observed mixing ratios (Thompson et al., 2009). Due to the difficulties in interpreting these measurements, the Ochsenkopf data were excluded in the global inversions of (Rödenbeck, 2005; Peters, 2010). A modeling framework consisting of a high-resolution Eulerian transport model, Weather Research and Forecasting (WRF) (<http://www.wrf-model.org/>) coupled to a diagnostic vegetation model, Vegetation Photosynthesis and Respiration Model (VPRM) (Mahadevan et al., 2008) is used to assess whether measurements can be represented sufficiently well when increasing the models' spatial resolution. The coupled model, WRF-VPRM (Ahmadov et al., 2007) simulates CO<sub>2</sub> concentrations at high spatial resolution using high-resolution CO<sub>2</sub> fluxes from net ecosystem exchange (NEE) and from fossil fuel emissions. In addition, a Lagrangian particle dispersion model, Stochastic Time-Inverted Lagrangian Transport Model (STILT) (Lin et al., 2003), driven with high-resolution



**Fig. 1.** (a) Map showing model domains used for WRF and STILT. STILT uses the larger domain covering Europe with two nests indicated by the blue rectangles. These two rectangles in blue represent the WRF domains, which are centered over OXK (50°01'N, 11°48' E, marked with “+”). A zoom of the WRF domain is shown in right-hand side of the main figure with an example of a DIMO flight track overlaid in grey lines. (b) Topography around OXK (the color gradient shows terrain height a.s.l.).

assimilated meteorological fields, is used to simulate the upstream influence on the observation point (i.e. the footprints). These footprints are then multiplied by VPRM fluxes (NEE) as well as fluxes from fossil fuel emissions in order to simulate CO<sub>2</sub> concentrations at the observation location. When the transport is adequately represented, the footprints calculated in the modeling system can be used to retrieve the source-sink distribution from CO<sub>2</sub> measurements over complex terrain at much higher spatial and temporal resolution than achievable with current global models.

The main goals of this study are: (1) to test the ability of high-resolution modeling tools to represent the spatial and temporal variability of CO<sub>2</sub> over complex terrain, compared to coarser models, (2) to infer the effect of mesoscale flows, such as mountain-valley circulations and mountain wave activities, on the observed atmospheric CO<sub>2</sub> fields and to assess how well these are reproduced in the high-resolution mod-

els, (3) to evaluate the models' reproducibility in capturing synoptic, seasonal and diurnal variability of observed CO<sub>2</sub> concentrations and (4) to assess the possibility of using these measurements in future inversion studies. In order to meet these goals, the simulations from the high-resolution modeling framework are compared with observations from various data streams as well as with simulations from a coarse resolution model. The target is to be able to retrieve fluxes from inverse modelling with an accuracy of 10 % on monthly time scales; hence this criterion is used to assess the model performance. As the simulated CO<sub>2</sub> concentrations are based on a combination of transport and flux modeling which are both associated with uncertainties, the method will yield an upper bound for the transport error compatible with the 10 % flux uncertainty. The paper is structured as follows: Sect. 2 describes briefly the data and the model set-up. In Sect. 3, the simulations from our high-resolution modeling framework are presented together with the observations as well as global model simulations. These results are discussed and conclusions are given in Sects. 4 and 5.

## 2 Data and modeling system

### 2.1 Tower and airborne measurements

The tower at Ochsenkopf is 163 m tall and is located in the second highest peak of Fichtelgebirge mountain range (1022 m a.s.l.; 50°1'48"N, 11°48'30"E) in Germany. The surrounded area of the tower is covered predominantly with conifer forest and has low population as well as industrial activity. The Ochsenkopf tall tower (from now on referred to as OXK) was instrumented as part of the European project – CHIOTTO (Continuous High-precision Tall Tower Observations of greenhouse gases) to establish a tall tower observation network for the continuous monitoring of the most important greenhouse gases over the European continent. OXK has been operated by the Max Planck Institute of Biogeochemistry, Jena, for continuous measurements of CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O, CO, SF<sub>6</sub>, O<sub>2</sub>/N<sub>2</sub>, and isotopes, in addition to meteorological parameters, and after re-equipping with instruments data are available since the beginning of 2006 (Thompson et al., 2009). For this study, we used high precision ( $\pm 0.02$  ppm) CO<sub>2</sub> measurements made at three heights (23 m, 90 m and 163 m) on OXK for different seasons. CO<sub>2</sub> is sampled at 2-minute intervals from all three heights in a 3-hour cycle with 1 h for each height. The meteorological observations from the tower: temperature and relative humidity at 90 m and 163 m, pressure at 90 m, and wind speed and direction at 163 m, are also analyzed.

Measurements from wind profilers can be used to infer the state of air flow and dynamics within the tropospheric column. These can be used to evaluate the model in predicting vertical gradients of meteorological variables, which are associated with the transport of tracer

constituents in the atmosphere. For this purpose, wind profiler measurements at Bayreuth, Germany (49.98° N, 11.68° E, 514 m a.s.l, <http://www.metoffice.gov.uk/science/specialist/cwinde/profiler/bayreuth.html>) are used. These comparisons shall give insight into the mesoscale flow patterns around OXK and help assess how well these are represented in the model.

Apart from tower-based data, we used the measurements from an airborne campaign with the METAIR-DIMO aircraft (<http://www.metair.ch/>) over Ochsenkopf. The high precision aircraft measurements, sampling air horizontally and vertically, are designed to understand the regional patterns of CO<sub>2</sub>, the influence of surface fluxes in the near-field, as well as atmospheric mesoscale transport and vertical mixing. In particular at Ochsenkopf, it is necessary to assess the influence of terrain-induced circulations on the mixing of atmospheric trace gases, which would create errors in inverse estimates of fluxes. The campaign was carried out during October 2008, covering an area around OXK (see Fig. 1) where the air was sampled for species such as CO<sub>2</sub>, CO and meteorological parameters, such as wind velocity, pressure, relative humidity and potential temperature, were measured. The boundary layer, up to several kilometers upwind of Ochsenkopf, was probed with multiple profiles during these flights. The fast and accurate measurement of CO<sub>2</sub> was achieved with an open path IRGA LI-7500 (greenhouse-gas analyzer), fitted to a LICO2 (modified closed path IRGA LI-6262) and then to flask samples, with a resolution of 20 Hz, which was down-sampled to 10 Hz to give an accuracy of better than 0.5 ppm. For more details about measuring systems, see <http://www.metair.ch/>.

## 2.2 Modeling system

We used two high-resolution transport models WRF (Eulerian) and STILT (Lagrangian), coupled to a biosphere model, VPRM, to simulate distribution of atmospheric CO<sub>2</sub>. Both of these coupled models, WRF-VPRM and STILT-VPRM were provided with same high-resolution surface fluxes as well as initial tracer concentrations at the boundaries.

VPRM computes biospheric fluxes (NEE) at high spatial resolution by using MODIS satellite indices (<http://modis.gsfc.nasa.gov/>), i.e. Enhanced Vegetation Index (EVI) and Land Surface Water Index (LSWI), and simulated WRF meteorological fields, i.e. temperature at 2 m and short wave radiation fluxes. VPRM uses eight vegetation classes with different parameters for each class to calculate CO<sub>2</sub> fluxes. These parameters were optimized against eddy flux measurements for different biomes in Europe collected during the CarboEurope IP experiment (<http://www.carboeurope.org/>). Further details on VPRM can be found in (Mahadevan et al., 2008).

High-resolution fossil fuel emission data, at a spatial resolution of 10 km, are prescribed from IER (Institut für Energiewirtschaft und Rationelle Energieanwendung),

University of Stuttgart, Germany (<http://carboeurope.ier.uni-stuttgart.de/>) to account for anthropogenic fluxes. Initial and lateral CO<sub>2</sub> tracer boundary conditions are calculated by a global atmospheric Tracer transport model, TM3 (Heimann and Koerner, 2003), with a spatial resolution of 4° × 5°, 19 vertical levels and a temporal resolution of 3 h. We use analyzed CO<sub>2</sub> fields (available at: <http://www.bgc-jena.mpg.de/~christian.roedenbeck/download-CO2-3D/>) that are consistent with atmospheric observations at many observing stations around the globe, generated by the forward transport of previously optimized fluxes (i.e. by an inversion).

In the coupled model, WRF-VPRM, the domain is set up for a small region (~ 500 × 500 km<sup>2</sup>, hereafter referred as “WRF domain”) centered over the OXK, and is nested with a horizontal resolution of 6 km (parent) and 2 km (nested) as well as with 41 vertical levels (thickness of the lowest layer is about 18 m) (Fig. 1a). Each day of simulation starts at 18:00 UTC of the previous day, and continues with hourly output for 30 h of which the first 6 h are used for meteorological spin-up. CO<sub>2</sub> fields for each subsequent 30-hour run are initialized after the meteorological spin up with the previous day’s final CO<sub>2</sub> fields. The coupled model STILT-VPRM (Matross et al., 2006) is set up with a domain covering most of Europe, and virtual particles were transported backward in time for a maximum of 15 days. Trajectories were driven with WRF meteorology until particles left the WRF domain, and with ECMWF (<http://www.ecmwf.int/>) meteorology (horizontal resolution of approximately 25 km) for the rest of the domain. The sub-grid scale turbulence in STILT-VPRM is modeled as stochastic Markov chain. In STILT-VPRM, receptors are either located at different measurement levels on the tower or at different altitudes covering the flight track of the aircraft. The vertical mixing height ( $z_i$ ) is slightly different in WRF and STILT, although the same meteorological (for the STILT nested domains) and surface flux fields were used. For more detailed information on these coupled models (WRF-VPRM and STILT-VPRM), the reader is referred to (Ahmadov et al., 2007; Nehr Korn, 2010; Pillai et al., 2010). Note that STILT-VPRM uses a different model domain (Europe) than WRF-VPRM, using additional meteorological information from ECMWF outside the WRF domain as mentioned above.

A continuous record of meteorological fields and CO<sub>2</sub> concentrations from a tower allows the evaluation of models for different seasons as well as for different measurement levels. Model simulations were carried out for May (spring), August (summer), October (autumn) in 2006, and March (winter) in 2008. In addition to this, simulations were carried out for October 2008 in order to evaluate the models against the DIMO aircraft measurements to assess the model’s ability to reproduce CO<sub>2</sub> distributions over the Ochsenkopf mountain region.

### 3 Results

Here we present high-resolution simulations of meteorology (by WRF) and CO<sub>2</sub> (by WRF-VPRM and STILT-VPRM) at 2 km resolution around OXK. The models are evaluated using wind profiler, tower and airborne measurements of meteorological parameters and CO<sub>2</sub> concentrations. These model evaluations assess the ability of the high-resolution model framework to simulate atmospheric transport and to capture the spatial and temporal variability of atmospheric CO<sub>2</sub>.

#### 3.1 Model evaluation: meteorology

##### 3.1.1 Wind profiler

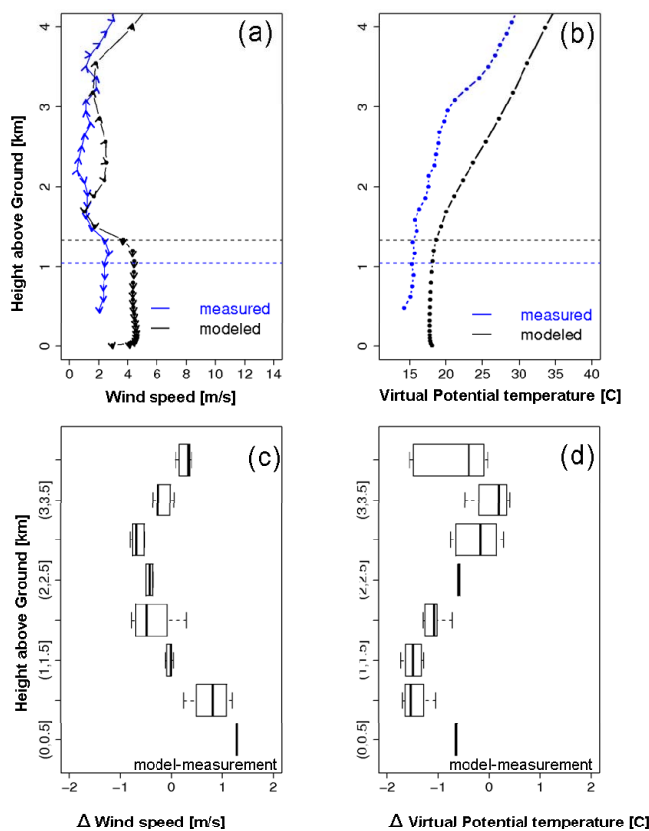
Vertical profiles of meteorological fields are validated for 2 to 30 August 2006 with the measurements provided by the Bayreuth wind profiler, located about 10 km south-west of OXK. For demonstration, a comparison of measured and modeled wind and temperature profiles on 3 August 2006 at 15:00 UTC is shown in Fig. 2a and b. The time period was chosen as representative for the model performance when the boundary layer is well-mixed. The observed prevailing wind direction was northerly for the atmospheric column below 2 km which was also reproduced by the model simulation. For a thin vertical layer, between 2.3 and 3.2 km, the prevailing wind direction changed to south-east; however the model simulated a north-westerly wind. Above 3.2 km, both observations and simulations indicated a south-westerly wind. The magnitude of the wind was overestimated in the model, particularly in the boundary layer (bias:  $\sim +2 \text{ m s}^{-1}$ ).

A model-measurement comparison of the vertical profile of virtual potential temperature ( $\theta_v$ ) showed an overestimation of simulated  $\theta_v$ . A relatively gradual increase in  $\theta_v$  (compared to simulations) was observed for the thin vertical layer between 2.3 and 3.2 km which could not be captured in the model. A possible reason for the decrease in  $\theta_v$  could be the intrusion of air from south-east direction on this layer (see Fig. 2a for wind direction) that existed for a short period of time.

To analyze the overall agreement, the monthly averages of profiles for wind-speed and  $\theta_v$ , both measured and simulated, are produced at 15:00 UTC and the model-measurement mismatches are shown in Fig. 2c and d. The result shows that the model overestimated wind-speed in the boundary layer and in contrast showed a slight underestimation for the free troposphere. In general, the model slightly underestimated  $\theta_v$  profiles, particularly in the boundary layer. Overall, the model could capture much of the variability in the vertical profiles of wind-speed and  $\theta_v$ .

##### 3.1.2 Tower

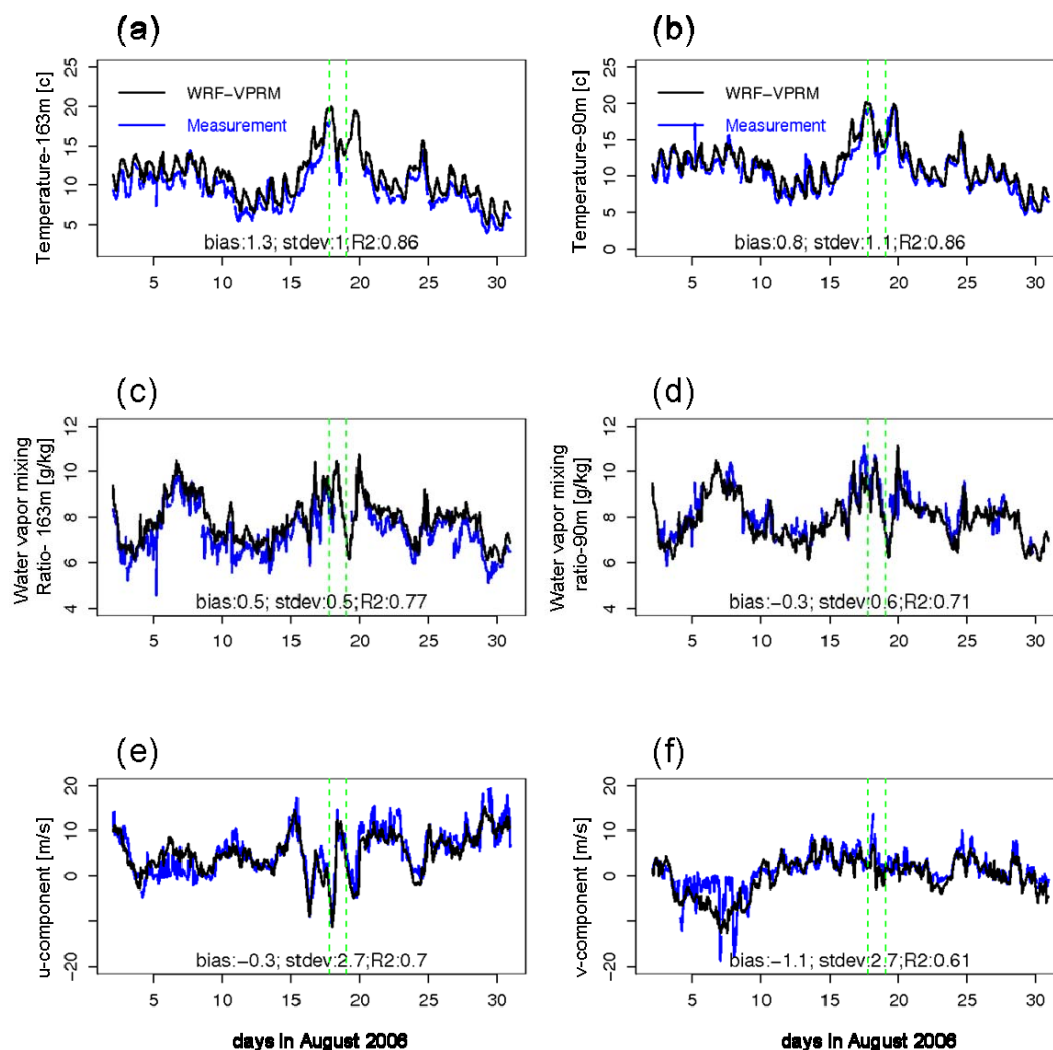
Evaluations of the modeled meteorology are carried out at different measurement levels on the tower for different seasons. An example of those validations is demonstrated here.



**Fig. 2.** (a–b) Profiles of observed vs. modeled wind fields and virtual potential temperature for 3 August 2006 at 15:00 UTC. The horizontal direction of wind is indicated with arrowheads. The dashed horizontal lines represent both observed (in blue) and simulated (in black) mixing heights calculated using bulk Richardson method. (c–d) the model-measurement mismatch for the monthly averages of these fields at 15:00 UTC, plotted against different altitude bins. The box indicates 95 % quartile, the whisker denotes minimum and maximum of deviations and the vertical bar inside the box denotes the median.

Figure 3 shows time series' of observed and WRF-simulated variables (temperature, relative humidity and wind components) for August 2006. The plot shows the prevailing weather situation and also the model capability to predict these variables, which can drive atmospheric CO<sub>2</sub> variability over OXK.

Simulated atmospheric temperatures at two different levels (90 m and 163 m) on the tower agree well with observations (squared correlation coefficient,  $R^2 = 0.86$  and bias = 0.8 to 1.3 °C) (Figs. 3a, b) and captured reasonably well the diurnal variability of temperature. Note that the model layers relative to the model terrain are used for all comparisons unless otherwise mentioned. This good temperature agreement suggests that uncertainties in the (simulated) temperature dependent VPRM respiration fluxes caused by temperature biases are expected to be small on synoptic time scales.



**Fig. 3.** Comparison of measured and modeled meteorological parameters for August 2006 at the OXK site: (a–b) temperature at 163 m and 90 m, (c–d) water vapor mixing ratio at 163 m and 90 m and (e–f) horizontal components of wind at 163 m. The green dotted vertical lines denotes the passage of a cold front investigated in detail (see Sect. 4.1).

The transport of moisture (comparable to CO<sub>2</sub> transport) in the model was validated by comparing the measured and simulated water vapor mixing ratio at two levels. The model agrees well with the observations ( $R^2 = 0.71$  to  $0.77$ ) with slight biases (Figs. 3c and d).

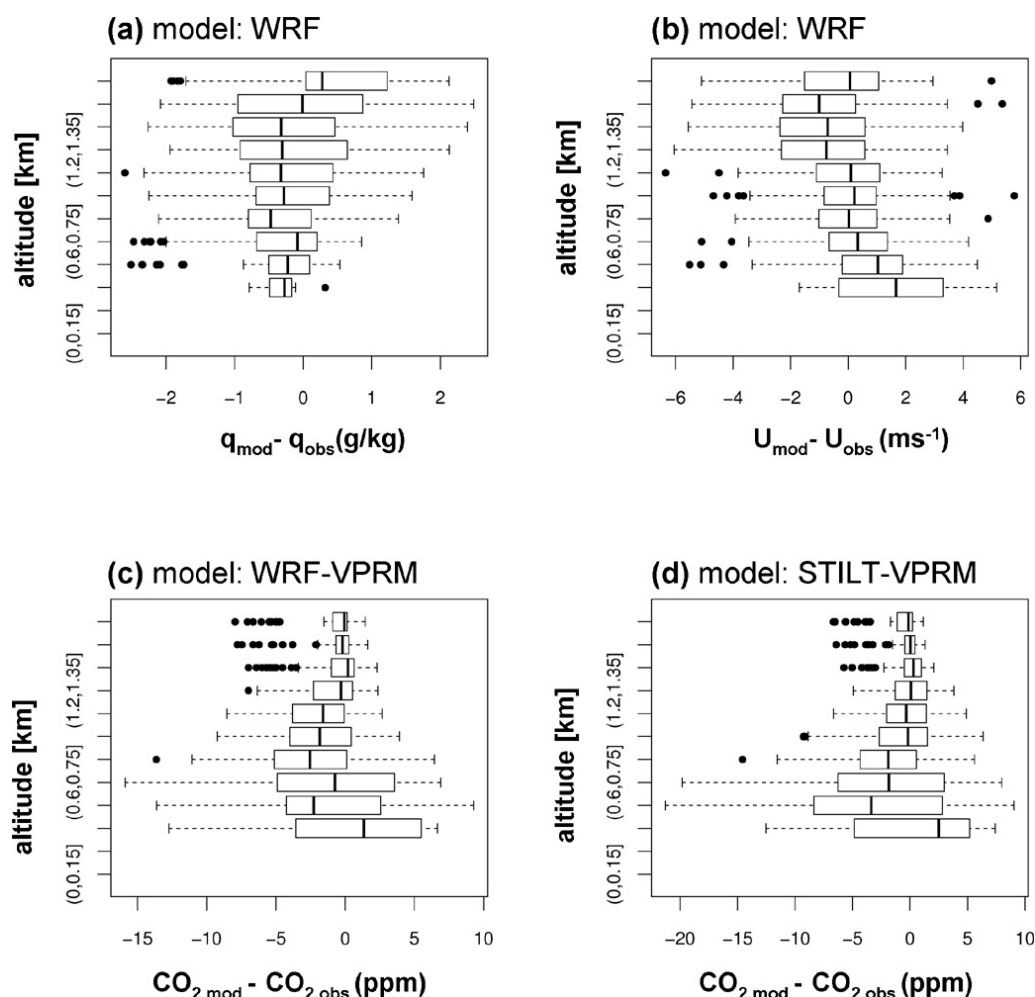
The wind speed and direction was also predicted reasonably well. A comparison of horizontal components of observed and modeled wind components  $u$  (east-west) and  $v$  (north-south) at 163 m (Figs. 3e and f) demonstrates fairly good agreement between observations and simulations ( $R^2 = 0.70$  and  $0.61$  respectively).

Table 1 gives the overall model performance (model bias, standard deviation of model-measurement mismatch and squared correlation coefficient of the model-measurement agreement) from comparing the hourly time series of observed and simulated meteorological fields at the avail-

able measurement levels for different seasons. The summary statistics indicate that WRF could follow the seasonal changes in the atmospheric transport and dynamics in most of the cases.

### 3.1.3 DIMO campaign

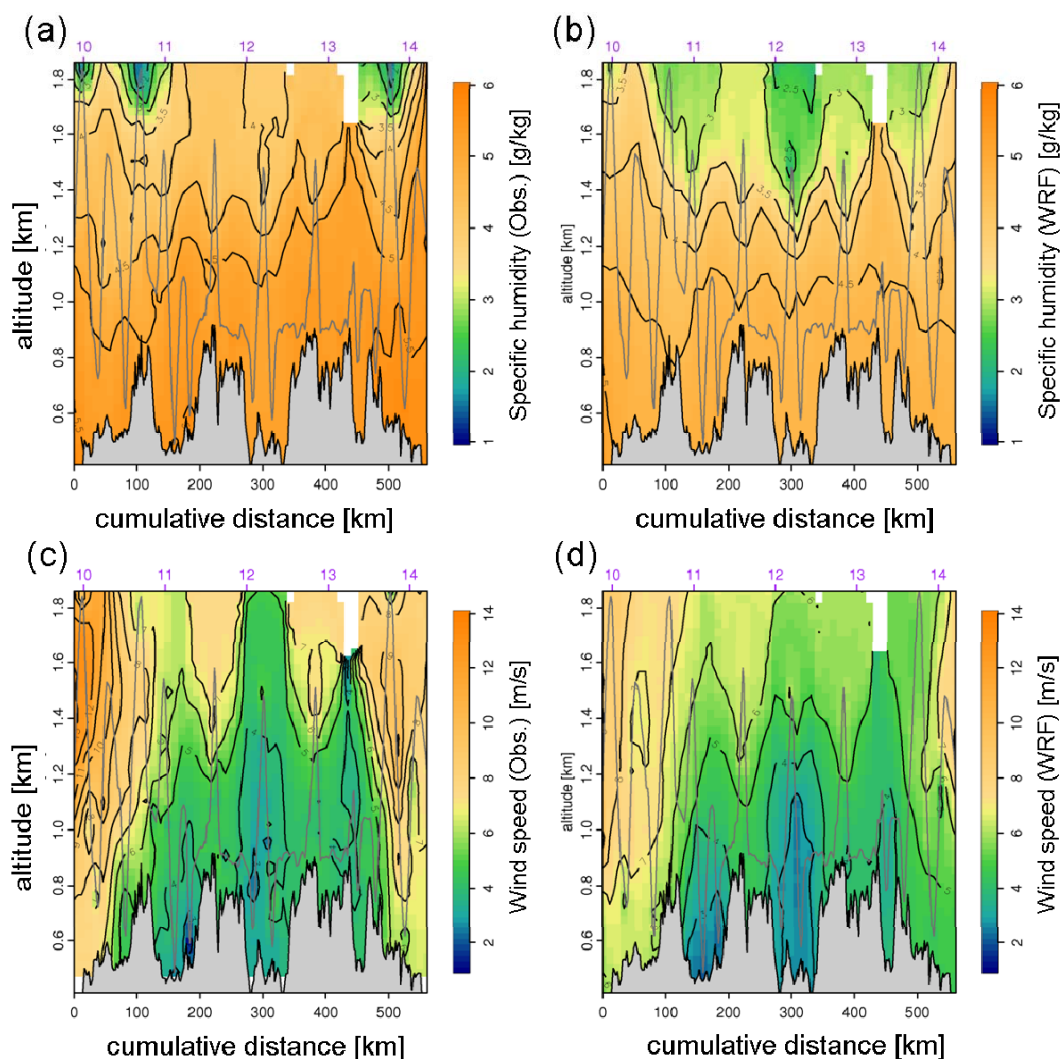
Vertical distributions of meteorological fields were validated against the DIMO profiles around the Ochsenkopf mountain region for all campaign days. The box-whisker plot (Figs. 4a, b) of the model-measurement mismatch (from all aircraft profiles) provides an overview of the model performance on simulating specific humidity and wind speed. In general, WRF meteorological simulations agree well with the DIMO observations as indicated by the lower median ( $+0.25 \text{ g kg}^{-1}$  for water vapor mixing ratio and  $-0.06 \text{ m s}^{-1}$  for wind speed



**Fig. 4.** The box-whisker plot of model mismatch (simulations-observations) using all aircraft profiles for (a) specific humidity, (b) wind speed and (c) CO<sub>2</sub> (WRF-VPRM) (d) CO<sub>2</sub> (STILT-VPRM). The box indicates 95 % quartile, the whisker denotes minimum and maximum of deviations and the vertical bar inside the box denotes the median. Black dots are outliers.

**Table 1.** Summary statistics of observed and simulated (WRF) meteorological fields (model bias (bias), standard deviation of the difference between the model and the data (sd) and squared correlation coefficient  $R^2$ ) using hourly time series at available measurement levels for different seasons. The bias and sd are in SI units of respective meteorological fields.

Season	Level	Temperature			Water vapor mixing ratio			u-component			v-component		
		bias	sd	$R^2$	bias	sd	$R^2$	bias	sd	$R^2$	bias	sd	$R^2$
Spring (May 2006)	163	1.2	1.4	0.81	0.7	0.5	0.87	0.9	3.1	0.92	1.2	2.3	0.66
	90	0.7	1.3	0.80	0.2	0.7	0.66	–	–	–	–	–	–
Summer (Aug 2006)	163	1.3	1.0	0.86	0.5	0.5	0.77	0.3	2.7	0.70	1.1	2.7	0.61
	90	0.8	1.1	0.86	–0.3	0.6	0.71	–	–	–	–	–	–
Autumn (Oct 2006)	163	0.2	1.7	0.68	0.6	1.0	0.79	2.2	3.4	0.81	0.2	3.0	0.65
	90	–0.1	1.6	0.67	–0.1	1.1	0.73	–	–	–	–	–	–
Winter (Mar 2008)	163	1.4	0.9	0.93	0.2	0.4	0.88	0.6	6.4	0.48	1.2	5.0	0.33
	90	1.2	1.0	0.91	–0.1	0.5	0.81	–	–	–	–	–	–



**Fig. 5.** Vertical cross section (using a distance weighted interpolation) of the observed and simulated meteorological fields as a function of distance flown by the aircraft for 19 October 2008: (a–b) specific humidity in  $\text{g kg}^{-1}$  (c–d) Wind speed in  $\text{m s}^{-1}$ . (a) and (c) represent measurements and (b) and (d) represent WRF simulations. The grey lines indicate flight track and the shaded grey region represents terrain elevation. See Fig. 7d for aircraft track showing altitude above ground. Time of the measurements/simulations is given in the top x-axis.

while using all available observations and simulations) and 95 % quartile ( $1.5 \text{ g kg}^{-1}$  for specific humidity and  $3.2 \text{ m s}^{-1}$  for wind speed). Noteworthy is that the model-measurement mismatch for water vapor mixing ratio increases with increasing height.

As an example, we demonstrate the model-measurement comparison for 19 October 2008 from 10:00 to 14:00 UTC. During this period, the air was sampled intensively near the top of OXK and the surrounding mountain ridges and valleys (Fig. 5c). Figure 5 shows the vertical cross-section of the observed and modeled meteorological fields (wind speed and specific humidity) as a function of distance flown by the aircraft (Cumulative Distance, hereafter referred to simply as distance). WRF reproduced specific humidity fairly well at the surface layers; however, it showed an underestimation

in the upper vertical levels (Fig. 5a, b). A relatively calm wind ( $2$  to  $5 \text{ m s}^{-1}$ ) was observed over Ochsenkopf mountain ranges during this period except in the early hours of the campaign. This was predicted well in WRF with negligible bias (Fig. 5c, d).

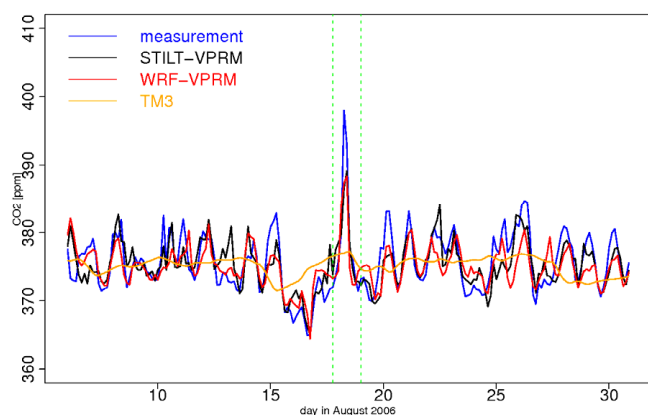
### 3.2 Model evaluation: CO<sub>2</sub> concentrations

Similar to Sect. 3.1, here we use observations of CO<sub>2</sub> fields at OXK and during the DIMO aircraft campaign for the evaluation of the models (WRF-VPRM and STILT-VPRM). As mentioned in the Sect. 1, we target at a monthly averaged flux uncertainty (in  $\mu\text{moles}/(\text{m}^2 \text{ s}^{-1})$ ) with the upper boundary of 10 %. This flux criterion can abide a monthly averaged transport model bias of 0.4 to 0.6 ppm, which is obtained



**Table 2.** Summary statistics of observed and simulated CO<sub>2</sub> fields (model bias (bias), standard deviation of the differences (sd) and squared correlation coefficient  $R^2$ ) using 3-hourly time series at available measurement levels for different seasons. Simulated fields are provided by TM3, STILT-VPRM and WRF-VPRM. The bias and sd are in ppm units.

Season	Level	TM3			STILT-VPRM			WRF-VPRM		
		bias	sd	$R^2$	bias	sd	$R^2$	bias	sd	$R^2$
Spring (May 2006)	163	-1.9	3.1	0.11	-1.7	3.0	0.33	1.4	2.7	0.41
	90	-1.7	3.2	0.16	-1.7	2.8	0.50	1.4	2.4	0.57
	23	-1.1	4.1	0.09	-1.6	2.8	0.58	1.6	2.8	0.58
Summer (Aug 2006)	163	0.5	4.0	0.01	0.6	2.8	0.50	0.8	2.9	0.46
	90	0.4	4.8	0.02	0.3	3.2	0.58	0.6	3.3	0.55
	23	0.8	5.0	0.01	-0.1	3.4	0.52	0.5	3.1	0.62
Autumn (Oct 2006)	163	2.6	3.9	0.39	-0.5	3.1	0.59	0.6	3.3	0.51
	90	3.4	4.7	0.29	-0.4	3.4	0.62	0.6	3.9	0.52
	23	4.6	5.5	0.21	-0.4	4.4	0.52	0.3	4.7	0.49
Winter (Mar 2008)	163	1.6	2.1	0.17	-0.5	2.2	0.20	0.5	2.3	0.23
	90	1.5	2.1	0.19	-0.8	1.8	0.42	0.4	2.2	0.30
	23	2.1	2.6	0.14	-0.8	2.4	0.37	0.5	2.6	0.32



**Fig. 6.** Comparison of measured and modeled CO<sub>2</sub> concentrations for August 2006 at 90 m on the OXK. A period between dashed green vertical bars denotes a synoptic event during 00:00 to 15:00 UTC on 18 August 2006 (see also Sect. 4.1).

by transporting biospheric CO<sub>2</sub> fluxes from uptake (gross ecosystem exchange) or release (ecosystem respiration) during the growing period with an additional flux uncertainty of 10 % on a monthly scale.

### 3.2.1 Tower

The observed atmospheric CO<sub>2</sub> concentrations at different measurement levels are compared with simulations generated by WRF-VPRM and STILT-VPRM for different seasons. For illustration, we show the time series comparison of CO<sub>2</sub> concentrations at 90 m level on the tower for the period from 2 to 30 August 2006 (Fig. 6). The period is chosen due

to its enhanced biospheric activity and the existence of strong diurnal patterns in transport and fluxes which can complicate the measurement interpretation. For comparison, the CO<sub>2</sub> analyzed fields from TM3 with 3-hourly time steps are also included. The observed atmospheric CO<sub>2</sub> shows large diurnal and synoptic variability and notably, these large variations in atmospheric CO<sub>2</sub> were not captured in the TM3 global model. Note that the generation of analyzed CO<sub>2</sub> fields (by atmospheric inversion) did not include OXK CO<sub>2</sub> data, so in this sense they can be used for independent validation. The comparison becomes more favorable when high-resolution transport and fluxes are used. Most of the observed temporal patterns in CO<sub>2</sub> concentrations on the tower is reproduced remarkably well in both high-resolution models ( $R^2 = 0.55$  to  $0.58$ ) when compared to TM3 ( $R^2 = 0.02$ , see Fig. 6). The high-resolution models slightly overestimated the CO<sub>2</sub> concentrations with biases ranging from 0.3 to 0.6 ppm (Table 2), which is in the targeted range (10 %) of the monthly averaged flux uncertainty. The better performance of high-resolution models points to the fact that most of the variations in CO<sub>2</sub> are due to surface flux variations and mesoscale transport processes on scales not resolved by TM3, which has a grid-cell size of several hundred kilometers. Also note that TM3 uses coarse resolution terrain elevation data.

In addition to August (summer) 2006, CO<sub>2</sub> concentrations are also validated for other seasons and the summary statistics (similar to Table 1) of the model-measurement comparison are given in Table 2. Observations from other levels (23 m and 163 m) on the tower are also used to assess the models' performance in reproducing the vertical structure of CO<sub>2</sub> in the atmospheric column. The summary statistics

clearly indicate that high-resolution models are able to predict reasonably well the temporal patterns of CO<sub>2</sub> (measured at three different vertical levels on the tower) for different seasons when compared to the coarse resolution model. Section 3.2.4 discusses further the seasonal variability of CO<sub>2</sub> concentrations.

In this context, it is interesting to assess what is the minimum spatial resolution of the model which is required to represent OXK (CO<sub>2</sub>) measurements that would enable to design the future regional inversion system at the lowest possible computational requirements. This assessment was accomplished by performing WRF-VPRM simulations at different spatial resolutions such as 6 km × 6 km, 12 km × 12 km and 24 km × 24 km and by evaluating those simulations against measurements. Table 3 gives the summary statistics of the model performance. The result indicates that there is a strong degradation of the model performance when decreasing the model spatial resolution to 24 km, compared to 6 km (100 % increment in model bias, 46 % increment in standard deviation of the difference and 150 % reduction in squared correlation coefficient). The model at 24 km resolution could not capture most of the nocturnal variability as compared to higher resolutions. The simulations from other resolutions (6 km and 12 km) can be argued to be of similar quality in most of the cases. This suggests that a minimum spatial resolution of 12 km is required to represent OXK CO<sub>2</sub> measurements.

### 3.2.2 DIMO campaign

The profiles of atmospheric CO<sub>2</sub> concentrations obtained from the aircraft campaign were used to examine how well the models can reproduce the vertical distribution of tracer concentrations over the Ochsenkopf mountain region. Figure 4c shows the statistical analysis of model-measurement mismatches using CO<sub>2</sub> profiles for all days in the campaign. The median of all residuals is 0.5 (1.1) ppm for STILT-VPRM (WRF-VPRM). The model-measurement mismatch of CO<sub>2</sub> for both models increases with decreasing heights, the opposite of what was found for water vapor. The reasons can be: (1) the large variability of CO<sub>2</sub> at the surface compared to higher levels (Pillai et al., 2010), (2) improper representation of boundary layer vertical mixing in the models and, (3) water vapor has sinks (precipitation) in the atmosphere, while CO<sub>2</sub> has not.

The same period that was chosen for DIMO meteorological validations is used also here as an example to demonstrate the vertical distribution of CO<sub>2</sub>. Figure 7 shows the vertical cross section of the observed and simulated CO<sub>2</sub> concentration as a function of distance for 19 October 2008 from 10:00 to 14:00 UTC. Compared to summer months, higher values of CO<sub>2</sub> are generally expected due to lower biosphere uptake and shallower vertical mixing. Accumulation of CO<sub>2</sub> in the valley south of OXK was observed in the morning (10:30–11:30 UTC) between the aircraft's cumulative flown distance

**Table 3.** Summary statistics of observed and simulated CO<sub>2</sub> fields for various model resolutions. The statistics includes model bias (bias), standard deviation of the differences (sd) and squared correlation coefficient ( $R^2$ ) which are calculated using 3-hourly time series data, separately for different data selections for the measurement level at 23 m during August 2006. Simulated fields are generated by WRF-VPRM. The bias and sd are in ppm units.

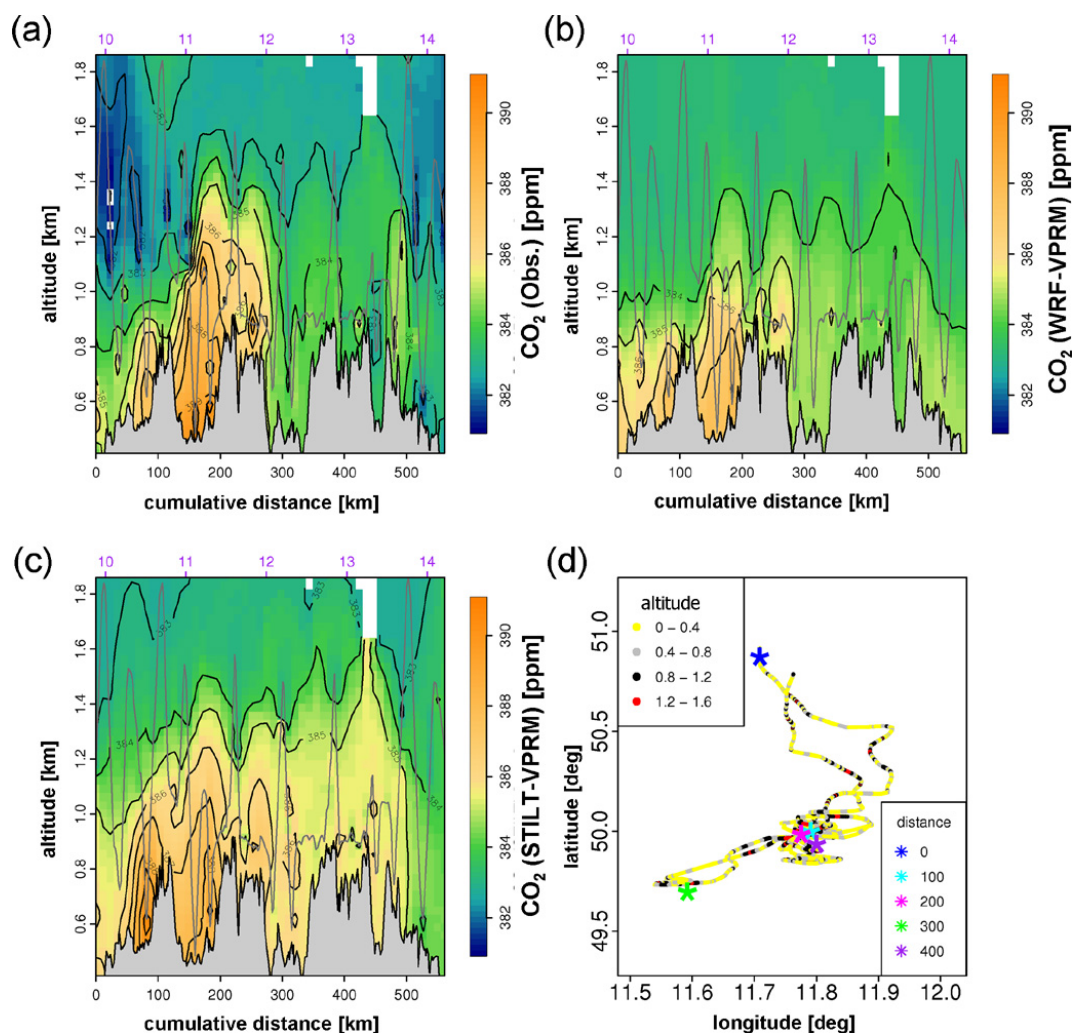
Data selection	Resolution km × km	WRF-VPRM		
		bias	sd	$R^2$
all [00:00 to 23:00 h]	6 × 6	0.3	3.4	0.52
	12 × 12	−0.3	3.5	0.48
	24 × 24	0.6	5.1	0.19
day-time only [12:00 to 18:00 h]	6 × 6	−0.1	2.4	0.53
	12 × 12	−0.6	2.7	0.38
	24 × 24	−0.6	2.9	0.28
night-time only [00:00 to 06:00 h]	6 × 6	0.7	3.8	0.32
	12 × 12	0.3	3.8	0.32
	24 × 24	2.4	6.5	0.04

range 120 and 200 km (see Fig. 7a). CO<sub>2</sub> can accumulate in valleys under shallow vertical mixing in the nocturnal boundary layer as well as under nocturnal drainage conditions in complex terrain. The valley-mountain gradient in CO<sub>2</sub> concentrations in the valley decreased rapidly in the afternoon with the establishment of convective mixing and consequently enhanced vertical turbulence. STILT-VPRM and WRF-VPRM were able to capture relatively well the CO<sub>2</sub> accumulation in the valley in the morning (distance between 100 and 200 km); however WRF-VPRM slightly underestimated the vertical extent of valley accumulation during this period. At noon (distance between 280 and 320 km), STILT-VPRM overestimated the CO<sub>2</sub> concentrations and this overestimation can also be seen in the afternoon when the boundary layer is well mixed.

## 4 Discussion

### 4.1 Synoptic variability

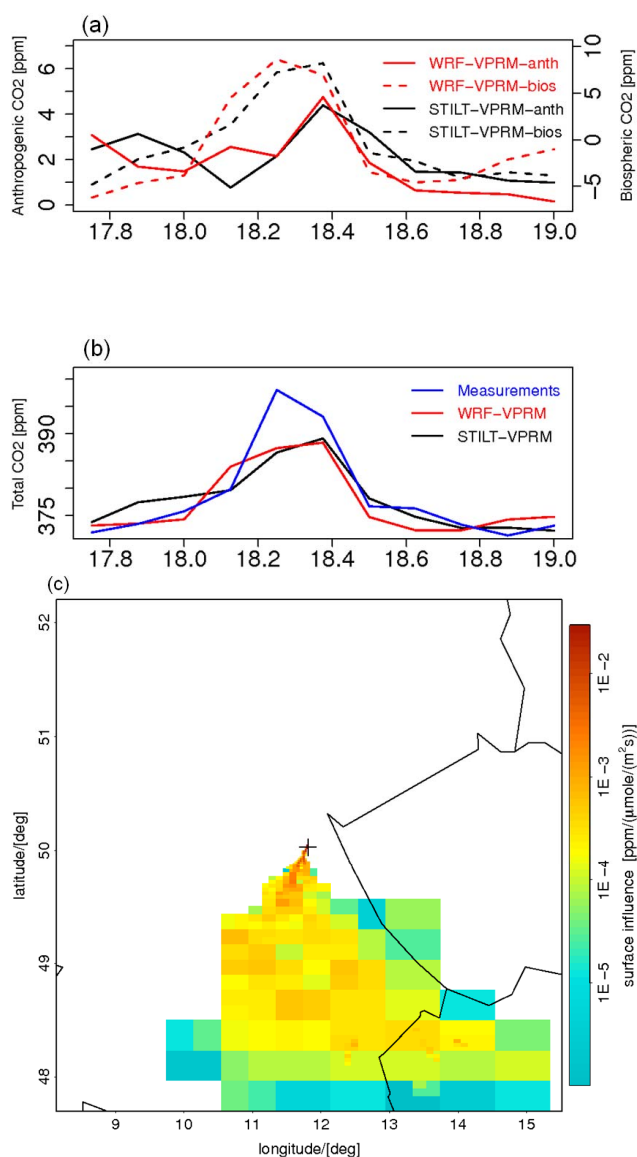
The observations show considerable synoptic variability in CO<sub>2</sub> concentrations which are driven by atmospheric transport and surface flux heterogeneity. These synoptic variations in tracer concentrations provide valuable information on spatiotemporal patterns of surface fluxes and thus can be used in atmospheric inversion to construct regional fluxes. A synoptic event (cold front), observed on 18 August 2006, during which the observed CO<sub>2</sub> showed an enhancement of more than 20 ppm, is analyzed in detail to examine how such variations are represented by the mesoscale models. In the beginning of the event, the air temperature dropped significantly with a relatively sharp increase in humidity (Fig. 3a



**Fig. 7.** Vertical cross section (using a distance weighted interpolation) of the observed and simulated CO<sub>2</sub> fields (given in ppm) as a function of distance flown by the aircraft (cumulative distance) for 19 October 2008: (a) measurements (b) WRF-VPRM (c) STILT-VPRM and (d) Flight track with color gradient showing altitude range (legend at the top left-hand side of the panel) above ground. The symbol “\*” denotes cumulative distance in km (legend at the bottom right-hand side of the panel). In (a–c), the time of measurements/simulations is given in the top x-axis.

to d). The wind speed was relatively high, reaching a maximum of  $15 \text{ m s}^{-1}$ . The atmospheric CO<sub>2</sub> observation shows a large peak during this period, which was captured by both models as seen in Figs. 6, 8a and 8b. However the models predict this elevated concentration with a considerable low bias of  $\sim 15$  ppm. During the event, the air was coming from the south-west, and the time integrated footprints derived from STILT (sensitivity of mixing ratio at 07:00 UTC on 18 August to surface fluxes integrated over the past 48 h), shows a strong influence from the highly industrialized area in the south-west part of Germany occurring 10 h prior to the measurement (Fig. 8c). Tracer simulations, where anthropogenic and biospheric contributions within the domain are separated, show a large contribution from respiration and emission fluxes for the event (Fig. 8a) and consequently an

increase in CO<sub>2</sub> concentration in the atmosphere (Fig. 8b), which reached a peak in the early morning, owing to the shallow mixing in the nocturnal boundary layer. These higher concentrations started decreasing with the development of the convective mixed layer combined with the drawdown of CO<sub>2</sub> by photosynthesis. The above analysis suggests that OXK during this event was highly influenced by air carrying a large contribution from respiration, but also emissions originating from densely populated and industrialized area. The underestimation of the CO<sub>2</sub> peak in the models could be due to several reasons: (1) uncertainties in vertical mixing (this is the more likely scenario as it would strongly affect the vertical distribution of tracer concentrations, producing large model-measurement mismatches) (2) uncertainties in advection (WRF underestimated the wind speed in the beginning



**Fig. 8.** Influence of surface fluxes on measured CO<sub>2</sub> concentration at OXK: (a) and (b) Time series of simulated anthropogenic and biospheric CO<sub>2</sub> signals (contribution of anthropogenic and biospheric fluxes to the total CO<sub>2</sub>) at 90 m on the tower during 17–18 August 2006. (c) Time integrated footprints derived by STILT on 18 August 2006 at 07:00 UTC for particles running –48 h (backward in time) from tower (indicated with + sign).

of the event and predicted south-easterly wind rather than the observed south-westerly wind direction. The strong south-westerly wind might be associated with advection of large plumes of CO<sub>2</sub> (respired and anthropogenic) to the measurement location (3) the underestimation of anthropogenic emissions in the inventory for this area of influence (uncertainties of emission inventories at small spatial and short temporal scales can easily be as large as 50 % (Olivier et al., 1999) (4) uncertainties in the VPRM respiration fluxes (note

that VPRM simulates respiration fluxes as a linear function of the simulated surface temperature (at 2 m). The uncertainty due to a temperature bias is likely to be small because the simulated temperature for this period is fairly in good agreement with observations. However, the respiration fluxes in reality are not only controlled by temperature but also by other factors such as soil moisture.) (5) underestimation of TM3 initial fields (it is more unlikely that a short term event, which originated outside of Europe domain, would have had an influence on this). This emphasizes the complexities of mechanisms involved in such short-term scale events. The vertical profiling of CO<sub>2</sub> (as like DIMO aircraft campaign) or wind profiler measurements can be helpful to assess the impact of vertical mixing on tracer concentrations).

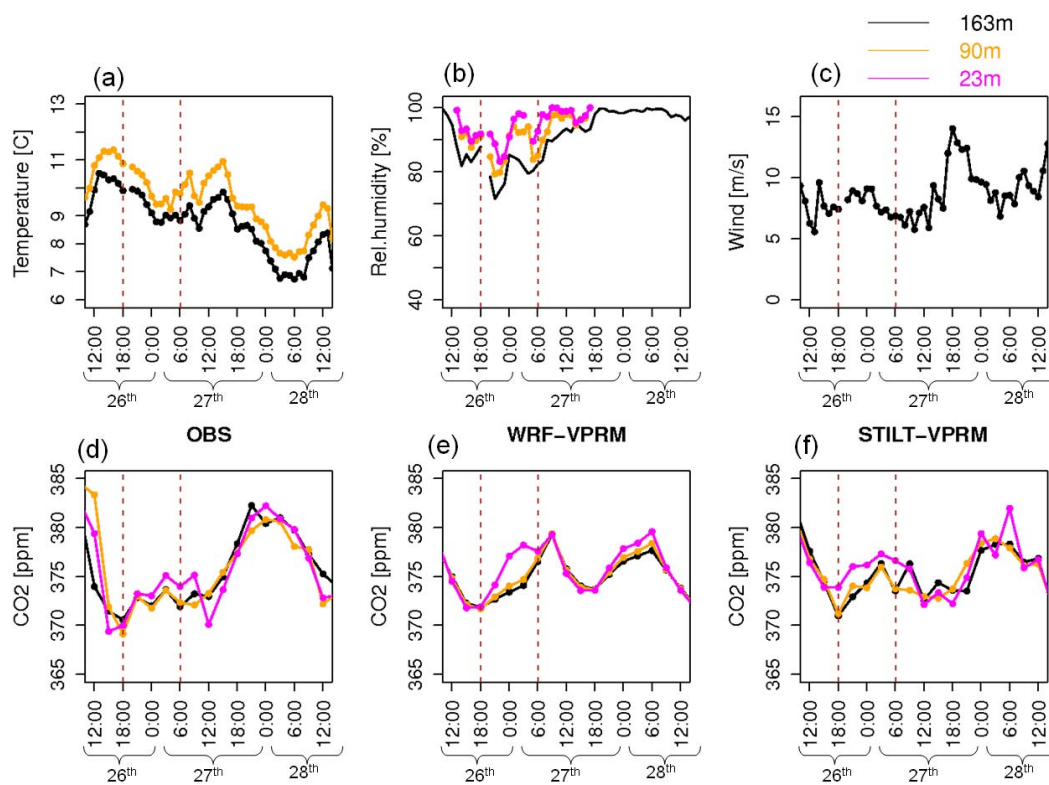
In general, both high-resolution models could capture the general trend of CO<sub>2</sub> variability during this synoptic event, by simulating well the influence of surface fluxes in the near-field and the atmosphere dynamics.

## 4.2 Orographic effect

The mountainous terrain can influence the regional circulation pattern around the tower site, resulting in local flow patterns which can have an impact on diurnal patterns in tracer concentration measurements. The local flow patterns are developed by the formation of (1) thermally forced mountain-valley circulations in response to radiative heating and cooling of the surface and (2) topographically induced stationary gravity waves (i.e., mountain waves) when stable flow encounters a mountain barrier. The downslope flows are more common at OXK during nighttime although mountain gravity waves are also likely in winter periods (based on WRF simulations as well as photographs taken during DIMO campaign).

### 4.2.1 Mountain-valley circulations

The mountain valley flows can change the atmospheric vertical mixing and can thus influence tracer measurements at OXK (Thompson et al., 2009). An example of such an event occurred at nighttime between 26 and 27 August 2006 is demonstrated in Fig. 9. During this period, the expected nocturnal CO<sub>2</sub> build up at OXK was found to be nearly absent owing to the thermally induced drainage flow. The data shown are the time series of meteorological and CO<sub>2</sub> observations at each level on the tower for a period from 26 to 28 August 2006. The period between the brown vertical dashed lines in Fig. 9 shows evidence of mountain-valley circulation. Also the period was under weak synoptic pressure gradient conditions (as indicated by the simulated potential temperature) with a prevailing westerly flow (as indicated by the simulated wind speed) (Fig. 10a, c). The observed temperature and wind speed during this period (Fig. 9a, b) also suggest that the conditions were favorable for the formation of a buoyancy-driven downslope flow. Following radiative



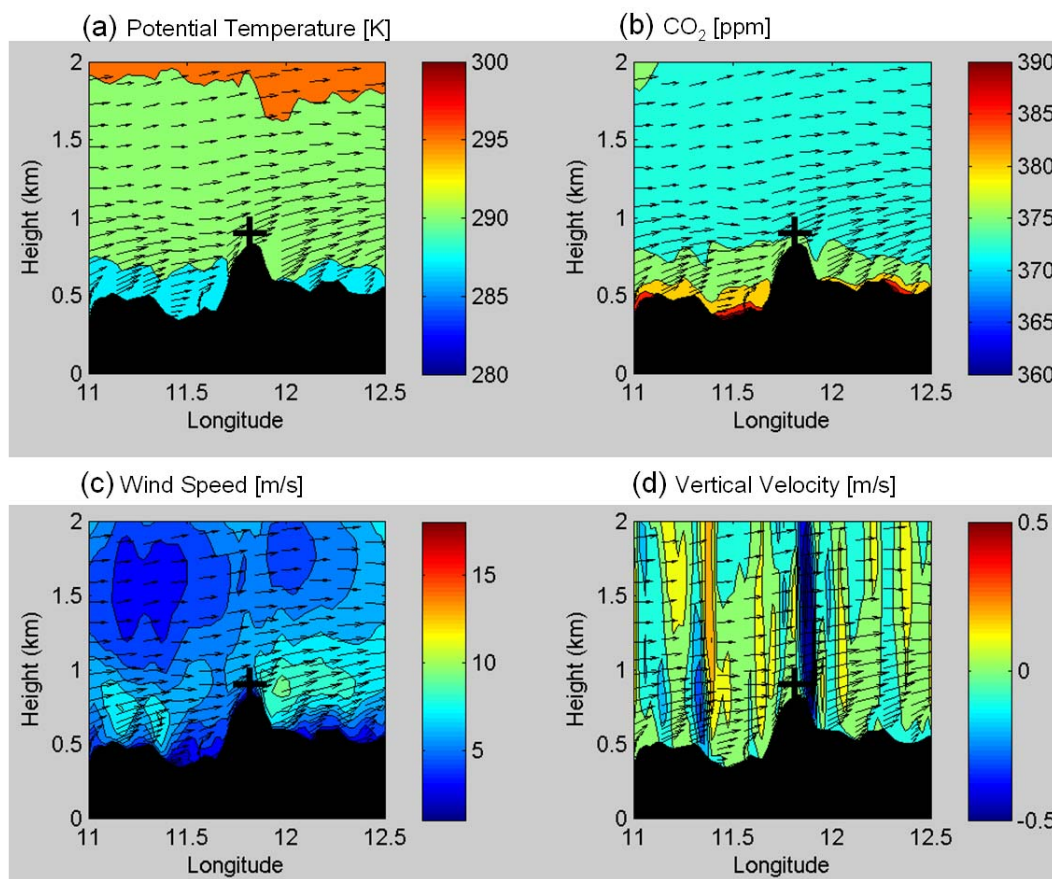
**Fig. 9.** Time series of meteorological parameters and CO<sub>2</sub> concentrations for different levels at OXK site during 26–28 August 2006: (a–c) observed air-temperature, relative humidity and wind speed respectively (d–f) CO<sub>2</sub> concentration, observed and modeled by WRF and STILT, respectively. The area between dashed brown vertical bars denotes the period under mountain-valley circulation. The x-axis shows hours in UTC; the horizontal extent of curly bracket at the bottom of x-axis shows the day on August 2006.

cooling of the surface on 26 August, relatively dry air intruded from the free troposphere into the nocturnal boundary layer, which was observed as a sharp decrease in the relative humidity (Fig. 9b). Noticeable time lags in the transition from moist to dry air were seen at the different sampling levels, which also indicate the intrusion of air from above. The evidence of dry air subsidence from the residual layer can also be seen later at 06:00 UTC on 27 August. Consequently, a decrease in CO<sub>2</sub> concentration was observed at 00:00 UTC and at 06:00 UTC on 27 August due to the replacement of air by the residual layer containing lower CO<sub>2</sub> concentration. STILT-VPRM captured well the lowering of CO<sub>2</sub> concentration at 06:00 UTC in response to the drainage flow and simulated well-mixed tracer concentrations in the nocturnal boundary layer. However WRF-VPRM showed an unrealistic accumulation of CO<sub>2</sub> concentration at the lower level which might be associated with the underestimation in the vertical extent of the entrainment air reaching the tower site. The presence of katabatic flow on the lee side of the mountain was predicted in WRF, indicated by the negative vertical velocity (downward movement of air) and increased wind speed along the mountain slope (Fig. 10d). The (simulated) impact of drainage flow on the tracer concentrations

on the lee side of the mountain can be seen as a region of lower CO<sub>2</sub> contours in Fig. 10b.

#### 4.2.2 Mountain wave activity

The buoyancy driven upslope and downslope flows, which are discussed above, are less common in winter due to low surface heating. As mentioned earlier, under stable stratified nocturnal boundary conditions, mountain gravity waves can be formed when air flow is perturbed with a barrier (e.g. mountain). Propagation of gravity waves transporting mass and energy in the stable boundary layer can affect tracer concentrations measured at the tower. The possible occurrence of gravity waves can be assessed by estimating the Froude number (Stull, 1988),  $Fr$  (the ratio of inertial to gravitational forces,  $= \frac{U}{(N \times h)}$ ) which relates the prevailing horizontal wind speed ( $U$ ), mountain height ( $h$ ) and buoyancy oscillation frequency (Brunt-Väisälä frequency,  $N$ -calculated as a function of potential temperature). When  $Fr$  is near unity, the wavelength of the air flow is in resonance with the mountain size, creating trapped mountain lee waves which results in strong downslope winds and enhanced turbulence on the lee side of the mountain.

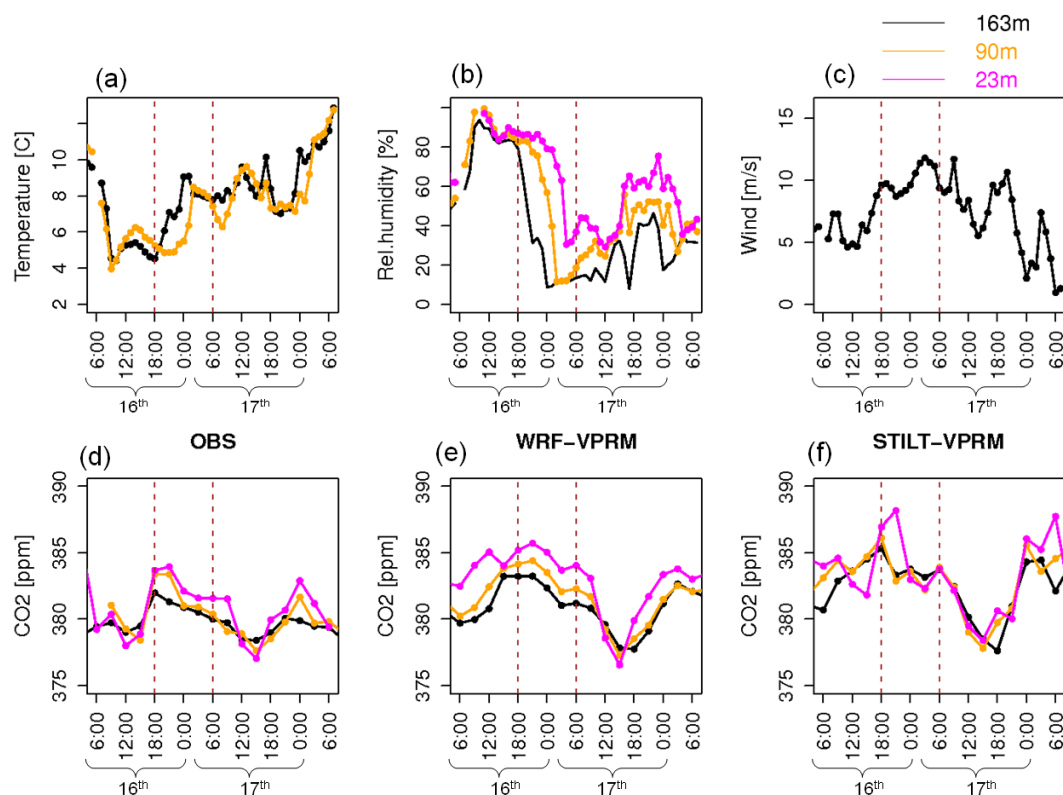


**Fig. 10.** Vertical cross section along OXK latitude ( $50^{\circ}01' \text{ N}$ ) on 27 August 2006 at 01:00 UTC, showing WRF-VPRM simulated (a) Potential temperature in Kelvin (b) CO<sub>2</sub> concentration in ppm (c) Wind speed in  $\text{m s}^{-1}$  and (d) Vertical velocity in  $\text{m s}^{-1}$ . The overlaid arrows indicate prevailed wind direction at different altitudes; the symbol “+” indicates OXK location.

However, the mountain wave activity is much more complex in reality and is difficult to interpret its effects on measurements. An ideal case of such an activity was occurred at a nighttime between 16 and 17 October 2006 (between brown dashed lines in Fig. 11). A temperature inversion was observed during this period (Fig. 11a) indicating the stable atmospheric conditions. The sharp decrease in observed relative humidity on the tower under relatively high wind speed indicates the presence of possible mountain wave activity with intrusion of dry air on the lee side of the mountain. These meteorological features were predicted reasonably well by the WRF model and the west-east cross section of simulated vertical velocity shows the downward movement of air at the lee side of the mountain (Fig. 12d). Note that the WRF simulations might not always capture the waves correctly and the caution has to be taken to interpret the structures of the vertical velocity fields which can also be formed due to the numerical noise. The increased gradient in the simulated potential temperature, together with higher values of simulated vertical velocity ( $50 \text{ cm s}^{-1}$ ) and strong wind speed, suggests the occurrence of mountain wave phe-

nomena at the OXK site (Fig. 12). The Froude number was found to be close to unity, indicating the likelihood of gravity wave (mountain wave) activity. In addition to this, the simulated wavelengths  $\lambda (= \frac{U}{N})$  for the region over the mountain were found to be close to the mountain height, showing the existence of vertically propagating mountain waves.

Following the collapse of the convective boundary layer on 16 October, CO<sub>2</sub> started to build up in the nocturnal shallow boundary layer and showed a distinctive gradient between layers for a few hours between 18:00–21:00 UTC. These nocturnal developments of CO<sub>2</sub> were captured in STILT-VPRM; however the vertical mixing between levels at 23 m and 90 m was underestimated. Corresponding to the prevailing mesoscale feature, the observed nocturnal gradient in tracer concentrations disappeared in response to the descent of air from the free troposphere. This was reproduced well in STILT-VPRM, while WRF-VPRM showed the decreasing tendency of CO<sub>2</sub> concentrations on this period but with an unrealistic gradient between the layers (00:00 to 06:00 UTC during 16–17 October 2006), which might be due to the underestimated mixing process. Note that vertical



**Fig. 11.** Time series of meteorological parameters and CO<sub>2</sub> concentrations for different levels at Ochsenkopf tower site during 16–17 October 2006: (a–c) observed air-temperature, relative humidity and wind speed respectively (d–f) CO<sub>2</sub> concentration-observed, modeled by WRF and STILT respectively. The area between dashed brown vertical bars denotes the period under mountain wave activity. The x-axis shows hours in UTC; the horizontal extent of curly bracket at the bottom of x-axis shows the day on October 2006.

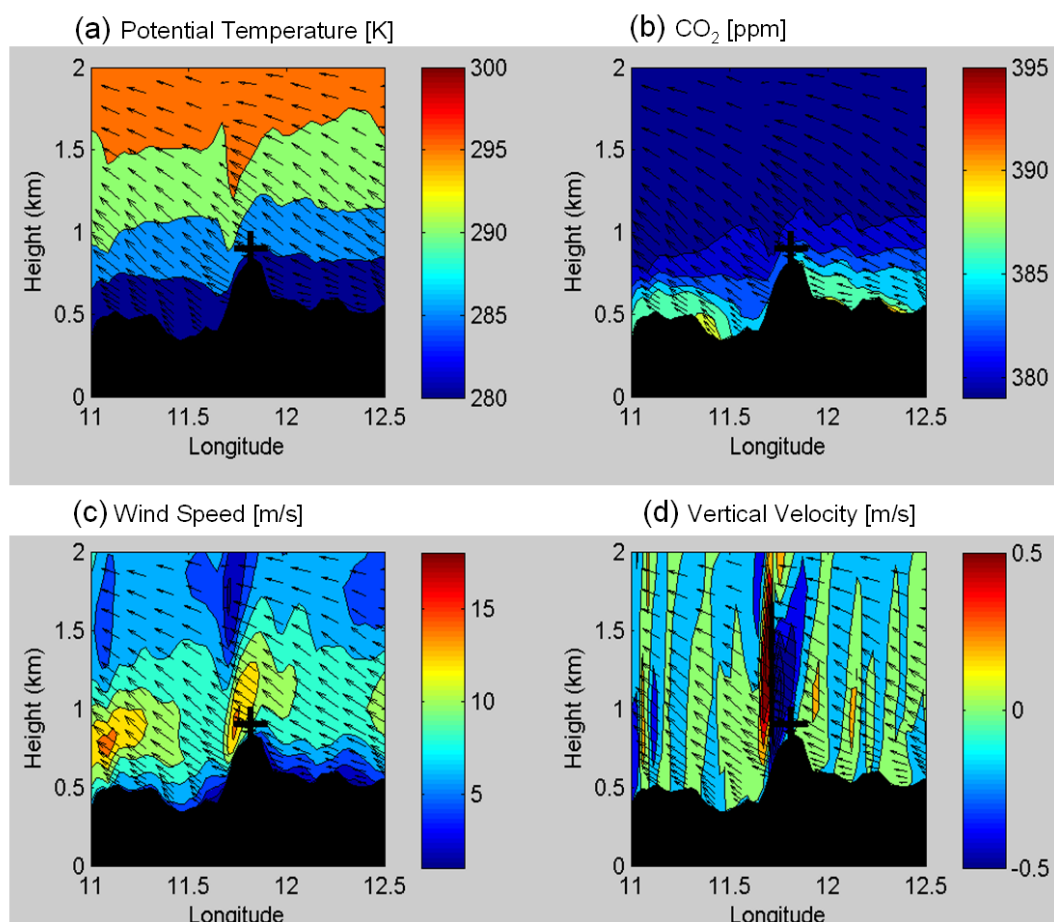
mixing is parameterized slightly differently in WRF-VPRM and STILT-VPRM. The influence of mountain waves on generating turbulent vertical mixing of nocturnal tracer concentrations at the lee side of the valley can be seen in the WRF-VPRM simulations (Fig. 12b). Owing to the strong downward movement of air and vertical mixing, a layer of lower CO<sub>2</sub> concentration was simulated for the western slope of the mountain, despite the nocturnal build-up period. The nocturnal build-up of CO<sub>2</sub> under shallow mixing and weak biological CO<sub>2</sub> uptake were simulated for the other valleys (Fig. 12b).

The above two case studies suggest that changes in the atmospheric transport and mixing in response to mesoscale phenomena, such as mountain-valley circulations and mountain wave activities, can strongly affect the diurnal patterns of CO<sub>2</sub> concentrations at OXK, and that these can be represented well in mesoscale models at the resolution of 2 km.

### 4.3 Seasonal variability

Different seasonal aspects, such as changes in thermal circulation patterns (changes in solar radiation), changes in diurnal patterns of vertical mixing, effects of snow cover and

diurnal variations in surface fluxes, can have an important influence on measured tracer concentrations. Seasonal changes in the diurnal patterns of CO<sub>2</sub> concentration are observed at Ochsenkopf mountain station as it can be influenced by heterogeneous land sources and sinks as well as by synoptic atmospheric conditions. Figure 13 shows averaged diurnal cycles of observed and modeled CO<sub>2</sub> at different measurement levels and for different seasons. Except for the level 163 m in winter and autumn, the CO<sub>2</sub> concentration maxima were observed during nighttime due to the accumulation of CO<sub>2</sub> concentration in the shallow nocturnal boundary layer. The measurement level at 163 m during winter and autumn is more representative of free tropospheric or residual layer air, as indicated by the weak diurnal changes in observed concentrations and by the decoupling relative to the lower levels. The slight daytime increase at the 163 m level, delayed by about six hours compared to the lower levels, is consistent with the daytime mixing of air previously trapped in the stable mixed layer, containing remnants of respired CO<sub>2</sub> from the previous night. The amplitude of the diurnal cycle is larger in spring and summer months (~8 ppm), consistent with the enhanced biospheric activity (photosynthesis and ecosystem respiration), whereas the amplitude is



**Fig. 12.** Vertical cross section along OXK latitude ( $50^{\circ}01''$  N) on 17 October 2006 at 02:00 UTC, showing WRF-VPRM simulated (a) Potential temperature in Kelvin (b) CO<sub>2</sub> concentration in ppm (c) Wind speed in  $\text{m s}^{-1}$  and (d) Vertical velocity in  $\text{m s}^{-1}$ . The overlaid arrows indicate wind direction at different altitudes.

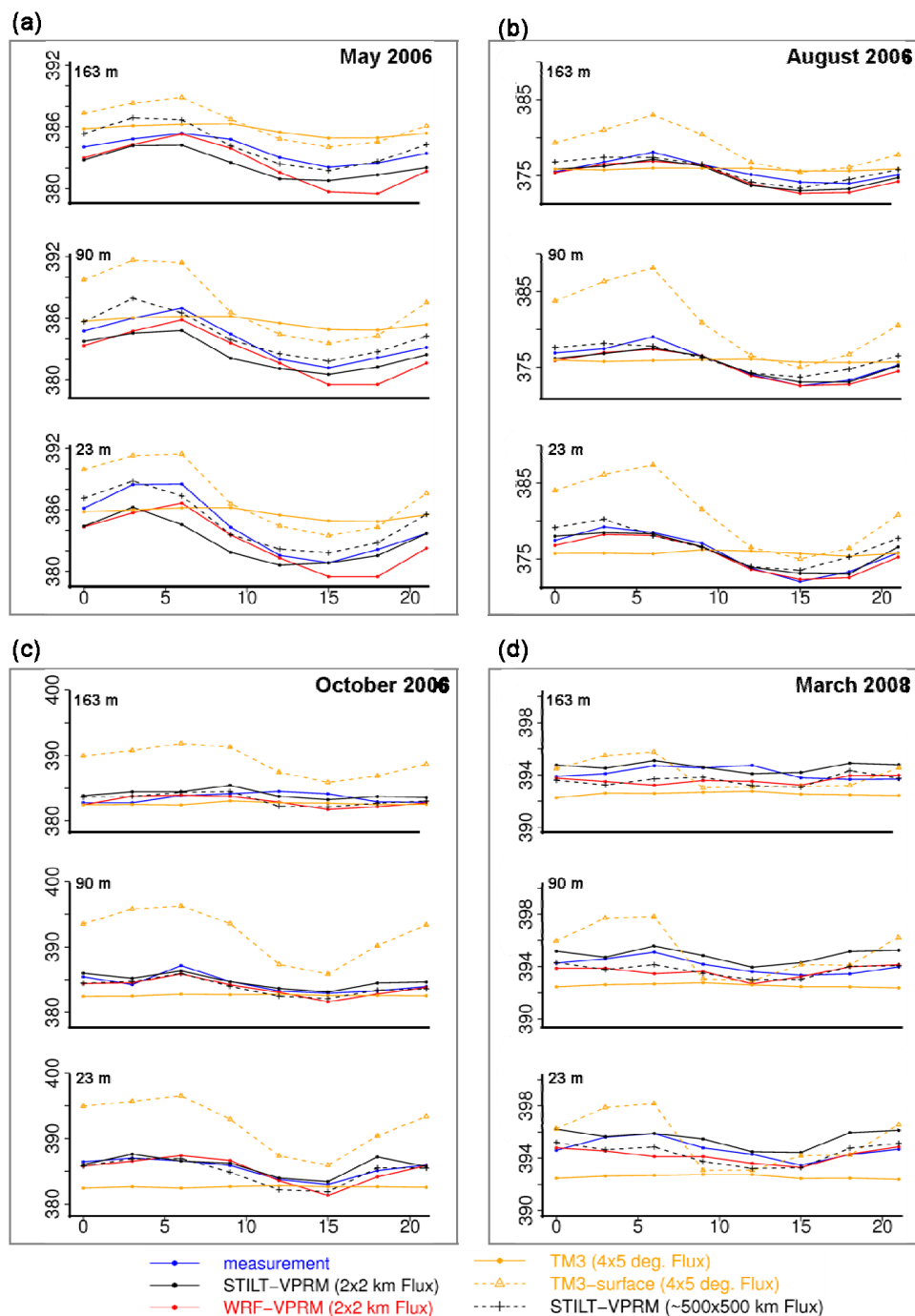
smaller in autumn and winter months owing to the reduced diurnal variability in the terrestrial fluxes. The low values of CO<sub>2</sub> are noticeable in August (active growing season) due to enhanced biospheric CO<sub>2</sub> uptake. The model-measurement agreement is fairly good for higher resolution models, except for the level 163 m in winter and autumn seasons where both models overestimate the vertical mixing. The coarse resolution TM3 analyzed CO<sub>2</sub> fields (taken from 940 hPa) TM3 pressure level which corresponds to the measurement levels above sea level, i.e. relative to the sea level; indicated as “TM3” in Fig. 13) show little diurnal change during all seasons and at all levels. On the other hand, TM3 analyzed CO<sub>2</sub> fields corresponding to the model levels close to the measurement levels from the surface, i.e. relative to the model terrain (taken from 1013 hPa and 1002 hPa TM3 pressure levels corresponding to the levels on the tower; indicated as “TM3-surface” in Fig. 13) show large diurnal variability due to the strong influence of surface fluxes near the ground, but with large positive biases in most of the cases. This discrepancy can lead to potential biases in flux esti-

mates when using measurements from a site like OXK, as discussed above. Again, this suggests the importance of using high-resolution models to resolve the large variability of atmospheric CO<sub>2</sub> concentrations in response to variability in surface fluxes and mesoscale transport. In order to examine whether the poor performances of TM3 are caused by the coarse resolution flux fields (horizontal resolution:  $4^{\circ} \times 5^{\circ}$ ), we run STILT-VPRM with biospheric fluxes aggregated to  $\sim 500 \text{ km} \times 500 \text{ km}$  resolution, comparable to the TM3 resolution. CO<sub>2</sub> simulated by this coarse resolution version of STILT-VPRM shows remarkable similarity to the high-resolution simulations by STILT and WRF in the diurnal cycle for the different seasons.

#### 4.4 Vertical distribution of CO<sub>2</sub> concentrations

The vertical profiling of atmospheric CO<sub>2</sub> during aircraft campaigns provides more information on vertical mixing in the atmosphere and provide the opportunity to evaluate current transport models. The discrepancies in predicting atmospheric mixing can lead to a strong bias in the simulated





**Fig. 13.** Averaged diurnal cycle of observed and modeled CO<sub>2</sub> for OXK at different measurement levels and for different seasons: (a) May 2006 (spring), (b) August 2006 (summer), (c) October 2006 (autumn) and (d) March 2008 (winter). In each plots, top to bottom panels represents CO<sub>2</sub> at 163 m, 90 m and 23 m respectively. x-axis: hour; y-axis: CO<sub>2</sub> concentration in ppm.

vertical distribution of CO<sub>2</sub> concentrations. An example of such an effect can be seen in Figs. 5 and 7. The underestimation of the vertical extent of CO<sub>2</sub> accumulation (as mentioned in Sect. 3.2.2, Fig. 11a, b) can be caused by the overestimation of vertical mixing in WRF. The effect of this overestimation can also be seen in the modeled specific humidity

(Fig. 5b) as low values (underestimation) in the upper layers. Note that the wind speed was predicted well in WRF with negligible bias.

It should also be mentioned that the difference in observed and modeled wind speed found at the Ochsenkopf valley for another day of the campaign (23 October 2008) generated an

underestimation of CO<sub>2</sub> concentration in both WRF-VPRM and STILT-VPRM (figure not shown). WRF underestimated the flow of air, advected from upstream locations and consequently failed to capture the huge contribution of the advected respired signal to the measurement locations. STILT-VPRM also shows a similar underestimation of CO<sub>2</sub> concentration for the same reason.

These two case studies of model evaluation with the airborne measurements show the necessity of accurately predicting the mesoscale atmospheric transport, such as advection and convection, as well as vertical mixing. Both models are able to capture the spatial variability of measured CO<sub>2</sub> concentration in the complex terrain for most of the cases and the discrepancy between models and measurements are mainly attributed to the difference in representing atmospheric PBL dynamics.

## 5 Summary and conclusions

High-resolution modeling simulations of meteorological fields and atmospheric CO<sub>2</sub> concentrations, provided by WRF-VPRM and STILT-VPRM, are presented together with measurements obtained from the Ochsenkopf tower (OXK) and from an aircraft campaign, to address the representativeness of greenhouse gas measurements over a complex terrain associated with surrounding mountain ranges. The spatial and temporal patterns of CO<sub>2</sub> are reproduced well in high-resolution models for different seasons when compared to the coarse model (TM3). This emphasizes the importance of using high-resolution modeling tools in inverse frameworks, since a small deviation in CO<sub>2</sub> concentration can lead to potentially large biases in flux estimates. The actual reduction in uncertainties of flux estimates when using high-resolution models (compared to lower-resolution models) in the inverse framework needs to be further investigated.

The measurements of CO<sub>2</sub> at OXK show diurnal, synoptic and seasonal variability of CO<sub>2</sub> due to different aspects such as changes in the diurnal patterns of vertical mixing, diurnal variations in surface fluxes, effect of front passage, changes in thermal circulation patterns etc. These variations in tracer concentrations provide valuable information on spatiotemporal patterns of surface fluxes and thus can be used in atmospheric inversions to construct regional fluxes. Both high-resolution models were able to capture this variability by simulating well the influence of surface fluxes in the near-field and the atmosphere dynamics. The model performance is assessed using a criterion of targeted monthly averaged flux uncertainty of 10 %.

The mesoscale flows, such as mountain wave activity and mountain-valley circulations, can have a strong influence on the observed atmospheric CO<sub>2</sub> at OXK by changing the vertical mixing of the tracer concentrations. The meteorological simulations by WRF indicate that the buoyancy driven drainage flows are more common at OXK during nighttime

(especially in summer) and mountain gravity waves are likely to occur in winter periods. Resolving these circulation patterns in models is a prerequisite for utilizing observations from mountain stations such as OXK with a reduced representation error.

The discrepancies in predicting vertical mixing can lead to strong biases in simulated CO<sub>2</sub> concentrations and these kinds of uncertainties are typical for complex terrain regions. The vertical profiling of CO<sub>2</sub> (like the DIMO aircraft campaign) or wind profiler measurements can be helpful in assessing the impact of vertical mixing on tracer concentrations. Our study shows that much of the variability in CO<sub>2</sub> concentrations can be reproduced well by appropriate representation of mesoscale transport processes, such as advection, convection and vertical mixing as well as surface flux influences in the near-field.

This study demonstrates the potential of using high-resolution models in the context of inverse modeling frameworks to utilize measurements provided from mountain or complex terrain sites. The model evaluation of different spatial resolutions suggests that a minimum resolution of 12 km is required to represent OXK mountain station. Our future work will focus on regional inversions using STILT-VPRM at the required resolution (e.g. 10 km × 10 km) with a nested option. The feasibility of using these high-resolution nests in global models has already been demonstrated by (Rödenbeck et al., 2009). This provides justified hope that measurements from mountain stations can be utilized in inverse modeling frameworks to derive regional CO<sub>2</sub> budgets at reduced uncertainty limits.

*Acknowledgements.* We thank Martin Heimann, Max Planck Institute of Biogeochemistry, Germany for continuing support and helpful discussions. We acknowledge Deutscher Wetterdienst (DWD), Germany for providing wind profiler data. We are also thankful to the whole Ochsenkopf tall tower team in Max Planck Institute of Biogeochemistry, Germany for their assistance in data processing.

The service charges for this open access publication have been covered by the Max Planck Society.

Edited by: P. Monks

## References

- Ahmadov, R., Gerbig, C., Kretschmer, R., Koerner, S., Neining, B., Dolman, A. J., and Sarrat, C.: Mesoscale covariance of transport and CO<sub>2</sub> fluxes: Evidence from observations and simulations using the WRF-VPRM coupled atmosphere-biosphere model, *J. Geophys. Res.-Atmos.*, 112, D22107, doi:22110.21029/22007JD008552, 2007.
- Ahmadov, R., Gerbig, C., Kretschmer, R., Krner, S., Rdenbeck, C., Bousquet, P., and Ramonet, M.: Comparing high resolution WRF-VPRM simulations and two global CO<sub>2</sub> transport models with coastal tower measurements of CO<sub>2</sub>, *Biogeosciences*, 6, 807–817, doi:10.5194/bg-6-807-2009, 2009.

- Denning, A. S., Zhang, N., Yi, C. X., Branson, M., Davis, K., Kleist, J., and Bakwin, P.: Evaluation of modeled atmospheric boundary layer depth at the WLEF tower, *Agr. Forest Meteorol.*, 148, 206–215, 2008.
- Enting, I. G.: Inverse problems in atmospheric constituent studies: III. Estimating errors in surface sources, *Inverse Probl.*, 9, 649–665, 1993.
- Gangoiti, G., M. M. Millan, R. Salvador, and Mantilla, E.: Long-range transport and re-circulation of pollutants in the western Mediterranean during the project Regional Cycles of Air Pollution in the west-central Mediterranean area, *Atmos. Environ.*, 35(36), 6267–6276, 2001.
- Geels, C., Gloor, M., Ciais, P., Bousquet, P., Peylin, P., Vermeulen, A. T., Dargaville, R., Aalto, T., Brandt, J., Christensen, J. H., Frohn, L. M., Haszpra, L., Karstens, U., Rödenbeck, C., Ramonet, M., Carboni, G., and Santaguada, R.: Comparing atmospheric transport models for future regional inversions over Europe - Part 1: mapping the atmospheric CO<sub>2</sub> signals, *Atmos. Chem. Phys.*, 7, 3461–3479, doi:10.5194/acp-7-3461-2007, 2007.
- Gerbig, C., Körner, S., and Lin, J. C.: Vertical mixing in atmospheric tracer transport models: error characterization and propagation, *Atmos. Chem. Phys.*, 8, 591–602, doi:10.5194/acp-8-591-2008, 2008.
- Gerbig, C., Dolman, A. J., and Heimann, M.: On observational and modelling strategies targeted at regional carbon exchange over continents, *Biogeosciences*, 6, 1949–1959, doi:10.5194/bg-6-1949-2009, 2009.
- Gourdji, S. M., Mueller, K. L., Schaefer, K., and Michalak, A. M.: Global monthly averaged CO<sub>2</sub> fluxes recovered using a geostatistical inverse modeling approach: 2. Results including auxiliary environmental data, *J. Geophys. Res.-Atmos.*, 113, D21115, doi:10.1029/2007JD009733, 2008.
- Gurney, K. R., Law, R. M., Denning, A. S., Rayner, P. J., Baker, D., Bousquet, P., Bruhwiler, L., Chen, Y.-H., Ciais, P., Fan, S., Fung, I. Y., Gloor, M., Heimann, M., Higuchi, K., John, J., Maki, T., Maksyutov, S., Masarie, K., Peylin, P., Prather, M., Pak, B. C., Randerson, J., Sarmiento, J., Taguchi, S., Takahashi, T., and Yuen, C.-W.: Towards robust regional estimates of CO<sub>2</sub> sources and sinks using atmospheric transport models, *Nature*, 415, 626–630, 2002.
- Heimann, M. and Koerner, S.: The global atmospheric tracer model TM3, Technical Reports, Max-Planck-Institute for Biogeochemie, 5, 131 p., 2003.
- Jacobson, A. R., Mikaloff Fletcher, S. E., Gruber, N., Sarmiento, J. L., and Gloor, M.: A joint atmosphere-ocean inversion for surface fluxes of carbon dioxide: 1. Methods and global-scale fluxes, *Global Biogeochem. Cy.*, 21, GB1019, doi:10.1029/2005GB002556, 2007.
- Lauvaux, T., Uliasz, M., Sarrat, C., Chevallier, F., Bousquet, P., Lac, C., Davis, K. J., Ciais, P., Denning, A. S., and Rayner, P. J.: Mesoscale inversion: first results from the CERES campaign with synthetic data, *Atmos. Chem. Phys.*, 8, 3459–3471, doi:10.5194/acp-8-3459-2008, 2008.
- Le Treut, H., R. Somerville, U. Cubasch, Y. Ding, C. Mauritzen, A. Mokssit, Peterson, T., and Prather, M.: Historical Overview of Climate Change, in: *Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change*, edited by: Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K. B., Tignor, M., and Miller, H. L., Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2007.
- Levin, I., Graul, R., and Trivett, N.: Long-term observations of atmospheric CO<sub>2</sub> and carbon isotopes at continental sites in Germany, *Tellus B*, 47, 23–34, 1995.
- Lin, J. C., Gerbig, C., Wofsy, S. C., Andrews, A. E., Daube, B. C., Davis, K. J., and Grainger, C. A.: A near-field tool for simulating the upstream influence of atmospheric observations: The Stochastic Time-Inverted Lagrangian Transport (STILT) model, *J. Geophys. Res.-Atmos.*, 108, 4493, doi:10.1029/2002JD003161, 2003.
- Lin, J. C., and Gerbig, C.: Accounting for the effect of transport errors on tracer inversions, *Geophys. Res. Lett.*, 32, L01802, doi:10.1029/2004GL021127, 2005.
- Mahadevan, P., Wofsy, S. C., Matross, D. M., Xiao, X., Dunn, A. L., Lin, J. C., Gerbig, C., Munger, J. W., Chow, V. Y., and Gottlieb, E. W.: A satellite-based biosphere parameterization for net ecosystem CO<sub>2</sub> exchange: Vegetation Photosynthesis and Respiration Model (VPRM), *Global Biogeochem. Cy.*, 22, GB2005, doi:10.1029/2006GB002735, 2008.
- Masek, J. G. and Collatz, J.: Estimating forest carbon fluxes in a disturbed southeastern landscape: integration of remote sensing, forest inventory, and biogeochemical modeling, *J. Geophys. Res.*, 111, G01006, doi:10.1029/2005JG000062, 2006.
- Matross, D. M., Andrews, A., Pathmathevan, M., Gerbig, C., Lin, J. C., Wofsy, S. C., Daube, B. C., Gottlieb, E. W., Chow, V. Y., Lee, J. T., Zhao, C. L., Bakwin, P. S., Munger, J. W., and Hollinger, D. Y.: Estimating regional carbon exchange in New England and Quebec by combining atmospheric, ground-based and satellite data, *Tellus B*, 58, 344–358, 2006.
- Nehrkorn, T., Eluszkiewicz, J., Wofsy, S. C., Lin, J. C., Gerbig, C., Longo, M., and Freitas, S.: Coupled weather research and forecasting—stochastic time-inverted lagrangian transport (WRF-STILT) model, *Meteorol. Atmos. Phys.*, 107, 51–64, 2010.
- Olivier, J. G. J., Bouwman, A. F., Berdowski, J. J. M., Veldt, C., Bloos, J. P. J., Visschedijk, A. J. H., and van der Maas, C. W. M.: Sectoral emission inventories of greenhouse gases for 1990 on a per country basis as well as on 1° × 1°, *Environ. Sci. Policy*, 2, 241–263, 1999.
- Pérez-Landa, G., Ciais, P., Gangoiti, G., Palau, J. L., Carrara, A., Gioli, B., Miglietta, F., Schumacher, M., Millán, M. M., and Sanz, M. J.: Mesoscale circulations over complex terrain in the Valencia coastal region, Spain - Part 2: Modeling CO<sub>2</sub> transport using idealized surface fluxes, *Atmos. Chem. Phys.*, 7, 1851–1868, doi:10.5194/acp-7-1851-2007, 2007.
- Peters, W.: Seven years of recent European net terrestrial carbon dioxide exchange constrained by atmospheric observations, *Glob. Change Biol.*, 16, 1317–1337, 2010.
- Pillai, D., Gerbig, C., Marshall, J., Ahmadov, R., Kretschmer, R., Koch, T., and Karstens, U.: High resolution modeling of CO<sub>2</sub> over Europe: implications for representation errors of satellite retrievals, *Atmos. Chem. Phys.*, 10, 83–94, doi:10.5194/acp-10-83-2010, 2010.
- Reiter, R., Sladkovic, R., and Kanter, H. J.: Concentration of trace gases in the lower troposphere, Part I: Carbon dioxide, *Meteorol. Atmos. Phys.*, 35, 187–200, 1986.
- Rödenbeck, C., Houweling, S., Gloor, M., and Heimann, M.: CO<sub>2</sub>

- flux history 1982–2001 inferred from atmospheric data using a global inversion of atmospheric transport, *Atmos. Chem. Phys.*, 3, 1919–1964, doi:10.5194/acp-3-1919-2003, 2003.
- Rödenbeck, C.: Estimating CO<sub>2</sub> sources and sinks from atmospheric mixing ratio measurements using a global inversion of atmospheric transport. Technical Report 6, Max-Planck Institut für Biogeochemie, Jena, Germany, 53 pp., 2005.
- Rödenbeck, C., Gerbig, C., Trusilova, K., and Heimann, M.: A two-step scheme for high-resolution regional atmospheric trace gas inversions based on independent models, *Atmos. Chem. Phys.*, 9, 5331–5342, doi:10.5194/acp-9-5331-2009, 2009.
- Sarrat, C., Noilhan, J., Lacarrère, P., Donier, S., Lac, C., Calvet, J. C., Dolman, A. J., Gerbig, C., Neininger, B., Ciais, P., Paris, J. D., Boumard, F., Ramonet, M., and Butet, A.: Atmospheric CO<sub>2</sub> modeling at the regional scale: Application to the CarboEurope regional experiment, *J. Geophys. Res.-Atmos.*, 112, D12105, doi:10.1029/2006JD008107, 2007.
- Stull, R. B.: *An Introduction to Boundary Layer Meteorology*, Kluwer Academic Publishers, Dordrecht, 666 pp. Webb, E.K., Pearman, 1988.
- Tans, P. P., Fung, I. Y., and Takahashi, T.: Observational constraints on the global atmospheric CO<sub>2</sub> budget, *Science*, 247, 1431–1438, 1990.
- Thompson, R. L., Manning, A. C., Gloor, E., Schultz, U., Seifert, T., Hänsel, F., Jordan, A., and Heimann, M.: In-situ measurements of oxygen, carbon monoxide and greenhouse gases from Ochsenkopf tall tower in Germany, *Atmos. Meas. Tech.*, 2, 573–591, doi:10.5194/amt-2-573-2009, 2009.
- Tolk, L. F., Meesters, A. G. C. A., Dolman, A. J., and Peters, W.: Modelling representation errors of atmospheric CO<sub>2</sub> mixing ratios at a regional scale, *Atmos. Chem. Phys.*, 8, 6587–6596, doi:10.5194/acp-8-6587-2008, 2008.
- van der Molen, M. K. and Dolman, A. J.: Regional carbon fluxes and the effect of topography on the variability of atmospheric CO<sub>2</sub>, *J. Geophys. Res.-Atmos.*, 112, D01104, doi:10.1029/2006JD007649, 2007.