The carbon balance from an atmospheric perspective

Inverse modeling of regional biospheric CO$_2$ fluxes

Lieselotte Tolk
Cover photo: Meteorological and COₒ concentration observation towers, Marmande, Southern France.

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Voorwoord en dankwoord

De wereld om ons heen, en het besef waar we deel van zijn, heeft iets fascinerends. In mijn studie stond systeem aarde centraal, en daar wilde ik meer van leren. Het relativerende besef van grote tijdlijnen, het ingenieus in elkaar grijpen van structuren, aan het eind van mijn studie was mijn nieuwsgierigheid daarnaar nog lang niet gestild. En zo begon de promotie. Met als onderwerp de robuustheid van de aarde, waarin klimaatverandering voor een groot deel wordt tegengegaan door de veerkracht van het systeem. Het romantische idee van modelleren op een regionale schaal, waar je letterlijk doorheen kan rijden. De variatie die ik probeerde te vangen kon je vanuit de trein voorbij zien flitsen. Hoe vaak heb ik niet op weg naar congressen met mijn neus tegen het raam van het vliegtuig gedrukt gezeten, in een oogopslag vrijwel het gehele domein van mijn model overziend. De onzichtbare stroming van CO₂ herkennend in de structuur van de wolken, de kleine variaties in de luchtbeweging. Op winterochtenden keek ik op de fiets altijd als vanzelfsprekend hoe de rookpluim van de VU warmtecentrale oprees, om te zien hoe hoog de atmosferische grenslaag die dag was. Het onderwerp van mijn promotie, de atmosfeer, kan je dus volledig omringen, en zo kun je ook opgaan in het modelleren ervan; we hebben tijdens het onderzoek zelfs onze eigen pseudo-werkelijkheid gecreëerd. En dit alles om uiteindelijk, op inverse wijze, de waarheid iets dichter te benaderen.

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1 Introduction

1.1 Background

Climate change has gained broad attention over the previous decades. The climate system is warming, which is evident from observations of increased global average air and ocean temperatures, melting of snow and ice, and the rising global average sea level. Moreover, there is a very high confidence that the global average net effect of human activities since 1750 has been one of warming. An important factor in this change of the climate system is the increase of atmospheric concentrations of greenhouse gases, which alter the balance of incoming and outgoing energy at the surface (Solomon et al., 2007).

The most important anthropogenic greenhouse gas is carbon dioxide (CO$_2$), which is released amongst others by fossil fuel burning. Atmospheric CO$_2$ contributes 63% of the gaseous radiative forcing responsible for anthropogenic climate change (Hofmann et al., 2006). Its concentrations have increased from the pre-industrial values of about 280 ppm to about 379 ppm in 2005, and 390 ppm in 2011, which exceeds by far the natural range over the last 650,000 years (e.g. Keeling and Whorf, 2005).

The interaction between the terrestrial biosphere and the atmosphere plays an important role in the global carbon balance, and determines partly the atmospheric CO$_2$ concentrations. The uptake of carbon by the biosphere is therefore an important component affecting, and mitigating, climate change (e.g. Canadell et al., 2007, Dolman et al., 2010). Because of the substantial impact of the biospheric fluxes on the atmospheric CO$_2$ concentration, it is important to improve our knowledge of the controlling processes, and to verify if the national emission reductions that are realized by enhanced biospheric uptake fulfill the obligations of the Kyoto framework or its successors.

Exactly the reason why biospheric fluxes are important to understand -because they affect the atmospheric CO$_2$ concentrations- provides also a method to do so. Spatial differences in the fluxes cause variations in the atmospheric CO$_2$ concentration fields. Observations of these atmospheric CO$_2$ concentration variations can thus also be used in reverse, to constrain the fluxes of the underlying terrestrial biosphere. This method is referred to as inverse modelling. The link between the surface fluxes and the observed variations in the atmosphere is obtained by modelling the atmospheric transport of the air parcel affected by surface exchange. Inverse methods thus provide an independent top-down approach to verify greenhouse gas emission based on observations of atmospheric concentrations of greenhouse gasses. Through inverse modelling the distribution and temporal evolution of CO$_2$ in the atmosphere are used to quantify surface fluxes, using numerical models of atmospheric transport as a key tool (e.g. Bousquet et al., 1999; Rayner and O’Brien, 2001; Gurney et al., 2002; Rödenbeck et al., 2003).
In this thesis such an inverse method is developed and tested for the regional scale of a few hundreds of kilometers. This is a novel application compared to previous inverse studies because of the relative small scale and the high level of detail of the models and observations used. We show in this study to what extent regional scale inverse studies can constrain the biospheric fluxes and provide an estimate of the carbon balance for a pilot area, the Netherlands.

For global and continental application the inverse method to estimate the carbon fluxes is already well established. However, these studies also showed the limitations of these less detailed approaches. Smaller scale regional inversions have therefore potentially several considerable advantages compared to coarser scale inversions, but modelling at this small and detailed scale also brings new challenges. This is described in more detail below, and against this background the purpose of this thesis is outlined.

1.1.1 Inverse modelling of carbon fluxes

Several studies showed that a terrestrial carbon sink should be present in the northern hemisphere, according to the pole-to-pole atmospheric CO$_2$ distribution, and atmospheric isotope and oxygen measurements (Tans et al., 1990; Ciais et al., 1995; Keeling et al., 1996; Rayner et al., 1999). Compared to our understanding of the system there was an excess in CO$_2$ uptake, which was referred to as the ‘missing sink’. The search for this missing sink was one of the main goals for inverse modelling of CO$_2$.

Inverse models have provided estimates of the distribution of carbon sinks and sources at a global scale, typically with a resolution in the order of continents to a few hundreds of kilometers. These studies showed large differences between the different models and algorithms used. This was pointed out in a comparison of various global inversion models that concluded that “a consensus had not yet been reached regarding the size and distribution of regional carbon fluxes obtained” (Gurney, 2002). These studies did show that the northern hemisphere was a substantial net sink of approximately 2.0-3.5 Pg C year$^{-1}$. However, the distribution of the northern hemisphere carbon uptake between the oceans, North America, Europe and Asia was still subject to many uncertainties (e.g. Fan et al., 1998; Kaminski and Heimann, 2001; Peylin et al., 2002).

Difficulties in global inverse models

The discrepancies between the results of different inversion studies appear related to a number of errors that occur in the global inversions. One of the most important was the error in the atmospheric transport model used to connect the CO$_2$ concentration observations in the atmosphere with the CO$_2$ fluxes at the surface (Rayner et al., 1995; Law et al., 1996; Gurney et al., 2002). Perfect modelling of the circulations and air movements in the atmosphere is virtually impossible. Atmospheric models remain an approximation of the atmospheric reality, and especially in global scale atmospheric models many parameterizations for example for convection and radiation are needed to simulate the atmospheric transport within the available computer power. Later, Stephens et al. (2007) showed that the transport error did not only cause a spread between the models, but also a bias in the results because of a systematic error in the simulation of the vertical atmospheric gradient. They concluded that northern terrestrial uptake of CO$_2$ plays a smaller role in the global carbon budget than previously thought. Part of the transport errors are also the so-
called “rectification” errors. The co-variation of the atmospheric transport and the seasonality and diurnal cycle of the terrestrial CO$_2$ fluxes may lead to substantial errors in the CO$_2$ flux estimate if the interaction between the two is not captured correctly, as was pointed out by Denning et al. (1996) and later at a smaller scale by Perez-Landa et al. (2007) and Ahmadov et al. (2007).

Besides an imperfect transport model, other errors related to inverse studies may also cause differences in the resulting CO$_2$ flux estimates. To allow the limited number of atmospheric CO$_2$ observations to constrain the surface fluxes, the amount of unknowns should also be limited. Therefore, some assumptions are needed about the spatial and temporal structures of the flux field, and aggregation over space and time is applied. Optimization over a large area and/or long time frame with only few unknowns to adjust the fluxes may lead to aggregation errors, because the inversion lacks flexibility to alter the prior structure of the fluxes. Aggregation to large regions was found to cause significant differences in the final results, with errors of the same order of magnitude as the fluxes themselves (Kaminski et al., 2001).

Another error, strongly related to the resolution of the inversion is the representation error. This error is introduced by the assumption in inversions that a point observation can be represented by the average CO$_2$ mixing ratio in a model grid box. However, when low resolutions, and thus large grid boxes, are used this assumption may fail. This will especially be the case above terrain with many small scale variations. This may cause substantial mismatches between the observed and simulated CO$_2$ concentrations that are not caused by erroneous surface fluxes –as is assumed in the inversions- but by variations of the CO$_2$ concentration within one grid box. The extent of representation errors was first quantified by Gerbig et al. (2003) and is also explored further, in this thesis.

Figure 1.1 Results from four recent inversions for the CO$_2$ flux estimates from atmosphere to land ecosystems over the period 2000-2004 (blue), compared to the land C sink estimate from published bottom-up accounting studies (green) and the estimated fossil fuel emissions (red). Bars denote the min–max range of different mean flux estimates from the four inversions, and whiskers the 1-sigma internal precision of each inversion or the 1-sigma uncertainty (replicated from Ciais et al., 2010).
Despite these caveats, these studies demonstrated the general feasibility of the inversion method and confirmed that the concept is promising. For example, the results at some locations were already found to be robust to the choice of transport model or methodological approach (Gurney et al., 2002). Over the last decade many studies have been performed to overcome the challenges in inverse modelling and to improve the carbon balance estimate, with a range of inversion methods. For example, the carbon fluxes have been estimated by optimizing biosphere model parameters rather than flux fields (e.g. Kaminski et al., 2002; Rayner et al., 2005), with a geostatistical approach that combined several constraints on carbon exchange (e.g. Michalak et al., 2004; Gourdji et al., 2008) and using data assimilation approaches that estimated weekly multiplicative factors at a continental scale (Peters et al., 2007). This resulted in an estimate of the mean northern hemispherical terrestrial CO$_2$ sink from the inversion models of 1.7 Pg C year$^{-1}$ over the period 2000–2004 (Ciais et al., 2010). The current estimates of the carbon fluxes including their uncertainty and their distribution over the continents is shown in figure 1.1.

1.1.2 Regional scale inversions

**Advantages of inverse modelling at high resolutions**

Parallel to the studies that aimed to constrain the fluxes at global to continental scales, regional scale inversions were developed, amongst others in this thesis. Modelling at a smaller scale has the advantage that a much larger part of the atmospheric signal may be used to constrain the carbon fluxes. A significant fraction of the information present in the signature of greenhouse gas concentrations observed within the atmospheric boundary layer is contained in relatively small spatial and temporal scales (Gerbig et al., 2003). In regional scale inversions a larger part of this information can be used, since more detail can be incorporated if the inversion is performed for a limited area rather than the full globe. Therefore, regional scale modelling provides a method to overcome a part of the difficulties and limitation of the global scale inversions (see previous section) and provides the possibility to use a much larger part of the atmospheric CO$_2$ signal to constrain the carbon balance.

An additional advantage of more detailed inverse modelling, is that the results of regional inversions, in contrast to global inversion results, can almost directly be linked with observations at the surface. These bottom-up measurements are performed with eddy covariance techniques, at towers or with aircrafts (Baldocchi et al. 2001; Valentini et al. 2000, Vellinga et al., 2010). In parallel, field studies can determine changes in vegetation and soil carbon stocks using biometric techniques. The flux estimates by these methods contain uncertainties, partly due to uncertainties in the measurements themselves, and for a large part due to uncertainties in the upscaling of a limited number of point measurements to an integral carbon balance for a full region (Schulze et al. 2000; Wirth et al. 2002; Curtis et al. 2002). Inverse modelling at the previously ‘missing scale’ of the regional level provides an independent check of the carbon flux estimates based on these bottom-up methods. Combining regional top-down and bottom-up methods may improve the quantification of the average carbon balance of ecosystems. Additionally, the surface measurement and upscaling techniques can be independently validated, which will help to further improve both bottom-up and top-down observation systems (Dolman et al., 2008).
Finally, and of considerable importance in climate mitigation policies, incorporating small scale variations in inversion studies can provide a tool to verify emissions at roughly national and perhaps sub-national levels. Therefore, it can potentially be used to check national emission reductions, as are reported to the United Nations Framework Convention on Climate Change (UNFCCC).

**Requirements for high resolution inverse modelling**

To provide input for the inversions at the required level of detail (national to sub-national levels), measurements at relatively detailed spatial and temporal levels are required, with a precision that matches that of the major processes determining the carbon sources and sinks. In the research program this PhD is a part of, high resolution observations are available, the required datasets are provided by parallel working packages within the program (further described in section 1.2).

Modelling at the high resolution brings extra challenges to the required modelling of atmospheric transport, and an accurate estimate of the uncertainty must be made. This includes the modelling of small scale variations in the wind patterns, for example due to differences at the surface. The contrast between the sensible heat fluxes over the land and the sea can for instance result in a seabreeze. Also between different types of vegetations, or cities and their surrounding, the contrast in sensible heat fluxes can cause variations in the atmospheric boundary layer height (the well mixed part of the lower atmosphere) and thus the atmospheric CO₂ concentration footprint. The challenges in small scale inverse modelling thus lay in correctly capturing both the large scale weather systems, and the more detailed atmospheric movements and their covariance with the carbon fluxes.

Concluding, to constrain fluxes at a regional scale an inverse modelling framework more tuned towards the smaller scales is required. The required level of detail needs to include high resolution modelling of (1) the variation of the CO₂ fluxes at the surface, and (2) atmospheric transport. The latter must include the variation due to the diurnal cycle, boundary layer mixing, orography, and the variations in the surface driving factors such as the surface heat flux and the surface roughness. The high resolution models, combined with high resolution observations of CO₂ concentration observations, provide a method to use a relatively large part of the atmospheric signal to constrain the carbon fluxes at a regional scale.

1.2 **Purpose and scope of this thesis**

**Background: the BSIK program**

This PhD research project was part of the Dutch ‘Besluit Subsidies Investeringen Kennisinfrastructuur’ (BSIK) program Climate for Space, section mitigation 2 (ME2): ‘Integrated observations and modelling of greenhouse gas budgets at the national level in the Netherlands’. In this project an advanced greenhouse gas information system - consisting of a comprehensive set of monitoring systems, combined with a complementary suite of 3D models- was developed, that would be able to quantify the magnitude, trends and associated uncertainties of the biogenic and anthropogenic greenhouse gas budgets at high spatial and temporal resolutions. New in this BSIK-ME2 program is the high resolution and the regional scale at which the observations and the forward and inverse modelling of sources and sinks of CO₂ are applied.
Formulation of the research questions in this thesis

The main research question addressed in this thesis is: “To what extent can we constrain the regional carbon fluxes with a high resolution atmospheric observation and modelling system?” This question can be subdivided in three components that are the focus of this thesis:

(1) the practical considerations, i.e. is it possible to develop a stable and robust nested modelling framework at the required high resolution;

(2) the performance of a high resolution inverse modelling system, i.e. what can be gained and what are the limitations when moving towards higher resolutions, and

(3) the application of the high resolution inverse modelling system to constrain the carbon balance, i.e. what can be learned about the carbon balance, in this study for the Netherlands as a pilot area.

The following tasks and objectives associated with these three components are fulfilled within this thesis:

Practical considerations

Develop a nested modelling framework for the estimation of sources and sinks of CO₂ at a regional scale:

- online coupling of atmospheric transport and surface flux modelling systems at a high resolution and develop a CO₂ nudging algorithm to prescribe CO₂ inflow and outflow for offline coupling between models at different scales;
- increase the resolution at which observations can be used in inversion studies in time and space, to use the high-frequency variation in the concentration time series, make use of all constraints imposed by the respective elements of the greenhouse gas information system;
- apply inversion algorithms based on Eulerian models at the regional scale.

Performance

Evaluate the performance and the possibilities of a regional scale inversion method, and its added value compared to coarser inversions:

- show the representation error reduction that can be obtained using a higher resolution modelling system.
- provide a quantitative assessment of the performance of a state-of-the-art atmospheric transport model and a range of inversion algorithms at the regional scale;

Application

Quantify the magnitude and associated uncertainties of the biospheric CO₂ surface fluxes for a pilot area, making use of various constraints imposed by the GHG information system:

- provide a carbon balance at spatial resolutions of roughly 50km (implying grid sizes of 10km) for a domain of 400x400km, for a single full year;
- provide a modelling framework that can be used as a prototype verification system for regional emissions.
1.2.1 Area and period

The high resolution forward and inverse studies are performed for two regions where greenhouse gas concentrations and various other meteorological parameters are measured at high temporal and spatial resolution. An intensive measurement campaign was the CarboEurope Regional Experiment (CERES) in South Western France which lasted for six weeks in the early summer of 2005. In this campaign meteorological parameters and atmospheric CO$_2$ concentrations were intensively measured with meteorological towers and airplanes, additionally detailed meteorological measurements were performed with radiosoundings, lagrangian balloons, a ceilometer and Rass-Sodar boundary layer profiling. In chapter 4 the area is further described. The details of this innovative experimental and modelling campaign are described in Dolman et al. (2006).

In 2008 a measurement campaign was performed in the Netherlands for a full year. During this period continuous meteorology and atmospheric CO$_2$ observations are available from four towers spread across the Netherlands. Additional, boundary layer depth measurements are available and carbon fluxes are measured directly, continuous by eddy covariance techniques at small towers, and weekly by aircraft measurements over tracks across the Netherlands. The background of this intensive measurement and modelling campaign and a general overview of the results can be found in Nol et al. (2010).

The observations from these campaigns form the basis of the forward and inverse modelling studies in this thesis.

1.3 Thesis line out

First the methodology that is applied to develop a high resolution inverse modelling system is presented in chapter 2. Thereafter four detailed studies of the practical considerations, the performance of the models in forward and inverse mode, and the application of the modelling system for the Netherlands is presented. In chapter 3 the forward simulation of CO$_2$ is assessed, including the performance of the surface energy flux model, the performance of the meteorological simulation and the quality of the boundary layer estimation. In this chapter also the importance of the atmospheric signal of the surface biospheric carbon fluxes is explored, to estimate the signal-to-noise ratio of the biospheric carbon signal compared to the uncertainty in the modelling system. In chapter 4 the added value of high resolution modelling compared to coarser resolution modelling is shown. The reduction of the representation error is quantified in this chapter. Next, in chapter 5, a range of state-of-the-art inversion methods is applied to the regional scale. In a detailed assessment the performance of the different inversion methods at the regional scale is explored. This chapter uses pseudodata to test regional inverse modelling. Subsequently the regional inverse modelling system is applied for the real situation in chapter 6. In this study the performance of the inversion is tested by the comparison with independent aircraft observations. This provides a constraint on the biospheric carbon fluxes for the Netherlands. Finally, in chapter 7 the results are summarized, including recommendations for future research. In Annex 1 the list of articles published during this PhD is included.
Method of inverse modelling

In the biospheric carbon balance two components determine the CO$_2$ fluxes: (1) the assimilation of carbon by photosynthesis, referred to as gross primary productivity (GPP) and (2) the release of carbon from the vegetation and the soil, referred to as respiration. The total biospheric carbon flux is the sum of these two components and is referred to with net ecosystem exchange (NEE). Both GPP and respiration change seasonally and diurnally. GPP on the one hand is mainly light driven, and is largest during sunny summer days. During the night, in absence of light, the GPP reduces to zero. Variations in respiration on the other hand, are mainly temperature driven. Therefore, respiration fluxes are also largest during warm summer days, but these fluxes continue during the night (for more detail on the calculation of the biospheric fluxes see section 2.2). The task of the inversions developed in this thesis is to optimize the carbon balance, and to provide thus a better estimate of the combination of these two components of the biospheric fluxes.

The inverse modelling system we use consists of a number of components, including the actual inversion method, the prior estimate of the biospheric carbon fluxes, an atmospheric transport model, the atmospheric CO$_2$ concentration observations and their uncertainty estimates. The different components of the carbon balance are optimized either separately (GPP and respiration) or as a total net flux (NEE). Additionally, in the most detailed approach the parameters in the biosphere model specifying the behavior of the carbon uptake by the vegetation and the respiration of the soil are optimized for each vegetation type.

In this chapter all components of the inverse modelling framework will be addressed. First the inversion method, in which the fluxes are optimized to match both the prior flux estimates and the CO$_2$ concentration observations in an optimal manner, will be explained. The key of this inversion method is the cost-function. The different parts of this function will in the subsequent sections be explained further, and a description of the models used to calculate these different parts will be given. In this way this chapter provides an overview of the modelling framework that forms the basis for the studies that are described in the next chapters. The used symbols are summarized in table 2.1.

2.1 Bayesian inversions

The core tool is a coupled atmosphere and vegetation model. This uses as input, besides many known variables, certain unknown variables determining the surface CO$_2$ fluxes and, consequently, the atmospheric CO$_2$ concentrations. These unknown variables can be the biospheric parameters or the linear multiplication factors for the biospheric fluxes, depending on the case. The state vector $\mathbf{x}$ contains the unknown variables as elements. Selected observations of CO$_2$ mixing ratios are contained in an observation vector $\mathbf{y}$. Running the model while using a state vector $\mathbf{x}$ yields predictions for the observations in $\mathbf{y}$, and these are called $H(\mathbf{x})$. Inversion means that
the unknown $x$ is optimized such that the ensuing $H(x)$ is as well as possible in tune with $y$ and with $x_{\text{prior}}$. Measuring this will involve an error covariance matrix $R$ for the observations contained in $y$.

Several approaches are used for inverse modelling, like Green’s function approach, Kalman filtering, adjoint models, geostatistical inversions and others (Heimann and Kasibhatla, 2000; Raupach et al., 2005). In this thesis all the inversions are performed with the Ensemble Kalman filter (EnKF). This approach was chosen because of its flexibility to perform non-linear optimizations, such as the optimization of parameters of the biosphere model (see section 2.2). In this Bayesian approach the optimum value between the prior knowledge and the information in the observations is established by minimizing a quadratic cost function:

$$J(x) = (x - x_{\text{prior}})^T P^{-1}(x - x_{\text{prior}}) + (y - H(x))^T R^{-1}(y - H(x))$$

(2.1)

In which $x$ denotes the state vector (the unknowns, such as the biospheric parameters or the linear multiplication factors for the biospheric fluxes), $y$ the observation vector (CO₂ mixing ratios), $P$ the error covariance matrix of $x_{\text{prior}}$, $R$ the error covariance matrix of the observations, $H$ is the observation operator, that contains the influence of the variables in the state vector ($x$) on the CO₂ mixing ratio at the observation locations. The subscript $\text{prior}$ denotes the prior estimate of the state vector, and $\text{post}$ the posterior, optimized estimate of the state vector. According to the Bayesian theory, the best $x$ is the one for which the cost function becomes minimal for Gaussian errors described by $P$ and $R$. This is the posterior $x$ or $x_{\text{post}}$. The remainder of this subsection is devoted to the solving of this optimization problem.

The optimum posterior state vector that minimizes this cost function (minimum least squares solution), and its error covariance matrix are:

$$x_{\text{post}} = x_{\text{prior}} + K(y - H(x_{\text{prior}}))$$

(2.2)

$$P_{\text{post}} = (I - KH)P_{\text{prior}}$$

(2.3)

Where $I$ is an identity matrix and $K$ is the Kalman gain matrix:

$$K = (P_{\text{prior}}H^T)(HP_{\text{prior}}H^T + R)^{-1}$$

(2.4)

In the Ensemble Kalman Filter method the information in the error covariance matrix $P$, and its projection in observational space $HP$ and $HPH^T$ are not calculated based on independently determined $H$ and $P$ matrices. Instead of the full calculation, an ensemble of state vectors that represent the statistical properties of $x_{\text{prior}}$ and $P_{\text{prior}}$ is used. Normally this is done to reduce the size of the matrices that are processed in the inverse system, which may become very large if the amount of unknowns is large. With this approach the size of the matrix has a maximum of $[n_{\text{members}} \times n_{\text{observations}}]$ instead of $[n_{\text{unknowns}} \times n_{\text{observations}}]$. Here, the Ensemble Kalman Filter is applied because of another advantage: this method of directly calculating $PH^T$ and $HPH^T$ from $x$ and $H(x)$ allows the use of a non-linear relation between the parameters ($x$) and the CO₂ mixing ratios ($H(x)$) as is the case in the parameter inversion used in chapter 5 and chapter 6.
The ensemble of state vectors, with N ensemble members, was created such that the normalized ensemble of deviations define the columns of matrix $X$ (Whitaker and Hamill, 2002):

$$X = \frac{1}{\sqrt{N-1}}(x_1 - \bar{x}, x_2 - \bar{x}, \ldots, x_N - \bar{x})$$  \hspace{1cm} (2.5)

which is the square root of the covariance matrix:

$$P = XX^T$$  \hspace{1cm} (2.6)

The ensemble members $x$ contain the unknowns, i.e. parameter values, or multiplication factors, depending on the inversion options applied in this thesis. All inversions are performed with ensembles containing 100 ensemble members. For each ensemble member the corresponding CO$_2$ mixing ratios at the observation locations were calculated. This is done in the coupled biosphere-atmosphere model (5PM coupled to B-RAMS3.2, (Pielke et al., 1992; Groenendijk et al., 2010) described in more detail below). Thus an ensemble of CO$_2$ mixing ratios was created:

$$H(X) = [H(x_1) - H(\bar{x}), H(x_2) - H(\bar{x}), \ldots, H(x_N) - H(\bar{x})]$$  \hspace{1cm} (2.7)

From the ensemble of state vectors ($X$) and the ensemble of corresponding CO$_2$ mixing ratios ($H(X)$) the Kalman gain matrix, and the posterior optimized values including their uncertainty was calculated with equations 2.2-2.4 combined with (Whitaker and Hamill, 2002):

$$HPH^T = \frac{1}{N-1}H(X)(H(X))^T$$  \hspace{1cm} (2.8)

and

$$PH^T = \frac{1}{\sqrt{N-1}}X(H(X))^T$$  \hspace{1cm} (2.9)

Due to the use of an ensemble instead of the full Kalman Filter, small extra covariances may be created. The impact of these small artificial covariances on the inversion result can be diminished by localization, in which only the optimized values that are constrained based on a minimum amount of observations are used. In this study we used the localization method and values established in Zupanski et al. (2007), a threshold value for the ratio between the prior uncertainty and the posterior uncertainty of 1.05 was applied.
2.2 Prior carbon flux and uncertainty

\[
(x - x_{\text{prior}})^T P^{-1} (x - x_{\text{prior}})
\]

The first part of the cost function consists of the state vector and its uncertainty. Since the problem would be ill-constrained without prior knowledge, a first estimate of the flux field is necessary. Carbon cycle research has needed to cope with a small and incomplete measurement network since the first observations of CO₂ at the top of Mauna Loa by David Keeling in 1957. Currently, the number of well-calibrated longer terms CO₂ records is still limited to no more than 150, and expansion is slow. As a result, only a limited part of the Earth surface can directly be constrained by such CO₂ observations. Additionally, due to atmospheric mixing some of the flux information disappears. For inverse modelling, this means that the problem in some areas becomes ill-constrained, such that multiple solutions for the unknowns are possible. The typical solution, also employed in numerical weather prediction and other applications, is to use a first-guess estimate of the unknowns to which the solution will revert in the absence of observations. In the presence of observations, this first-guess will be updated by the inverse technique. In numerical weather prediction, this solution is also motivated by the uncertainty of the observations, with the background being even more precise than some observations.

Whether the posterior flux field is closer to the prior flux estimate, or to the values indicated by the atmospheric CO₂ concentration observations depends on the ratio between the prior uncertainty and the transport and observation uncertainty. For the latter see section 2.3. Here the calculation of the prior carbon flux estimate is explained, including its uncertainty. The biospheric carbon fluxes consist on the one hand of the uptake from the vegetation by photosynthesis, and on the other hand of emission from the biosphere by respiration.

2.2.1 Photosynthetic CO₂ flux calculation

The biosphere model used in this study to calculate the prior NEE fluxes is 5PM (Groenendijk et al., 2010) extended with the use of leaf area index (LAI) to upscale the fluxes from the leaf to the canopy scale. In this model photosynthesis is calculated based on the Farquhar model (Farquhar et al., 1980) and heterotrophic respiration is based on the relationship by Lloyd and Taylor (1994). Here the calculation of carbon assimilation is described, and in the next section of respiration.

In the Farquhar approach assimilation of CO₂ by the vegetation is either limited by the amount of radiation or by the availability of the enzyme Rubisco, which is involved in the conversion of CO₂ into glucose and oxygen. Photosynthesis is formulated as the minimum of the light limited \( (w_j) \) or enzyme limited assimilation rate \( (w_c) \), corrected for the maintenance respiration of the vegetation \( (R_d) \):

\[
A = \min(w_c, w_j) - R_d
\]

(2.10)

The assimilation rate depends on the CO₂ concentration inside the leaf available for photosynthesis \( (\text{Ci}) \), the internal oxygen concentration \( (\text{O}) \), the compensation point for CO₂ \( (\Gamma^*) \) and the Michaelis-Menten parameters for CO₂ \( (K_c) \) and O₂ \( (K_o) \). The
latter are temperature dependent. The first rate, Rubisco-limited assimilation is calculated as:

$$w_c = V_{cm} \frac{C_i - \Gamma^*}{C_i + K_c \left(1 + \frac{O}{K_o}\right)}$$

(2.11)

where $V_{cm}$ is the maximum carboxylation capacity ($\mu$mol m$^{-2}$ s$^{-1}$). The second option, light limited assimilation is calculated as:

$$w_j = J \frac{C_i - \Gamma^*}{4(C_i + 2\Gamma^*)}$$

(2.12)

where $J$ is the electron yield, specified by:

$$J = \frac{\alpha d_{PAR} J_m}{\alpha d_{PAR} + 2.1 J_m}$$

(2.13)

in which $IPAR$ is the Photosynthetic Active Radiation ($\mu$mol photons m$^{-2}$ s$^{-1}$), $J_m$ the maximum potential electron transport rate ($\mu$mol m$^{-2}$ s$^{-1}$) and $\alpha$ the quantum yield (mol mol$^{-1}$). Assumed is that the plants aim for an optimum between the energy allocated to the potential electron transport rate and to the carboxylation capacity, and $J_m$ is linked to $V_m$ by (Collatz et al., 1991):

$$J_m = 2.5V_{cm}$$

(2.14)

Leaf internal CO$_2$ is estimated with the method described in Arneth et al. (2002) in which the value for $\Gamma$ was kept constant at 700 mol mol$^{-1}$. The atmospheric CO$_2$ mixing ratio is assumed to be 380 ppm during photosynthesis. During the project the model was refined with the inclusion of the dependence of the photosynthesis on LAI. In the inverse studies in this thesis the integration of the photosynthetic flux to the full canopy is based on MODIS leaf area index (LAI) observations (Sellers et al., 1996):

$$A_c = \Pi A_{n0}, \quad \Pi = \frac{1 - e^{-\frac{FLAI}{k}}}{k}$$

(2.15)

where $A$ is the assimilation, subscript $n0$ refers to leaves at the top of the canopy, subscript $c$ refers to total canopy and $k$ is the PAR extinction coefficient.

The selected parameters of the photosynthesis calculation for the parameter inversion are $V_{cm}$ and $\alpha$, which represent the enzyme limited part and the light limited part, respectively.

### 2.2.2 Respiration CO$_2$ flux

Due to the composition of carbon in the soil the respiration differs from site to site. Besides, the respiration rate is temperature dependent. In 5PM the heterotrophic respiration is calculated with the temperature dependent relationship by Lloyd and
Taylor (1994). The respiration is parameterized with a simple function with a site dependent parameter that accounts for the effective mass of carbon available for respiration and a temperature function that is the same for all ecosystems and substrate types. Lloyd and Taylor (1994) showed that the best fit to the data was obtained with an Arrhenius type equation, where temperature dependence of the activation energy ($E_0$) is included. This gives the following relationship for respiration:

$$R = R_{10} e^ \left( \frac{E_0}{\mathcal{R}} \left( \frac{1}{28315 - T_0} - \frac{1}{T - T_0} \right) \right)$$

(2.16)

where $R_{10}$ is the respiration rate at a reference temperature of $10^\circ C$, $E_0/\mathcal{R}$ is the activation energy divided by the universal gas constant, $T_0$ is a constant of 227.13 K and $T$ is soil temperature.

The selected parameters of the respiration calculation for the parameter inversion are $R_{10}$ and $E_0$ which represent the available substrate part and the temperature dependency, respectively.

### 2.2.3 Coupling of the biospheric and atmospheric model

This biospheric carbon flux model 5PM is coupled to the Regional Atmospheric Modelling System (RAMS) through the radiation, the temperature and humidity of the canopy air and influences the CO$_2$ mixing ratio at the lowest atmospheric level. The atmospheric model on the one hand provides input for the biospheric model through the total amount of radiation (which is converted to $I_{\text{PAR}}$), temperature and the vapor pressure deficit. On the other hand the CO$_2$ flux calculated with 5PM serves as input for the CO$_2$ flux in the lowest cell in the atmospheric model. Note that the 5PM model formulation does not include a water-limitation on photosynthesis, and also does not describe the opening and closing of stomates to regulate CO$_2$ uptake and water loss. The hydrological and carbon cycle are thus not coupled for this study, but might be important in more arid countries or under drought conditions.

Both photosynthesis and respiration depend on the land use. For this the Pelcom dataset is used, which is refined to the Corine 2000 land use maps. The leaf area index from the MODIS dataset is used to adjust the photosynthesis fluxes (equation 2.15).

### 2.2.4 Prior uncertainty of the flux-model parameters

The estimate of the prior uncertainty of the flux-model parameters is based on the independent optimizations of the 5PM biosphere model based on fluxnet bottom-up observations (Baldocchi et al., 2001), performed in the study by Groenendijk et al. (2010). They optimized parameters of this model ($V_{\text{max}}, \alpha, R_{10}$ and $E_0$) for the full canopy based on a large number of Fluxnet observations. The standard deviations of their optimizations were used as indication of the uncertainty of the prior estimate of the unknowns, with no correlations between the parameters. For the inversion in which the biosphere parameters are optimized this uncertainty can directly be implemented. To estimate the uncertainty in the GPP and Respiration the biospheric model is run, using the standard deviation of the biospheric parameters.
2.3 Atmospheric observations, transport and uncertainty

\[(y - H(x))^T R^{-1} (y - H(x))\]

The second part of the cost function consists of the comparison between the observed atmospheric CO$_2$ concentrations and the atmospheric concentration calculated with the atmospheric transport model, combined with the carbon flux field. The uncertainty of the CO$_2$ observations, and of the modelling system is included in the error covariance matrix $R$. Below the atmospheric observations used for the inversion in the pilot area of the Netherlands are described and the atmospheric transport model, RAMS coupled to the surface energy flux model Leaf-3 is introduced.

2.3.1 Atmospheric CO$_2$ mixing ratio observations

In the Netherlands four towers were used to observe the atmospheric CO$_2$ concentrations. These are reported as molar mixing ratio’s in ppm. At all four towers continuous observations are available for 2008 which were averaged to hourly values for this study. West of the center of the Netherlands, in Cabauw, observations are available up to an altitude of 200m. In the North, at the tower of Lutjewad, measurements are performed up to 60m height. In the middle of the Netherlands, at Loobos, observations up to 24m height are available, and at the east of the Netherlands, in Hengelman, up to 18 m height. The details of the measurements can be found in chapter 6, and in the papers by Vermeulen et al. (2011), Elbers et al. (2011) and Van der Laan et al. (2009a). The measurement precision ranged between <0.1 ppm at Lutjewad, to 0.2 ppm at Cabauw and Loobos, and 2 ppm at Hengelman. Only hourly values from 11 to 16 UTC are used for each day, since transport errors are likely to be too large for other hours. The difficulties in nocturnal transport modelling are further shown in chapter 3.

2.3.2 Transport model RAMS-Leaf and CO$_2$ nudging

Atmospheric transport of CO$_2$ is in all studies in this thesis simulated with the Regional Atmospheric Modelling System: RAMS (Pielke et al., 1992). The version used in this study is BRAMS-3.2. This is a non-hydrostatic model, together with its nesting options allowing it to be used in high resolution modes. RAMS is fundamentally a limited-area model, there is no lower limit to the domain size or to the cell size of the model's grid. In the simulations we applied two different turbulence schemes, the traditional Mellor Yamada scheme and the medium range forecast (MRF) model. The Mellor-Yamada scheme uses only local diffusion, based on the turbulent kinetic energy which is calculated using a prognostic equation, while the MRF uses a non-local turbulence parameterization within the convective boundary layer. The vertical resolution was highest in the lower part of the atmosphere, with 30m, and gradually increased with height. Meteorology, soil temperature and soil moisture were initialized with European Centre for Medium-Range Weather Forecasts (ECMWF) analysis data and the lateral boundary conditions were 6 hourly nudged to these ECMWF analysis (Uppala et al., 2005).

The transport of atmospheric CO$_2$ is relatively easily implemented in RAMS, since the code allows passive atmospheric transport of any number of scalars. Various
tracers are applied to model the transport of CO$_2$ through the atmospheric field. The number of tracers applied depends on the study and is further described in the specific chapters. The CO$_2$ fields are initialized and at the lateral boundaries 3 hourly nudged to reanalyzed CO$_2$ fields from CarbonTracker Europe (Peters et al., 2010).

The surface energy fluxes, that are drivers of the atmospheric turbulence, are computed by Leaf-3 (Walko et al., 2000). The lowest level above the surface in the RAMS model is the reference level at which atmospheric boundary layer values of temperature, vapour pressure and wind velocity are provided as upper boundary conditions to Leaf-3. Additionally, the direct and diffuse components of shortwave and near-infrared radiation incident at the surface are provided from the RAMS radiation scheme. As described in section 2.2.3 the biospheric model is coupled in the same manner.

During the analysis of simulations of RAMS we deduced and corrected an important error in the model. This is published in Meesters et al. (2008). Without correction, effective surface CO$_2$-fluxes on mountain slopes were found to be enhanced under certain common conditions to several times the parameterized fluxes. To solve the error the parameterization of the horizontal diffusion in the presence of a slope had to be corrected. After this correction a very good closure of the mass balance was obtained. The correction also modified the meteorological parameters, although the consequences were limited compared to the CO$_2$-fluxes.

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<th><strong>Ensemble Kalman Filter</strong></th>
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<th><strong>CO$_2$ flux calculation</strong></th>
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<td>$R_{10}$</td>
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Table 2.1, list of symbols used in the equations in chapter 2.
Modelling regional scale surface fluxes, meteorology and CO$_2$ mixing ratios for the Cabauw tower in the Netherlands

Abstract

We simulated meteorology and atmospheric CO$_2$ transport over the Netherlands with the mesoscale model RAMS-Leaf3 coupled to the biospheric CO$_2$ flux model 5PM. The results were compared with meteorological and CO$_2$ observations, with emphasis on the tall tower of Cabauw. An analysis of the coupled exchange of energy, moisture and CO$_2$ showed that the surface fluxes in the domain strongly influenced the atmospheric properties. The majority of the variability in the afternoon CO$_2$ mixing ratio in the middle of the domain was determined by biospheric and fossil fuel CO$_2$ fluxes in the limited area domain (640 x 640km). Variation of the surface CO$_2$ fluxes, reflecting the uncertainty of the parameters in the CO$_2$ flux model 5PM, resulted in a range of simulated atmospheric CO$_2$ mixing ratios of on average 11.7 ppm in the well-mixed boundary layer. Additionally, we found that observed surface energy fluxes and observed atmospheric temperature and moisture could not be reconciled with the simulations. Including this as an uncertainty in the simulation of surface energy fluxes changed simulated atmospheric vertical mixing and horizontal advection, leading to differences in simulated CO$_2$ of on average 1.7 ppm. This is an important source of uncertainty and should be accounted for to avoid biased calculations of the CO$_2$ mixing ratio, but it does not overwhelm the signal in the CO$_2$ mixing ratio due to the uncertainty range of the surface CO$_2$ fluxes.
3.1 Introduction

Terrestrial carbon uptake is an important process in the global carbon cycle. It removes a substantial part of the anthropogenic emitted CO$_2$ from the atmosphere (Canadell et al., 2007). A useful method to increase our understanding of the terrestrial CO$_2$ fluxes is inverse modelling of atmospheric CO$_2$ mixing ratio observations (e.g. Gurney et al., 2002). In this method the atmospheric signal is used to constrain the surface fluxes using an atmospheric transport model. The results of inversion calculations depend to a large extent on the quality of atmospheric modelling (Stephens et al., 2007).

Therefore, correct simulation of the atmospheric transport, and accounting for the uncertainties, is an important goal in inverse modelling of CO$_2$. Atmospheric transport is modelled at increasingly higher resolutions to capture the high spatial and temporal variability in observed CO$_2$ mixing ratios over the continent. Continental scale studies show that the forward simulation of CO$_2$ improved by increasing the horizontal resolution from a number of degrees (Gurney et al., 2002) to one degree or less (Geels et al., 2007, Parazoo et al., 2008). Further increasing the horizontal resolution to just a few kilometres in more limited domain studies (Dolman et al., 2006) was shown to improve the CO$_2$ mixing ratio simulation at observation stations in uneven and coastal terrain, because of the models ability to simulate mesoscale circulations, like sea breezes and topography induced katabatic flows (Nicholls et al., 2004; Riley et al., 2005; Van der Molen and Dolman, 2007; Sarrat et al., 2007; Ahmadov et al., 2009). This also avoids representation errors by resolving a larger part of the variability in the CO$_2$ mixing ratio (Corbin et al., 2008; Tolk et al., 2008).

Despite these achievements correct modelling of the CO$_2$ mixing ratios remains challenging. Model intercomparisons of global (Stephens et al., 2007; Law et al., 2008), continental (Geels et al., 2007) and mesoscale models (Van Lipzig et al., 2006; Sarrat et al., 2007) showed discrepancies in the meteorology and CO$_2$ modelled of different models. In the simulation of CO$_2$ mixing ratios both advection and entrainment play an important role (Vila et al., 2004; Casso-Torralba et al., 2008) and the quantification of uncertainties in these physical processes is one of the major questions in transport modelling. Comparisons at a coarser scale with observations showed that an erroneous simulation of the advection (Lin and Gerbig, 2005) and of vertical mixing (Gerbig et al., 2008) can lead to uncertainties in the simulated CO$_2$ mixing ratio of several ppm. Here we study at regional scale the effect of surface flux uncertainties on these transport errors.

In the present study a high resolution simulation is performed with the non-hydrostatic Regional Atmospheric Modelling System (RAMS; Pielke et al., 1992). The performance of the simulation is assessed with meteorological and CO$_2$ observations. We address a potential source of error in the simulated atmospheric vertical mixing: the simulation of the surface energy fluxes. Its uncertainty is estimated based on a comparison of different models (RAMS, WRF and ECMWF) and by using different parameter values in the surface flux model within RAMS. The model simulations are compared with both surface flux observations and with atmospheric CO$_2$ mixing ratio observations.

We coupled the biospheric CO$_2$ flux model 5PM to the RAMS atmospheric transport model, in order to study the coupled exchange of energy, moisture and CO$_2$. In this framework the impact of the surface energy fluxes on the simulation of atmospheric
transport and consequently on the CO₂ mixing ratio is quantified. Novel in our approach is that we distil the impact of the uncertainty in the simulated surface energy fluxes on the atmospheric CO₂ mixing ratio, and that we quantify this CO₂ transport error in a Eulerian approach.

Also, the uncertainty in the CO₂ surface fluxes is addressed. With the coupled RAMS-5PM simulation system these are propagated into a range of CO₂ mixing ratios. This indicates the minimal performance of the atmospheric transport model required for the use in inversion studies, since the uncertainty in the transport modelling should not exceed the uncertainty related to CO₂ surface flux uncertainty. The parameters in the biospheric model 5PM have been optimized in a previous study for a number of eddy correlation flux observations (Groenendijk et al., 2009). Innovative in this study is that we show at mesoscale a realistic uncertainty range of CO₂ mixing ratios due to uncertainties in the CO₂ surface fluxes, based on independently determined a-priori flux estimates.

Finally, we separate the contribution of different CO₂ sources and sinks to the CO₂ mixing ratio at Cabauw, i.e. the influence of the advection of CO₂ into our domain (background contribution), the fossil fuel emissions, sea-air CO₂ exchange, and terrestrial respiration and assimilation fluxes. The relative importance of the different CO₂ contributions indicates which uncertainties in the surface CO₂ fluxes are important and which can be neglected. Additionally, the relative contribution of the near field versus the far field fluxes on the CO₂ mixing ratio is shown, another important subject in regional scale inverse modelling (Zupanski et al., 2007; Lauvaux et al., 2008; Gerbig et al., 2009).

The paper is organized as follows: in Sect. 3.2 the simulation set-up is described, in Sect. 3.3 the performance of the model is validated against meteorological observations, Sect. 3.4 describes the simulated CO₂ fluxes and mixing ratios compared to observations and in Sect. 3.5 the implications of our results for the interpretation of the observations, future forward and inverse CO₂ simulations are discussed.

Figure 3.1. Simulation domain with 2 nested grids. The star indicates Cabauw, the square the location of the radiosonde release, the triangles indicate the scintillometers and the dots the eddy correlation observations.
3.2 Methods

3.2.1 Simulation period and domain

We performed simulations with the Regional Atmospheric Modelling System (RAMS) for 22 days in June 2006. In this time of year the biogenic assimilation fluxes during daytime of CO$_2$ were large. This period was selected because it covers a number of meteorological regimes with different wind directions and frontal passages, influencing the atmospheric properties and carbon exchange. South-easterly winds coincided with clear sky conditions, while northerly and south-westerly winds caused more cloudy conditions.

A two way nested grid was used (Figure 3.1) centred on the Netherlands at 52.25°N and 5.2°E, with a 320 x 320km domain at 4 km resolution nested in a 640 x 640 km domain at 16 km resolution (Table 3.1). The centre of the domain is relatively flat, with a maximum elevation of ~100m. The south-east part of the domain has more orography, up to ~500m. The dominant land use types in the area are cultivated lands (crops and grasslands) and urban areas. Large cities and industrial areas of the Netherlands, Belgium and the German Ruhr Area are within the domain. To the north and the west the Netherlands is bounded by the North Sea.

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</tr>
<tr>
<td>Soil textural class</td>
</tr>
<tr>
<td>Leaf Area Index</td>
</tr>
<tr>
<td>Fossil fuel emissions</td>
</tr>
</tbody>
</table>

*Table 3.1. Specification of the simulation settings*
3.2.2 Simulation setup

The atmospheric simulations were performed with the non-hydrostatic mesoscale model RAMS (Pielke et al., 1992), which has already been used to simulate the behaviour of CO$_2$ in the atmosphere in a number of studies (e.g. Denning et al., 2003; Nicholls et al., 2004; Sarrat et al., 2007; Ter Maat and Hutjes, 2008). The version used in this study is B-RAMS-3.2, including adaptations to secure mass conservation (Medvigy et al., 2005; Meesters et al., 2008). For vertical diffusion, we built in the turbulence scheme as described in section 2 of Hong and Pan (1996) (corrections: division by h should be added in their equation 4, and removed in their equation 9). This scheme uses a non-local turbulence parameterization within the convective boundary layer. Inclusion of this within the medium range forecast (MRF) model has been shown by Troen and Mahrt (1986), Holtslag et al. (1995) and Hong and Pan (1996) to simulate the daytime boundary layer structures more realistically than local mixing schemes. In our simulations with RAMS we applied this non-local scheme also to the CO$_2$-transport. Cumulus convection was not parameterized in the simulations. The surface energy fluxes were simulated using Leaf-3 (Walko et al., 2000). The vegetation Leaf Area Index (LAI) of the MODIS database was used.

Meteorology, soil temperature and soil moisture were initialized with ECMWF analysis data (Uppala et al., 2005). In order to be consistent with the RAMS soil wilting point (wp) and field capacity (fc), the ECMWF soil moisture ($\eta$) was scaled towards RAMS soil variables based on a soil wetness index (SWI):

$$SWI = \frac{\eta - \eta_{wp}}{\eta_{fc} - \eta_{wp}}$$  \hspace{1cm} (3.1)

$$\eta_{Rams} = \eta_{wp,Rams} + SWI_{ECMWF} (\eta_{fc,Rams} - \eta_{wp,Rams})$$  \hspace{1cm} (3.2)

Optimized CO$_2$ mixing ratio fields at 1x1$^\circ$ resolution from CarbonTracker Europe (Peters et al., 2009) were used for initial and boundary conditions of the CO$_2$ mixing ratio. The simulations were nudged every 3 hours to CarbonTracker CO$_2$ mixing ratios and every 6 hours to the ECMWF analysis meteorology with a nudging relaxation time scale of 900 seconds. The nudging extended inward from the lateral boundary by 5 grid cells and the centre of the domain was free of nudging.

3.2.3 CO$_2$ fluxes

CO$_2$ fluxes from fossil fuel burning were included in the simulations based on the IER database at 10 km resolution (carboeurope.ier.uni-stuttgart.de). The CO$_2$ fluxes from the coastal sea inside the domain were calculated based on climatologic estimates of the partial pressure of CO$_2$ in the sea (Wanninkhof, 1992; Takahashi et al., 2002). Biospheric CO$_2$ surface fluxes were modelled with 5PM (Groenendijk et al., 2009). This model was coupled to RAMS through the radiation, the temperature and humidity of the canopy air and influences the CO$_2$ mixing ratio at the lowest atmospheric level. The CO$_2$ assimilation does in this model not depend on the energy fluxes of RAMS through the stomatal conductance (Collatz et al., 1991) or on Leaf Area Index (LAI) (Sellers et al., 1996). In 5PM the photosynthesis is calculated following Farquhar et al. (1980), where photosynthesis is either limited by the carboxylation rate, which is enzyme limited, or by the light limited RuBP regeneration rate. The most important assimilation parameters in this model are the
maximum carboxylation capacity ($V_{c_{\text{max}}}$) and the light use efficiency ($\alpha$). Respiration was calculated with the relationship by Lloyd and Taylor (1994):

$$ R = R_{10} \frac{E_0}{R} e^{\frac{1}{28315-T_0}} e^{\frac{1}{T-T_0}} $$

(3.3)

where $R_{10}$ is the respiration rate at a reference temperature of 10°C, $E_0/R$ is the activation energy divided by the universal gas constant, $T_0$ is a constant of 227.13 K and $T$ is soil temperature. For further specifications of 5PM see Groenendijk et al. (2009).

Groenendijk et al. (2009) optimized the parameters of this model ($V_{c_{\text{max}}}$, $\alpha$, $R_{10}$ and $E_0$) for the full canopy based on a large number of Fluxnet observations (Baldocchi et al., 2001). We applied parameter values optimized for the temperate zone, for the period of May-July for all years (Table 3.2). The parameter values used in our simulations were kept constant in time. Simulations were performed with CO$_2$ fluxes calculated based on the best guess parameter values. For respiration and assimilation of the most abundant vegetation species (crops and grass) we also simulated fluxes using the upper and the lower parameter values within the standard deviation of the parameter estimate. In this way a range of CO$_2$ mixing ratios was simulated based on the different CO$_2$ flux parameter settings. In the rest of this work, we report the range of uncertainties, i.e. the difference between the highest and lowest values in our set of simulations. Further specifications on the design of the simulations are given in Table 3.1.

3.2.4 Observations

A large number of observations of the atmospheric properties and the surface fluxes were available for model validation. Data from continuous CO$_2$ mixing ratio measurements, performed by a Licor 7000 with a precision of 0.05 ppm, and meteorological data from the tall tower at Cabauw at a height of 20m, 60m, 120m and 200m were used. Also, atmospheric observations for temperature, humidity, wind speed and direction were available at 110 synoptic 2 meter stations over the Netherlands and from the radiosondes that were released twice a day at De Bilt, which is about 25km north-east of the Cabauw site. Observations of the surface fluxes were available for sensible heat, latent heat and CO$_2$ fluxes from eddy correlation measurements (Aubinet et al., 2001; Dolman et al., 2002; Wilson et al., 2002; Jacobs et al., 2007; Braam, 2008; Aubinet et al., 2009). Additionally, scintillometer measurements provided extra sensible heat flux measurements over a horizontal path of 0.35 - 5km (De Bruin et al., 2004). The locations are specified in Figure 3.1 and in Table 3.3.

3.3 Results: Meteorological performance of the model

3.3.1 Consistency of the simulation in time

The simulated period of 22 days covered a number of different weather regimes with different wind directions, solar radiation and temperature (Figure 3.2). East to south-easterly winds brought clear weather, with increasing temperature and relative large day-night temperature amplitudes, like at 9-14 June 2006 (doy 160-165). In general, northern and south-westerly winds brought more cloudy conditions with reduced radiation, lower temperatures and smaller nocturnal cooling.
Assimilation  \(|V_{c_{\text{max}}} (\mu \text{mol m}^{-2} \text{s}^{-1})| \quad \alpha (\text{mol mol}^{-1}) \quad n \text{ sites}
\begin{align*}
\text{Grass} & \quad 70 \pm 30 (40) & \quad 0.4 \pm 0.15 (0.4) & \quad 10 \\
\text{Crops} & \quad 100 \pm 50 (100) & \quad 0.4 \pm 0.15 (0.4) & \quad 5 \\
\text{Needle leaf forest} & \quad 80 & \quad 0.5 & \quad 10 \\
\text{Broadleaf forest} & \quad 100 & \quad 0.5 & \quad 2 \\
\text{Urban vegetation} & \quad 80 & \quad 0.4 & \quad - \\
\end{align*}

Respiration  \(|E_{0}/\mathcal{R} (\text{K})| \quad |R_{10} (\mu \text{mol m}^{-2} \text{s}^{-1})| \quad n \text{ sites}
\begin{align*}
\text{Full domain} & \quad 200 \pm 110 (310) & \quad 4.0 \pm 1.2 (3.5) & \quad 10 \\
\end{align*}

Table 3.2. \(\text{CO}_2\) flux parameter settings based on Groenendijk et al. (2009). \(V_{c_{\text{max}}}\) is the full canopy maximum carboxylation capacity, \(\alpha\) the light use efficiency for the full canopy, \(E_{0}/\mathcal{R}\) is the respiration activation energy divided by the universal gas constant, \(R_{10}\) is the respiration rate at 10 °C and \(n\) sites indicates the number of sites used in the optimizations of the parameters. Where uncertainty ranges are shown the best guess, upper and lower estimates of the parameters are used in the simulations. In between brackets the parameter values that returned the best \(\text{CO}_2\) mixing ratios.

Here we show the results of the standard simulation used in this study. For this simulation, the standard RAMS settings have been modified to obtain a more realistic Bowen ratio, as will be described in Sect. 3.2. The model reproduced the synoptic variations over the full 22-day period without any re-initialization of the simulation (Figure 3.2 and Table 3.4). This was achieved by prescribing boundary conditions from reanalysis products such as ECMWF meteorology and CarbonTracker \(\text{CO}_2\) mixing ratios. A change in the large-scale atmospheric situation was thus passed on to the inner domain for which RAMS simulated, mimicking the effect of a re-initialization. A large advantage of not needing to re-initialize the RAMS model over multi-week periods is that mass continuity of tracers and a balance of the physical equations for energy and water was ensured.

A comparison of the statistics for the first and last half of the period showed the consistency of the model performance in time (Table 3.4). Hourly temperature (\(T\)) and humidity (\(q\)) were simulated comparably well in both periods. Radiation showed a better performance in the first half of the period, which can be attributed to the occurrence of clouds in the second half of the period, rather than to a drift of the simulated meteorology with time. Incoming solar radiation and its reduction by clouds was mostly simulated with the correct amplitude and frequency. However, the exact location of the clouds and subsequently the timing of the radiation reduction sometimes deviated from the observations, as was also seen in similar mesoscale model studies (Denning et al., 2003; Van Lipzig et al., 2006; Parazoo et al., 2008).

3.3.2 Uncertainties in the surface energy fluxes

Surface energy fluxes are important drivers of processes in the atmosphere, influencing amongst others the atmospheric \(T\), \(q\) and vertical mixing. Uncertainties in the surface energy fluxes thus may be an important source of uncertainty in the simulation of the atmospheric properties and are addressed in this section.

We compared the simulated energy fluxes with eddy covariance and scintillometer measurements (Figure 3.3) and made a comparison with two other models: WRF and ECMWF. Additionally, we studied the sensitivity of the simulated sensible (\(H\) and
latent (LE) heat fluxes to changes in the surface flux calculation by Leaf3, and its effect on the atmosphere. This revealed that the simulations at some days either captured the observed surface energy fluxes, or the observed T and q vertical profile in the planetary boundary layer (PBL), but could not reconcile both. The atmospheric observations and the comparison with other models suggested a higher Bowen ratio (i.e. the ratio of sensible to latent heat flux, $\beta$) than simulated with standard Leaf3 settings. Possible options for such an increased $\beta$ are shown in Table 3.5 and described below, with a focus on T and H because of their importance for atmospheric vertical mixing.

The energy fluxes showed a large variation between low (crops, grasslands) and high (forest) vegetation types (Figure 3.3, note the different scale on the y-axis for low and high vegetation). These differences were driven by differing vegetation characteristics such as the low aerodynamic resistance and stomatal conductance in forest and were reproduced in the RAMS simulations.

With the standard Leaf3 vegetation characteristics (green line in Figure 3.3) most of the eddy correlation observations were captured reasonably well. The scintillometer observations at Maas-en-Waal and Haarweg were slightly underestimated. With these settings the PBL T was underestimated and q overestimated at clear days with eastern winds, in comparison with radiosonde observations (Figure 3.4 and Table 3.5), the Cabauw tall tower and synoptic 2m observations (not shown).

We compared our findings with the ECMWF (Uppala et al., 2005) forecast simulations and with a simulation performed with WRF (Skamarock et al., 2008) using the MRF PBL scheme and either ECMWF or NCEP boundary conditions for the same domain and period. Both simulations matched the observed T well (not shown), but also failed to match the observed H for grass and crops (light and dark blue lines in Figure 3.3).

<table>
<thead>
<tr>
<th>Site name</th>
<th>Vegetation type</th>
<th>Longitude</th>
<th>Latitude</th>
<th>Observation</th>
<th>Data providers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cabauw (Ca1)</td>
<td>Grass</td>
<td>4.93</td>
<td>51.97</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>TT CO$_2$</td>
<td>A. Vermeulen; ECN</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>TT meteo</td>
<td>F. Bosveld, H. Klein Baltink; KNMI</td>
</tr>
<tr>
<td>De Bilt</td>
<td>Grass, forest, urban</td>
<td>5.18</td>
<td>52.1</td>
<td>RS</td>
<td>F. Bosveld, H. Klein Baltink; KNMI</td>
</tr>
<tr>
<td>Haarweg (Haa)</td>
<td>Grass</td>
<td>5.63</td>
<td>51.97</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Sc</td>
<td>A. Moene; Wageningen University</td>
</tr>
<tr>
<td>Horstermeer (Hor)</td>
<td>Grass</td>
<td>5.04</td>
<td>52.14</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td>Lonzee (Lon)</td>
<td>Crops</td>
<td>4.75</td>
<td>50.55</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td>Loobos (Loo)</td>
<td>Needle Forest</td>
<td>5.74</td>
<td>52.17</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td>Lutjewad (Lut)</td>
<td>Crops</td>
<td>6.37</td>
<td>53.38</td>
<td>EC</td>
<td><a href="http://www.carboeurope.org">www.carboeurope.org</a></td>
</tr>
<tr>
<td>Maas en Waal (MeW)</td>
<td>Crops, grass, trees</td>
<td>5.7</td>
<td>51.82</td>
<td>Sc</td>
<td>A. Moene; Wageningen University</td>
</tr>
</tbody>
</table>

Table 3.3. Observation specifications. EC is eddy correlation measurements, Sc is scintillometer, RS is radiosonde and TT is tall tower.
Figure 3.2. Observed and simulated time series at the Cabauw of (a) short wave radiation, (b) potential temperature, (c) wind speed and (d) wind direction at 200m.
### Table 3.4. Statistics of the simulation, in comparison with observations of the potential temperature (T) and CO$_2$ at 20m and 200m, humidity (q) at 2m and the incoming shortwave radiation (rshort) at Cabauw, for the full period, the first and the second half of the simulation period. Humidity is compared to the simulated canopy air humidity, CO$_2$ and T with simulated atmospheric values.

<table>
<thead>
<tr>
<th></th>
<th>Full period</th>
<th></th>
<th>First half</th>
<th></th>
<th>Second half</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R$^2$</td>
<td>RMSE</td>
<td>R$^2$</td>
<td>RMSE</td>
<td>R$^2$</td>
<td>RMSE</td>
</tr>
<tr>
<td>T 200m</td>
<td>0.90</td>
<td>1.2 K</td>
<td>0.92</td>
<td>1.2 K</td>
<td>0.87</td>
<td>1.1 K</td>
</tr>
<tr>
<td>T 20m</td>
<td>0.87</td>
<td>1.4 K</td>
<td>0.92</td>
<td>1.3 K</td>
<td>0.80</td>
<td>1.5 K</td>
</tr>
<tr>
<td>q 2m</td>
<td>0.51</td>
<td>1.1 g kg$^{-1}$</td>
<td>0.47</td>
<td>1.3 g kg$^{-1}$</td>
<td>0.65</td>
<td>0.8 g kg$^{-1}$</td>
</tr>
<tr>
<td>Rshort</td>
<td>0.78</td>
<td>143.4 W m$^{-2}$</td>
<td>0.88</td>
<td>113.2 W m$^{-2}$</td>
<td>0.64</td>
<td>165.6 W m$^{-2}$</td>
</tr>
<tr>
<td>CO$_2$ 200m</td>
<td>0.21</td>
<td>5.9 ppm</td>
<td>0.15</td>
<td>5.8 ppm</td>
<td>0.23</td>
<td>6.3 ppm</td>
</tr>
<tr>
<td>CO$_2$ 20m</td>
<td>0.67</td>
<td>10.1 ppm</td>
<td>0.71</td>
<td>11.0 ppm</td>
<td>0.55</td>
<td>9.8 ppm</td>
</tr>
</tbody>
</table>

Sensitivity tests showed that the strength of LE and H depended strongly on (1) the water availability, (2) the minimal stomatal resistance, which determines the plants’ resistance to transport of water and CO$_2$ and (3) the fraction of the surface that is vegetated (Table 3.5).

(1) Decreasing the soil moisture content led to a strong increase in $\beta$, because of the decrease in evaporation from the soil and transpiration from the plants. (2) Also a doubling of the minimal stomatal resistance, a rather uncertain parameter in Leaf3 (Walko et al., 2000), for grass and crops from 100 sm$^{-1}$ to 200 sm$^{-1}$ increased $\beta$. (3) With standard Leaf3 settings the vegetation fraction of grass and crops did not exceed $\sim$70%, even with a high LAI. We increased the vegetation fraction to 90% when the LAI is larger than 1, in line with for example the settings in the ECMWF surface model. This increase led to a considerable increase in H and the atmospheric T (Table 3.5).

Simulations with these adapted settings returned an overestimation of H at most of the low vegetation sites (e.g. with adaptations (2) and (3), red line in Figure 3.3), but returned a rather well simulated PBL T and q (red lines in Figures 3.2 and 3.4). We will refer to the simulation with increased stomatal resistance and vegetation fraction and standard soil moisture as the ‘high $\beta$ simulation’, while the simulation with standard Leaf3 vegetation characteristics will be referred to as the ‘low $\beta$ simulation’.

These two cases however do not capture the full range of uncertainty in beta, as even the low beta simulation sometimes still overestimates H and underestimates LE (Figure 3.3 and table 3.5). Decreasing for example the stomatal resistance as suggested for Cabauw by Jackson et al. (2003) would further reduce $\beta$ in such situations (table 3.5). The uncertainty in surface energy fluxes may thus even be larger than inferred here from the atmospheric observations, indicating that our uncertainty estimates may be conservative.
Figure 3.3. Sensible heat flux for crops, grasslands and forest at 11 and 12 June 2006 (doy 162 and 163), for locations and full names see table 3.3. The black dots indicate for Maas en Waal (MeW) and Haarweg (Haa) scintillometer observations and for the other sites eddy correlation observations. Green indicates the RAMS simulation with a low Bowen ratio, and red with a high Bowen ratio (see text for explanation), dark blue is the WRF simulation and light blue is the ECMWF forecast simulation.

We tested the sensitivity of our findings to the moment of initialization. When initialized 6 hours, 18 hours or over 5 days in advance, the simulated noon temperatures deviated 2.0, 2.5 or 3.1 K from the observations, respectively (Table 3.5) using the settings yielding the low β. Hence, the largest part of the temperature underestimation built up within a few hours and was rather independent of the moment of initialization. For the high β simulation the results were robust to a change of the moment of initialization (not shown).

The fact that the surface flux observations and the atmospheric observations both suggest different optimal β’s indicated an uncertainty in what the correct β should be in the simulations for the full domain. Further discussion on this will be presented in Sect. 5. We will use the simulation with the high β (and hence lowest T and q bias in the atmosphere) to investigate the structure of the simulated CO₂ fields. This simulation corresponds to the standard run that was discussed in Sect. 3.1. In the next section the effects of the uncertainty in the surface energy fluxes on the atmospheric vertical mixing are addressed.
### Table 3.5. Overview of the sensitivity tests. Results are given for 11 June 12:00.

Simulation settings: Pre-sim is the time simulated before this moment, SM is the soil moisture content, $r_{\text{min}}$ is the minimal stomatal resistance of the low vegetation, veg. frac. is the vegetation fraction. Results: Bowen ratio ($\beta$), sensible ($H$) and latent ($LE$) heat flux, all for Cabauw; and observed potential temperature ($T$) for De Bilt at 500 m height (radiosonde observation), and its difference ($T_{\text{sim}} - T_{\text{obs}}$) with the simulated value. Sim. ID identifies the two simulations further used in this study (for more information see the text). The grey blocks indicate the change compared to the preceding simulation.

<table>
<thead>
<tr>
<th>Pre-sim. days</th>
<th>SM $m^3 m^{-3}$</th>
<th>$r_{\text{min}}$ s/m</th>
<th>veg. frac. %</th>
<th>$\beta$</th>
<th>$H$ W/m$^2$</th>
<th>$LE$ W/m$^2$</th>
<th>$T_{\text{obs}} - T_{\text{sim}}$ K</th>
<th>Sim. ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.75</td>
<td>0.23</td>
<td>100</td>
<td>70</td>
<td>0.17</td>
<td>70</td>
<td>408</td>
<td>3.1</td>
<td>low $\beta$</td>
</tr>
<tr>
<td>0.75</td>
<td>0.23</td>
<td>100</td>
<td>70</td>
<td>0.17</td>
<td>72</td>
<td>423</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>0.23</td>
<td>100</td>
<td>70</td>
<td>0.16</td>
<td>70</td>
<td>447</td>
<td>2.0</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>0.19</td>
<td>100</td>
<td>70</td>
<td>0.30</td>
<td>113</td>
<td>380</td>
<td>1.1</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>0.23</td>
<td>40</td>
<td>70</td>
<td>0.09</td>
<td>44</td>
<td>481</td>
<td>2.3</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>0.23</td>
<td>200</td>
<td>70</td>
<td>0.27</td>
<td>106</td>
<td>389</td>
<td>1.5</td>
<td></td>
</tr>
<tr>
<td>0.25</td>
<td>0.23</td>
<td>200</td>
<td>90</td>
<td>0.29</td>
<td>128</td>
<td>441</td>
<td>0.9</td>
<td>high $\beta$</td>
</tr>
</tbody>
</table>

#### 3.3.3 Atmospheric temperature and humidity profiles

The results of the simulations with (1) low $\beta$ and (2) high $\beta$ were compared with the radiosonde observations in De Bilt (e.g. Figure 3.4). Generally a well-mixed PBL developed that has a lower potential temperature and is moister than the free troposphere. At clear nights cooling near the surface led to a shallow (200 m) and stable PBL.

Simulations with the MRF turbulence scheme showed a better performance than the standard RAMS Mellor Yamada turbulence scheme (Figure 3.4). Still, the height of the PBL was not always captured correctly and the jump of $T$ and $q$ was less pronounced than observed. Increasing the vertical resolution to 60 instead of 25 vertical layers in the lower 3 km of the atmosphere did not change this. This may be due to the limited horizontal resolution of 4 km, or to uncertainties in the parameterization of vertical transport, like lack of subsidence, too much entrainment or an incorrect free tropospheric lapse rate of $T$ or $q$. The free tropospheric values are generally assumed reasonable due to the use of ECMWF analysis boundary conditions.

Simulation of the nocturnal PBL is even more challenging. The atmospheric stability during clear nights was systematically underestimated by the model, which is a common feature for most atmospheric transport models (Geels et al., 2007; Gerbig et al., 2008). In the simulation the nocturnal surface signal reached up to ~400m while in the observations it was limited to ~200m. The poorly simulated height of the PBL will cause discrepancies in the mixing ratios which are not directly related to the magnitude of the CO$_2$ fluxes.
The depth of the PBL is amongst others driven by the surface sensible heat fluxes. Uncertainty in these, as described in Sect. 3.2, will thus lead to uncertainties in the PBL depth. At days when the PBL height was clearly defined the root-mean-square error (RMSE) of the noon PBL height was for both simulations ~350m. The simulation with a relative low β (1, green line in Figure 3.4) showed a mean bias of ~100m, while the simulation with a higher β (2, red line in Figure 3.4) had a positive mean bias of ~75m. The uncertainty in the surface fluxes can thus explain part of the uncertainty in the simulated PBL height as for example indicated for ECMWF simulations in Gerbig et al. (2008).

Figure 3.4. Simulated and observed potential temperature (a) and humidity (b) profiles at De Bilt, and CO₂ mixing ratio (c) profiles at Cabauw, 11 June 2006, at 12:00 (left) and 24:00 (right). Black indicates the radiosonde (a, b) or tall tower (c) observations, red the simulation with a high Bowen ratio, green the simulation with a low Bowen ratio. Blue indicates the simulated temperature and humidity with a low Bowen ratio, but with the Mellor Yamada instead of MRF turbulence scheme.
3.4 Results: CO₂ fluxes and mixing ratios

The framework of the simulated meteorology as described in the previous sections allows us to study the coupling between the surface CO₂ fluxes and the atmospheric CO₂ mixing ratios. First, we will address the uncertainties in the CO₂ fluxes. Secondly, we will show how these propagate into a range of simulated CO₂ mixing ratios which is compared to the observations at the Cabauw tall tower. Finally, the contribution of the different CO₂ fluxes and the background CO₂ to the total CO₂ mixing ratio is unravelled.

3.4.1 CO₂ flux variability

The parameters optimized in the biosphere model 5PM showed a rather large variability in time and space, which is reflected in the uncertainty in the average CO₂ flux parameter values (Table 3.2). The range of CO₂ fluxes (Figure 3.5) simulated with these parameter settings, which were optimized based on European observations for the temperate zone, agreed well with observations and literature values (Jacobs et al., 2007) for our much smaller domain.

CO₂ fluxes simulated with the parameters that gave an unbiased result compared to the observed CO₂ mixing ratio at 200m at Cabauw are indicated in yellow in figure 3.5 and in brackets in Table 3.2. Note that in a follow-up study we intend to formally estimate the parameters of the 5PM model based on the forward results presented here, rather than simply selecting an unbiased set of values.

Respiration fluxes show a soil temperature driven diurnal and synoptic variation, which is represented by the model (Figure 3.5a). Additionally, the observed respiration fluxes showed differences between sites in magnitude and diurnal amplitude, not observed in T and not included in the model. These kind of variations are meant to be implicitly included in the parameter uncertainties. The observed respiration at Cabauw, Horstermeer and Lonzee are in the lower part of the uncertainty range, while the observations at Lutjewad are often near the top of the range.

Assimilation fluxes were inhomogeneous in space and time as well (Figure 3.5b). Generally, the uptake by crops was higher than by grass, as was correctly simulated. Also the observed assimilation reduction at days with limited radiation was captured by the model (within the limitations of the RAMS radiation calculations). Observed assimilation at Lutjewad is relatively high and near the maximum of the uncertainty range, while Lonzee and Cabauw are near the minimum and Horstermeer is in the middle of the range.

Both simulated respiration and assimilation at Lonzee were in the beginning of the period outside the uncertainty range from observations, most likely because the CO₂ flux calculations were not LAI dependent. To overcome this the biosphere model should be extended with spatially explicit, time-varying LAI (e.g. Sellers et al., 1996), which should also give a better representation of the spatial variability of the assimilation fluxes.

Our uncertainty estimates agreed with variability in Dutch grass sites estimated by Jacobs et al. (2007). The standard deviations of their respiration parameters were almost the same as in our study. Their photosynthesis model, and therefore these parameters are different, but the range is also comparable to the range used in this study, with 20-60% variations on the parameters in the GPP model. They concluded
that within small regions with relatively uniform climatic conditions the variability may be similar to the one observed at European larger scales, as is applied here.

3.4.2 \( \text{CO}_2 \) mixing ratios

Uncertainties in the \( \text{CO}_2 \) respiration and assimilation fluxes had a significant influence on the \( \text{CO}_2 \) mixing ratio when the air had passed land areas. The different \( \text{CO}_2 \) flux parameter settings returned a range of simulated \( \text{CO}_2 \) mixing ratios (Figure 3.6). This range varied in time between 1 ppm and 25 ppm, with a 22-day average of 11.7 ppm in the well mixed afternoon PBL (at 200m height). Small ranges were related to northern or south-westerly wind directions (Figure 3.2), when the air predominantly originated from over sea and the land signal is suppressed, while a broader range occurred when the continental signal was large, i.e. with south-easterly wind, low wind speeds or frontal passages. This broad range indicates that the atmospheric mixing ratio potentially contains much information about the \( \text{CO}_2 \) fluxes within the simulation domain. This agrees with studies from Lauvaux et al. (2008) and Zupanski et al. (2007) and shows the potential for future inversion on this temporal and spatial scale.

As mentioned previously, the uncertainties in the simulation of the meteorology discussed in Sect. 3.3 give rise to uncertainties in the simulated \( \text{CO}_2 \) transport. Here we give an overview of the impact of those features on the simulation of the \( \text{CO}_2 \) mixing ratios.

The uncertainty in the surface energy fluxes (Sect. 3.3.2) and consequently the vertical mixing (Sect. 3.3.3) results in an uncertainty in the \( \text{CO}_2 \) mixing ratio. To quantify this the results of the simulations with relative low (1) and high (2) simulated \( \beta \), were compared for \( \text{CO}_2 \) (Figure 3.7). These two simulations (with the same \( \text{CO}_2 \) flux parameter settings) returned a difference in the afternoon \( \text{CO}_2 \) mixing ratio of on average 1.9 ppm.

This was to a small extent due to changes in the \( \text{CO}_2 \) fluxes between the two simulations. The RMSE of the total flux change was 0.69 \( \mu \text{mol m}^{-2} \text{s}^{-1} \). Changes in the respiration caused by the temperature difference (RMSE = 0.63 \( \mu \text{mol m}^{-2} \text{s}^{-1} \)) were systematic. Assimilation fluxes slightly changed due to changes in cloud cover formation (RMSE = 0.29 \( \mu \text{mol m}^{-2} \text{s}^{-1} \)), and their difference over the full period was near to zero. Hence, the effect of respiration change on the \( \text{CO}_2 \) mixing ratio was relatively large compared to the assimilation change. Compensating for this by adjusting the \( R_{10} \) left a difference of 1.7 ppm. This uncertainty in the \( \text{CO}_2 \) mixing ratio is caused by the difference in vertical mixing and horizontal advection, due to the surface flux uncertainty.

Other difficulties were related to the simulation of the nocturnal \( \text{CO}_2 \) mixing ratio, which is up to now, because of the known large uncertainties in the transport model vertical mixing schemes in stable conditions, not used in inversion studies (Gurney et al., 2002; Stephens et al., 2007; Geels et al., 2007). Our simulations confirm that the simulation of nocturnal \( \text{CO}_2 \) is biased, because of the simulation of a too deep nocturnal PBL (see Sect. 3.3.3). The absolute nocturnal \( \text{CO}_2 \) mixing ratio accumulation was not simulated correctly, leading to a low \( R^2 \) of the \( \text{CO}_2 \) mixing ratio time series at 200m (Table 3.4) and simulated mixing ratios at 60-200m that were during some nights totally outside the range of simulated \( \text{CO}_2 \) mixing ratios. As such it is clear that the representation of the nocturnal boundary layer in mesoscale models requires improvement.
Figure 3.5. CO$_2$ respiration (a) and assimilation (b) fluxes for 2 grass (Ca1 and Hor) and 2 crops (Lut and Lon) sites. In black the observations. The red band is the range of CO$_2$ fluxes simulated with a spread of biosphere model parameters (table 3.2). Yellow shows the simulation that best fits the CO$_2$ mixing ratio observations.
Nevertheless, a significant part of the diurnal variation, especially at lower sample levels, is captured by simulations. During the nights CO\(_2\) accumulates near the surface and mixing ratios of over 450 ppm were seen at 20m (Figure 3.6). In the morning the PBL became unstable and the signal of the lower layers was mixed onto higher levels. This was for example reflected by early morning peaks at 200m height, in the observations as well as the simulations. During a number of nights a sudden drop of simulated and observed mixing ratios was seen in the mixing ratio at 20 and 60m around midnight, this is most likely due to the formation of a low level jet (e.g. Bosveld et al., 2008), for example at 11, 12 and 19; doy 162, 163 and 170.

Another important source of uncertainty is the simulated location and the timing of the cloud cover (Sect. 3.3.1). At partly clouded days, this led to an error in simulation of the CO\(_2\) fluxes and the depth of the PBL, and consequently biases in the CO\(_2\) mixing ratio. Therefore, the exact simulated mixing ratios at these days should be regarded as more uncertain. Frontal passages may cause a comparable misrepresentation of the simulated concentrations (e.g. at 25 June; doy 176).

### 3.4.3 Different tracer signals at Cabauw

To study the relative importance of the different sources and sinks influencing the CO\(_2\) mixing ratios we separated the simulated CO\(_2\) mixing ratios at Cabauw into contributions from (a) background CO\(_2\) entering through the lateral boundaries and (b) fluxes from within the RAMS domain. The latter were further separated into contributions from assimilation and respiration of different vegetation types, sea-air fluxes and fossil fuel emissions, which were included in the simulation as separate atmospheric tracers (Figures 3.7 and 3.8).

Assimilation and respiration fluxes were important in determining the CO\(_2\) mixing ratio. They had an average influence during the day of -10.5 and 7.8 ppm respectively, with peaks up to ~30 ppm at 200 m (Figures 3.7 and 3.8a). In the nocturnal PBL the respiration tracer showed peaks up to ~60 ppm at 20 m (not shown). The total biosphere signal, i.e. the sum of the respiration and assimilation, was because of the cancelling opposite signs more modest and had an average influence of 3.2 ppm.

Generally, the crops tracer was the most abundant assimilation tracer, even though Cabauw is a grassland site (Figure 3.8b). This was due to the relatively high assimilation of crops compared to grass (Figure 3.5b) combined with the large area of crops in the domain (Figure 3.1).

In our domain the fossil fuel was also an important contributor to the total signal. Plumes with high fossil fuel tracer concentrations originating from the industrial sources moved over the domain. The major sources were the Ruhr Area, southeast of the Netherlands, the ports in the southwest of the Netherlands and in Belgium, and smaller diffuse sources found over the total domain. Afternoon values in the well mixed PBL varied between 2-8 ppm and the average mixing ratio of the fossil fuel fluxes was almost as large as the biospheric signal whereas its afternoon variance is half that of the biospheric signal (Figure 3.8c).
Figure 3.6. CO$_2$ concentration at 4 heights at Cabauw tower. In black the observations. The red band is the range of CO$_2$ mixing ratio simulated with a spread of CO$_2$ flux parameters (table 3.2), it reflects the effect of uncertainties in the surface CO$_2$ fluxes on the CO$_2$ mixing ratios.

The contribution of the sea-air CO$_2$ fluxes to the total signal was very limited at these time scales (Figures 3.8a and c), although on a global scale the exchange of CO$_2$ by the oceans plays an important role. The average flux of $\sim$0.02 μmol m$^{-2}$ s$^{-1}$ at the North Sea was a negligible compared to the continental fluxes in the domain.

CO$_2$ mixing ratios entering the domain through the lateral boundaries showed a strong diurnal cycle over land, and a much smaller cycle over the sea. When the wind direction was from the east or south the low daily continental values in the background mixing ratio, caused by assimilation over the continent outside of our simulation domain, reached Cabauw. This was for example seen at 12 and 13 June (doy 163 and 164) when the background concentration was reduced by $\sim$10 ppm. Because the influence on the mixing ratios in the middle of the domain can be considerable, the quality of the boundary conditions in a limited domain simulation is important.
Figure 3.7. Contribution of the background CO$_2$ to the mixing ratio at Cabauw 200m (a) and the cumulative contribution of the CO$_2$ fluxes in the domain (b). The variation in the CO$_2$ mixing ratio is mainly determined by the fossil fuel, respiration and assimilation fluxes, where atmospheric signal from assimilation by crops dominates over grass assimilation.

3.5 Discussion & conclusions

We simulated three weeks in June 2006 with the B-RAMS-3.2 mesoscale model at 4km resolution. The simulations were able to reproduce the observed time series of the meteorological variables and CO$_2$ mixing ratios satisfactorily for most of the three week period. The model performance showed no drift and comparison with data remained acceptable throughout the full simulation. We found only limited sensitivity of the model performance to the moment of initialization. This, combined with the absence of significant drift, shows the possibility of a non-stop simulation without divergence of the results from the observations. Hence, in our simulations a re-initialization of the meteorology was not necessary. The advection of the ECMWF meteorological and CarbonTracker CO$_2$ mixing ratio boundary conditions over the domain prevents a runaway of the results in a dynamical and continuous way. This opens the way towards seasonal inversions at a high resolution.

The simulations with the RAMS MRF scheme showed a better performance than the standard Mellor Yamada scheme. This is in line with the findings of Holtslag et al. (1995) and confirms the importance of the parameterizations of turbulence and entrainment (Vila et al., 2004; Casso-Torralba et al. 2008) for the simulation of the atmospheric profiles.

Also a realistic simulation of surface energy fluxes is important for the simulation of atmospheric transport. Comparison with other models (WRF, ECMWF) and observations revealed a discrepancy between the simulations and the surface observations on the one hand and the atmospheric observations on the other hand. For a number of days the observed T profile could not be reconciled with H
observations, something also seen in previous studies (e.g. Holtslag et al., 1995; Ek and Holtslag, 2004). At those times, the observed PBL height could also not be reproduced with a simple mixed layer model (Vila and Casso-Torralba, 2007) based on the observed $H$.

The atmospheric observations suggest that the total Bowen ratio ($\beta$) over the full domain may be higher than indicated by the surface observations. This may be due to heterogeneity of the energy fluxes within one vegetation type (e.g. Baldocchi et al., 2001) which is not included in our land surface scheme. Also, the limited amount of observations over grass and crops, especially in the eastern part of the domain, and energy balance closure problems (Wilson et al., 2002) of ~30% for the Cabauw surface flux observations (Braam, 2008) may add uncertainty to the total surface energy flux estimate over the domain. Moreover, (freestanding) houses, trees and roads may lead to a different domain averaged $\beta$ than observed with the surface observations over vegetated terrain only. Hence, optimizations for a single site (e.g. Jackson et al., 2003) may lead to another estimate of the surface energy fluxes than optimizations with atmospheric properties, which reflect larger scale processes and fluxes over a larger area (e.g. Uppala et al., 2005).

The uncertainty in the sensible heat flux adds uncertainty to the simulation of the vertical mixing, i.e. the simulated shallow and deep convection and the PBL height, and consequently horizontal advection. A comparison of simulations with standard Leaf3 settings with a relative low $\beta$ (suggested by the surface observations) and with adjusted settings with a relative high $\beta$ (suggested by atmospheric observations and the ECMWF and WRF simulations) was made.

![Figure 3.8. Average contribution of the different tracers to the diurnal $CO_2$ mixing ratio (a and b) and its variance (c) at 200m at Cabauw. (a) shows the influence of the assimilation (assim), respiration (resp), sea and fossil fuel (FF) fluxes. In (b) the assimilation flux influence is separated by vegetation type: urban vegetation, broadleaf forest (Blf), needle leaf forest (Nlf), crops and grass. In (c) the variability is shown which is due to variations in the biospheric (bio), fossil fuel (FF), and sea fluxes, and in the background mixing ratio (BG).](image-url)
The surface energy flux and the resulting atmospheric transport uncertainty caused a difference in the simulated CO₂ mixing ratio of on average 1.7 ppm. The estimate of the surface flux uncertainty used in our work is conservative, and represents a minimal value to take into account in future inversion studies. It is in the same order of magnitude as other estimated CO₂ modelling errors, such as due to misrepresentation of smaller scales (0.5-3 ppm; Van der Molen and Dolman, 2007; Tolk et al., 2008), and much larger than the measurement accuracy.

The change in energy fluxes led to a difference in the noon PBL height of ~22%. A comparable sensitivity of the PBL height to changes in the surface energy fluxes (20%) was found by Vila and Casso-Torralba (2007) in a simple mixed layer study for Cabauw. Gerbig et al. (2008) showed at a lower model resolution that uncertainty in the PBL height of 40% gave a uncertainty of 3.5 ppm in the CO₂ mixing ratio. The ~20% change in PBL height and consequent 1.7 ppm range due to surface energy flux uncertainty found here can thus explain a part of those errors.

As a consequence of the change in turbulent mixing, the horizontal advection also changed. The wind change had a standard deviation of 0.85 ms⁻¹ and 0.98 ms⁻¹ in u and v direction, respectively. This is about 40% of the random error found by Lin and Gerbig et al. 80 km resolution. It suggests that the simulated change in CO₂ mixing ratios is importantly influenced by changed advection resulting from the changes in turbulent mixing.

Hence, changing horizontal and vertical transport due to uncertainties in surface energy fluxes can explain an important part of the errors found in previous studies at a coarser resolution. To avoid biased CO₂ mixing ratio estimates, a comparison with observations of the simulated wind direction, wind speed and PBL height and, if needed, adjustment of the surface fluxes like described in Sect. 3.3.2 is recommended as first step in an inversion.

The surface CO₂ fluxes in the domain strongly influenced the simulated CO₂ mixing ratios at Cabauw, causing by far the most of afternoon CO₂ mixing ratio variability (Figure 3.8c). A realistic variation of parameter settings for the calculation of CO₂ fluxes (Groenendijk et al., 2009) resulted in a range of simulated CO₂ mixing ratios that spans on average 11.7 ppm. This atmospheric signal will in future inversion studies be used to constrain the surface CO₂ fluxes. The rather broad range indicates the potential for inversions, even though transport errors are in the order of several ppm. It confirms, with a complementary approach, the findings of Lin and Gerbig (2005) and Gerbig et al. (2008) and is in line with previous studies that stress the importance of the near field fluxes for the CO₂ mixing ratios over the continent (Zupanski et al., 2007; Lauvaux et al., 2008; Gerbig et al., 2009).

Although grass is the dominant vegetation type near Cabauw (Figure 3.1) its atmospheric CO₂ mixing ratio is strongly affected by the assimilation of crops. This is due to the large magnitude of crops assimilation, the large area covered with crops, advection of the atmospheric signal and at wind still days entrainment from the residual boundary layer (Casso-Torralba et al. 2008, Vila et al., 2004). Hence, the information in the atmospheric mixing ratio measurements is not limited to the very local fluxes within the nearest tens of kilometres. We conclude therefore that the scale of tens to hundreds of kilometers is convenient for future inversions of the atmospheric CO₂ mixing ratio signal at the tall tower of Cabauw.

Another important contributor to the CO₂ mixing ratio at Cabauw are the fossil fuel CO₂ fluxes. At these small scales uncertainties in the timing and exact location of the
fluxes are important. The general assumption in global inversions that the fossil fuel fluxes are well known (Gurney et al., 2002) may be true for aggregated values in space and time (annual country totals) but is certainly not true for the scales in time and space that are modeled here. Because of the relative importance of the fossil fuel atmospheric signal, uncertainties in the timing and magnitude fossil fuel fluxes should be quantified and taken into account in future regional inversion studies.

The time series of grass and crops assimilation tracers as simulated for Cabauw were correlated (r=0.67). This suggests that the ability of the observed atmospheric CO$_2$ to distinguish between these vegetation types will be limited. The respiration and assimilation flux signals cancel each other during the day (correlation = -0.80), providing a relatively modest net atmospheric signal that may not constrain the two fluxes separately. During the night, when assimilation stops, the contribution of the respiration tracer to the total CO$_2$ mixing ratio becomes large compared to the contribution of the assimilation tracers. Potentially, nocturnal mixing ratios will be able to provide us therefore with a constraint on the division between respiration and assimilation (Ahmadov et al., 2009).

However, simulation of the nocturnal PBL is an important and long known source of uncertainty (e.g. Geels et al., 2007). The stability of the atmosphere at clear nights was systematically underestimated in our simulations which will lead to biased CO$_2$ mixing ratio estimates. Before simulated nocturnal CO$_2$ mixing ratios can be used in inversion studies they must at least be corrected for the PBL height. More importantly, the simulation of the nocturnal PBL should be improved as indicated for example by Steeneveld et al. (2008). The ability of the simulations to capture variations in the atmospheric stability at small temporal scales is promising. Because of the potential high value of the nocturnal mixing ratios in separating assimilation and respiration fluxes we plan to focus more work on this issue in the future.

Summarizing, the influence of the surface CO$_2$ and energy fluxes on the simulated atmospheric CO$_2$ mixing ratio, the temperature and humidity is large, especially at days with a continental footprint. This shows that atmospheric observations potentially contain much information about these fluxes at the scale of our simulation, i.e. at a spatial scale of tens to hundreds of kilometres. Most of the variability in the CO$_2$ mixing ratio is caused by fluxes within the domain, mainly by biospheric fluxes. Also the fossil fuel CO$_2$ fluxes play a role and their uncertainty should be taken into account in inversions for such an urbanized and industrialized area. Difficulties identified in the simulation of CO$_2$ mixing ratios that reduce the information content of the simulated mixing ratio are (a) the systematic underestimation of the stability of the nocturnal PBL at clear nights which may lead to a biased CO$_2$ estimate, (b) incorrect timing of cloud formation, (c) uncertainty in the diurnal PBL height due to uncertainties in the parameterization of vertical transport and (d) the uncertainties in the driving of the atmospheric mixing by the surface energy fluxes. We quantified the latter and show it is with ~1.7 ppm an important source of uncertainty in the CO$_2$ mixing ratio in the afternoon well-mixed PBL. Besides these shortcomings the atmospheric mesoscale simulation was shown to simulate the meteorological situation over the Netherlands non-stop for three weeks with reasonable accuracy. This, combined with the large simulated range of atmospheric CO$_2$ mixing ratios due to the spread in the CO$_2$ flux parameter settings provides a promising starting point for future inversion studies at the mesoscale.
3.6 Acknowledgements

This work has been executed in the framework of the Dutch project “Climate changes Spatial Planning”, BSIK-ME2 and the Carboeurope Regional Component (GOCE CT2003 505572). W. Peters was supported by NWO VIDI grant 864.08.012. We gratefully acknowledge the researchers who carried out measurements in the BSIK and CarboEurope consortia, with special thanks to A. Moene for providing the scintillometer data, F. Bosveld and H. Klein Baltink for the meteorological data, and E. Moors, J. Elbers, W. Jans, D. Hendriks, M. Aubinet, B. Heinesch, L. Francois and M. Carnol for the eddy correlation observations. ECMWF is acknowledged for providing meteorological observational and analysis data. Further, we would like to thank J. Vila for helpful discussions and H. ter Maat for his contribution to the RAMS simulations.
4 Modelling representation errors of atmospheric CO₂ mixing ratios at a regional scale

Abstract

Inverse modelling of carbon sources and sinks requires an accurate quality estimate of the modelling framework to obtain a realistic estimate of the inferred fluxes and their uncertainties. So-called ‘representation errors’ result from our inability to correctly represent point observations with simulated average values of model grid cells. They may add substantial uncertainty to the interpretation of atmospheric CO₂ mixing ratio data. We simulated detailed variations in the CO₂ mixing ratios with a high resolution (2 km) mesoscale model (RAMS) to estimate the representation errors introduced at larger model grid sizes of 10-100 km. We found that meteorology is the main driver of representation errors in our study causing spatial and temporal variations in the error estimate. Within the nocturnal boundary layer, the representation errors are relatively large and mainly caused by unresolved topography at lower model resolutions. During the day, convective structures, mesoscale circulations, and surface CO₂ flux variability were found to be the main sources of representation errors. Interpreting observations near a mesoscale circulation as representative for air with the correct footprint relative to the front can reduce the representation error substantially. The remaining representation error is 0.5-1.5 ppm at 20-100 km resolution.

This chapter is published as Tolk, L.F., A. G. C. A. Meesters, A. J. Dolman, W. Peters, 2008. Modelling representation errors of atmospheric CO₂ mixing ratios at a regional scale, Atmospheric Chemistry and Physics, 8, 6587-6596.
4.1 Introduction

Understanding the variation in atmospheric CO\textsubscript{2} concentration is the key to prediction and quantification of global climate change. Terrestrial CO\textsubscript{2} fluxes have a major impact on the CO\textsubscript{2} mixing ratios and it is therefore important to understand their spatial and temporal variation. Since the atmosphere is on the short term an incomplete mixer of the CO\textsubscript{2} surface fluxes, observations of CO\textsubscript{2} mixing ratios can be used to quantify the magnitude and strength of the surface fluxes. At the global scale, such inversion studies have increased our knowledge about the terrestrial source-sink distribution, but exact estimates of the sources and sinks still vary considerably (e.g. Fan et al 1998; Bousquet et al., 1999; Gurney et al., 2002; Rödenbeck et al., 2003; Baker et al., 2006). The difference between the results of the various studies are associated with errors in the simulated atmospheric transport (Gurney et al., 2002; Yang et al., 2007; Stephens et al., 2007), aggregation of the surface fluxes over large areas (Kaminski et al., 2001), errors due to a poor representation of the diurnal and seasonal covariance of the surface fluxes with the boundary layer height, i.e. ‘rectification’ errors (Denning et al., 1996; Perez-Landa et al., 2007; Ahmadov et al., 2007) and errors introduced by the assumption that a point observation can be represented by the average CO\textsubscript{2} mixing ratio in a model grid box, i.e. representation errors (Gerbig et al., 2003a, b; Lin et al., 2004; Van der Molen and Dolman, 2007, Corbin et al., 2008).

These errors may be reduced by increasing the resolution of global atmospheric transport models or by employing high resolution regional models (e.g. Peters et al., 2004; Karstens et al., 2006; Geels et al., 2007; Perez-Landa et al., 2007; Sarrat et al. 2007a, b; Ahmadov et al., 2007). With higher resolutions the simulated CO\textsubscript{2} mixing ratios are potentially more accurate, because more small scale phenomena that cause variations in the CO\textsubscript{2} distribution are explicitly resolved. This becomes increasingly important as observations in the boundary layer are used to constrain surface fluxes in more detail at the regional scale (e.g. Carouge 2006; Lauvaux et al., 2007; Peters et al., 2007; Zupanski et al., 2007).

One important error associated with the use of continental CO\textsubscript{2} mixing ratio observations in inversions is studied here in more detail: the representation error (RE). Previous studies showed that the error can be substantial when a grid cell at relatively coarse resolutions over the continent is assumed to be representative of a point observation (Gerbig et al., 2003a, b; Van der Molen and Dolman, 2007). In global scale inversions, large REs can be avoided by selecting ‘background’ observations and rejecting observations that are influenced too strongly by local sinks and sources (Houweling et al., 2000). However, in smaller scale inversions, observations over the continent are used to constrain the fluxes. The RE due to subgrid variability in the mixing ratios over the continent must thus be taken into account. From an analysis of aircraft profiles in the COBRA experiment in North America, Gerbig et al. (2003a) suggested that models may require horizontal resolution smaller than 30 km to capture the most important spatial variations of atmospheric CO\textsubscript{2} in the boundary layer over the continent. Van der Molen and Dolman (2007) found comparable results in a modelling study over Siberia.

In this paper, REs are studied in more detail using a high resolution mesoscale model. This provides the opportunity to assess the spatial and temporal distribution of the RE and its variability due to meteorological circumstances and surface properties. We aim to determine the main features and the major causes of REs, at
scales from 10 to 100 km resolution. In section 4.2, the model configuration and the calculation of the RE will be described. Section 4.3 will show the results of the simulations and the main contributors to REs. These will be discussed in section 4.4, where also some options to reduce the RE will be addressed.

4.2 Methods

4.2.1 Representation error calculation

In this study, the RE is estimated based on the spatial variability of the CO₂ mixing ratio simulated with the Regional Atmospheric Modelling System (RAMS) at 2 km resolution. We calculate the error introduced when trying to represent the values in the 2 km resolution set with the mean value at a coarser resolution of 10, 20, 50 and 100 km. The calculations are performed at an hourly time step, independently for each of the vertical model levels, using terrain following grid boxes. The RE is defined by the standard deviation of the CO₂ mixing ratio simulated at 2 km resolution within the coarser grid boxes of 10x10, 20x20, 50x50 and 100x100 km:

$$\sigma_{CO_2} = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (x_i - x_{coarse})^2}$$  (4.1)

$$x_{coarse} = \frac{1}{n} \sum_{i=1}^{n} x_i$$  (4.2)

Where \( \sigma_{CO_2} \) is the RE, \( n \) is the number of 2 km resolution grid cells within the coarser grid cell, \( x_i \) the CO₂ mixing ratio of the 2 km resolution grid cell, and \( x_{coarse} \) is the average CO₂ mixing ratio within the coarser grid cell. Additionally, the RE is calculated based on linear interpolation of the low resolution values. In these calculations \( x_{coarse} \) is replaced by the interpolated CO₂ mixing ratio \( x_{interpol} \). This is a linear interpolation between the mean of the grid cell and its adjoining cells. We excluded the calculation of RE_{interpol} at 100 km resolution because the boundary cells required for this calculation cover almost the full domain.

The size of the statistical sample (\( n \)) from which the RE is calculated is minimally 25 and maximally 2500 in the 10x10 km and 100x100 km cases respectively. The calculation of the RE is equal to the approach in Gerbig et al. (2003a), Lin et al. (2004) and Van der Molen and Dolman (2007). Note that in the studies of Gerbig et al. (2003a) and Lin et al. (2004) the size of the statistical sample was not limited due to the large number of observations, and the relatively small measurement error was included, which is non existent in our model study.

4.2.2 Simulation setup

The atmospheric simulations are performed with the non-hydrostatic mesoscale model RAMS (Pielke et al., 1992), which has been used to simulate the behaviour of CO₂ in the atmosphere in a number of studies (e.g. Denning et al., 2003; Nicholls et al., 2004; Sarrat et al., 2007b; Perez-Landa et al., 2007, Corbin et al., 2008). The version used in this study is BRAMS-3.2, including the adaptations to secure mass conservation (Medvigy et al., 2005; Meesters et al., 2008). The surface fluxes are calculated using Leaf-3 (Walko et al., 2000) which was extended with the Farquhar
photosynthesis model (Farquhar et al., 1980; Sellers et al., 1996) to calculate surface fluxes of CO₂. The standard vegetation parameters of Leaf-3 are used and completed with maximal rate of Rubisco activity (Vc\(_{\text{max}}\)) based on values from Wullschleger (1993) and Sellers et al. (1996). Respiration is simulated with an exponential (Q\(_{10}\)) temperature–respiration relationship, in which the Q\(_{10}\) and R\(_0\) values as estimated by Van Dijk and Dolman (2004) are used. Further specifications of the simulations are given in Table 4.1.

The simulations are performed for two days of the CERES experiment in South Western France (Figure 4.1) in spring 2005. See Dolman et al. (2006) for further details of this experiment. The 300x300 km domain with a resolution of 2 km is nested in a 1200x1200 km domain at 10 km resolution. It is bounded in the west by the Atlantic Ocean and in the south by the Pyrenean mountain massif with tops over 3000 m height. The area is characterized by several large areas of homogeneous land cover, with the Les Landes pine forest in the west, woods and pastures in the northeast, and large areas of cultivated plots in the rest of the domain (Figure 4.1). Two major cities are located in the southeast (Toulouse) and northwest (Bordeaux) corners of the domain.

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<td>Vegetation model</td>
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<td>Domain centre</td>
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<td>Meteorology, Soil moisture and Temperature</td>
<td>ECMWF ERA40 reanalysis dataset (<a href="http://www.ecmwf.int">www.ecmwf.int</a>)</td>
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<tr>
<td>CO₂ mixing ratio</td>
<td>1. Homogeneous 382 ppm</td>
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<td>2. 375 ppm below, 382 above 1000m</td>
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<th>Boundary conditions:</th>
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<tr>
<td>Meteorology</td>
<td>6 hourly nudged to ECMWF data</td>
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<td>CO₂ mixing ratio</td>
<td>Zero gradient</td>
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<th>Surface characteristics:</th>
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<tr>
<td>Land use</td>
<td>1. Pelcom database (<a href="http://www.geo-informatie.nl/projects/pelcom">www.geo-informatie.nl/projects/pelcom</a>)</td>
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<td>2. Modis biomes and LAI (modis-land.gsfc.nasa.gov/vi.htm)</td>
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<td>Topography</td>
<td>USGS dataset (<a href="http://www.atmet.com">www.atmet.com</a>)</td>
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<td>Soil textural class</td>
<td>UN FAO dataset (<a href="http://www.atmet.com">www.atmet.com</a>)</td>
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<tr>
<td>Fossil fuel emissions</td>
<td>IER database (carboeurope.ier.uni-stuttgart.de)</td>
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*Table 4.1. Simulation specifications. Where two options are mentioned the second is used for sensitivity tests.*
In this study two different days were simulated to compare the influence of different meteorological circumstances on the REs. The first day, 27 June 2005, was very warm with anti-cyclonic clear sky conditions. The wind came mainly from the southeast and allowed the formation of a sea breeze in the afternoon. On the second selected day, 6 June 2005, north-western winds prevailed. This day was cooler, and some cumulus clouds formed in the afternoon in the northern part of the domain.

The two selected days were part of intensive observation periods within the CERES campaign. The simulations were compared to the available observations and the most important findings were described in the model intercomparison of 5 mesoscale models by Sarrat et al. (2007b). That comparison shows the ability of the models to represent the atmospheric CO$_2$ distribution satisfactorily, in general agreement with the observations. They conclude that the complex spatial distribution as well as the temporal evolution of CO$_2$ in interaction with the surface fluxes are realistically simulated compared to the aircraft observations. Our model, BRAMS 3.2 performed satisfactory in most aspects. Any possible further influences of discrepancies between the simulations and the observations on the estimate of the RE are addressed in the discussion section.

The surface fluxes in the standard simulations are calculated based on the Pelcom land use map with a homogeneous LAI per land use class (www.geo-informatie.nl/projects/pelcom). To test the sensitivity of the RE to the formulation of the surface cover, land use maps derived from the Modis satellite data were used (modis-land.gsfc.nasa.gov/vi.htm), where the LAI can vary per pixel. Additionally, simulations were performed in which the CO$_2$ flux was prescribed spatially homogeneous, as a function of time.
The standard simulations for the two days were thus kept very similar, i.e. with similar land use maps and LAI and similar initialization of the CO₂ mixing ratio, so that the differences between the two days represent the influence of meteorology on the RE.

4.3 Results

Our simulations show that a number of processes contribute to the total RE, and their relative contribution is different on both simulated days. REs are always associated with strong horizontal gradients in the CO₂ distribution. There are large variations across the spatial domain due to differences in land-surface type and topography. In the next sections, we will separately discuss each process contributing to the total RE, which spans a range from 0.5 ppm to as much 10 ppm. First, we will illustrate the dominant mesoscale circulation patterns to provide appropriate background for the analysis.

4.3.1 Mesoscale circulations

The simulations show that the RE has a large spatial and temporal variability. The two simulated days show a clear distinction, where the REs during the day on 27 May exceed those on 6 June. The largest difference between the two days is the synoptic wind direction, which originates from the southeast on 27 May and from the west on 6 June. On 27 May mesoscale circulations formed, these were suppressed on 6 June.

During the night of 27 May the south-eastern wind moved air with a high CO₂ mixing ratio, because of respiration, from the land over the sea. Since the CO₂ fluxes over the sea are relatively small the CO₂ mixing ratios remain high there during the following day. In the course of the day a sea breeze developed. The direction of the sea breeze was at 27 May opposite to the synoptic wind direction. The converging winds led to the formation of a front (Figure 4.2a). A gradient of about 10 ppm formed between the high nocturnal mixing ratios over the ocean and the depleted mixing ratios over the land perpendicular to the coast line. This was also described by Dolman et al. (2006), Sarrat et al. (2007a) and Ahmadov et al. (2007).

![Figure 4.2. CO₂ mixing ratio in ppm and wind speed and direction at 250m agl at 14:00 UTC, 27 May 2005 (a) and 6 June 2005 (b). The opposing wind directions on 27 May lead to large CO₂ mixing ratio gradients which are absent on 6 June.](image-url)
Additionally, the relatively high sensible heat flux above the forest resulted in a deep boundary layer compared to its surroundings. On 27 May both the large scale and sea breeze wind directions are directed towards the forest. This prevented advection of the deep boundary layer that formed above the forest over the rest of the domain.

In contrast, on 6 June the synoptic wind was directed from sea to land and similar to the main direction of the sea breeze. Neither advection of the nocturnal high mixing ratios from land to sea, nor the formation of a convergence zone during the day takes place (Figure 4.2b). The effects of the sea breeze on the CO₂ mixing ratio are thus suppressed by the westerly wind on 6 June. Also, the high boundary layer over the forest is advected. This eliminates the strong contrast between the depth of the boundary layer over the forest and its surroundings. At 6 June background CO₂ mixing ratios from the ocean are advected over the land, where it is depleted due to CO₂ uptake at the surface during the day (Figure 4.2b).

4.3.2 Representation errors due to mesoscale circulations

The large mixing ratio contrasts over small distances induced by mesoscale circulations may lead to a large RE. On 27 May a higher RE is simulated than at 6 June (Figure 4.3). At locations that are not affected by mesoscale circulations, the REs on 27 May are comparable to those observed on 6 June. The high RE on 27 May is located in grid cells near of the edges of the convergence zone (Figure 4.4). Near the front a RE of ~2.5 ppm is found at 10 km resolution, and ~5.5 ppm at 100 km resolution.

On 27 May, the CO₂ depleted air from the boundary layer is lifted in the convergence zone. This leads to a band with high REs along the eastern edge of the convergence zone which dominate the average RE over the domain. The highest REs during the day are found around the top of the boundary layer next to the convergence zone (Figure 4.5).

Also in the rest of the domain and on 6 June the RE is high around the mean height of the top of the boundary layer (Figure 4.5b). This is a result of the difference between convection cells and their surroundings, causing strong horizontal gradients between the depleted boundary layer and free tropospheric air. On 6 June this effect stretches over a larger vertical range (Figure 4.5b), causing horizontal variations in the CO₂ mixing ratio up to 3000m height during the day.

Figure 4.3. Domain average RE at 250m above the surface for 12:00 27 May 2005 (red) and 12:00 6 June 2005 (black). This shows the increase of the RE with decreasing resolution, and the higher RE when mesoscale circulations are important on 27 May. The grey and green semi-transparent lines show estimates of the RE from previous studies (Gerbig et al., 2003 and Van der Molen and Dolman, 2007).
Over the sea the boundary layer is very shallow and therefore the largest REs are limited to the lower part of the atmosphere. For example, the RE at 250m height as shown in Figure 4.4 is small since it is above the boundary layer. Within the boundary layer over the sea the RE depends strongly on the wind direction. On 27 May the edges of air masses influenced by nocturnal land fluxes and transported from land during the night causing high REs. The high mixing ratios from the land contrast here with the background mixing ratios over the sea. On 6 June, the wind from the ocean brings ‘background’ air which is not influenced by any strong near field terrestrial fluxes. The REs over most of the sea are therefore very small over the sea on 6 June.

4.3.3 Representation errors due to topography

During the night the presence of the high mountains of the Pyrenees in the south of the domain strongly influences the RE at lower altitudes. In the simulations for both days a band with high CO₂ mixing ratios accumulates at the foot of the Pyrenees. It strongly contrasts with the lower mixing ratios in the flatter areas and at the tops of the mountains. This leads to a high RE near the surface during the night. After sunrise, over the land the high CO₂ mixing ratios at the foot of the Pyrenees are decreased due to the growth of the boundary layer, entrainment and CO₂ uptake at the surface. Over the sea, the high CO₂ mixing ratios are preserved in the shallow boundary layer and lead to enhanced REs during the whole day.

Smaller scale topographic features also induce RE. During the night, accumulation of CO₂ is simulated in valleys with up to a hundred meters altitude difference. The CO₂ mixing ratio variations induced by small scale variations in the surface altitude, remote of the Pyrenees, cause a RE of 0.5-3 ppm at 10 km resolution, and ~3 ppm at 100km resolution. The exact RE due to topography will depend on the specific meteorological circumstances and on the strength of the surface CO₂ fluxes. After sunrise, the gradients in the CO₂ mixing ratios formed during the night decrease and consequently the representation error is reduced near the surface.

4.3.4 Representation errors due to flux variability

During the day, areas of contrasting vegetation types and accompanying contrasting CO₂ fluxes cause large scale variations. An increase in the stomatal conductance causes a simultaneous increase of the CO₂ flux and the transpiration, at the expense of the sensible heat flux. This leads to an inverse relation between the CO₂ fluxes and the boundary layer depth. The surface signal is diluted stronger at locations with a deep boundary layer. CO₂ mixing ratio gradients introduced by CO₂ flux heterogeneity strengthen this effect and increase the RE. The CO₂ flux variability also strengthens the effect of the mesoscale circulations. Ahmadov et al. (2007) showed the covariance (3D-rectifier) between the mesoscale circulations and the CO₂ fluxes. The unresolved flux variability within one grid cell increases with the size of the grid cells. Its influence becomes therefore more pronounced at lower resolutions.

4.3.5 Relative contribution of the representation error components

The relative importance of the different sources of RE depends on the resolution, time and location. When a mesoscale circulation develops like on 27 May, it overwhelms the other sources of RE at all resolutions in the grid cells near the front (e.g. Figure 4.4). With decreasing resolution, the high RE caused by the sea breeze front influences a larger area as the size of the grid cells increases.
Figure 4.4. Spatial distribution of the RE [ppm] at 10 km resolution; 250m above the surface at 14:00 UTC 27 May 2005. Blue indicates sea and green land. The highest REs are located near the edge of the mesoscale circulation front.

Figure 4.5. Variations of the representation errors in ppm on 27 May 2005 (a.) and 6 June 2005 (b.) with time and altitude. The representation errors are averaged over the area north of 44.16°N. The circles in a. indicate the height of the boundary layer in the convergence zone and the triangles the main boundary layer height over the rest of the land area at 27 May, in b. the circles represent the more homogeneous main boundary layer height over the land on 6 June.
Without sea-breeze circulation, the main source of RE along the coast (see Figure 4.1) is the gradient between the mixing ratios over land and sea. Here linear interpolation can reduce the RE substantially, as is shown for 6 June in figure 4.6. More inland (Figure 4.1), linear gradients are less important and $RE_{interp}$ differs just slightly from the RE based on the standard means (Figure 4.6).

We performed two simulations with spatially homogeneous land CO$_2$ fluxes: with land CO$_2$ fluxes comparable to the forest fluxes or comparable to the fluxes of the crops. The REs in the simulations with homogeneous fluxes are mainly caused by convective structures. Gradients between the updraft and downdraft mixing ratios hamper the estimate of the mean boundary layer mixing ratio (e.g. Weckwerth et al., 1996 and Lothon et al., 2007). The strength of the gradient, thus the RE, depends on the strength of the surface fluxes (Figure 4.7). The simulations showed that the RE due to convective structures is about 0.05-0.5 ppm at 10 km resolution (figure 4.7). These values are comparable to the uncertainty of 0.2 ppm estimated from the COBRA data (Gerbig et al. 2003a). At high resolutions the RE is dominated by these CO$_2$ mixing ratio variances due to convective structures.

At lower resolutions, the RE due to CO$_2$ surface flux variability is, next to mesoscale circulations, the major source of REs. At 100 km resolution the RE simulated with heterogeneous fluxes is higher than the RE from either of the simulations with homogeneous CO$_2$ fluxes (Figure 4.7). At 6 June, the mean CO$_2$ flux over the domain is comparable to the average of the forest and crop CO$_2$ fluxes. The mean of the mixing ratio variances ($RE^2$) of the two different homogeneous flux simulations compares well with the $RE^2$ of the heterogeneous flux simulation (Figure 4.7). Their difference increases with resolution. An estimate of the relative contribution of the flux variability to the RE is indicated in figure 4.7 with the grey area.

![Figure 4.6. CO$_2$ mixing ratio variances ($RE^2$) on 12:00 6 June 2005, based on interpolated (dashed line) and standard mean (solid line) values of the coarse grid are used. The blue lines represent the $RE^2$ along the coast and the black lines the $RE^2$ more inland. See figure 4.1 for the areas for which these $RE^2$s are estimated.](image)
Figure 4.7. CO\textsubscript{2} mixing ratio variances (RE\textsuperscript{2}) on 12:00 6 June 2005 for the simulations with heterogeneous fluxes (black) and horizontal homogeneous fluxes similar to the simulated forest fluxes (green), crop fluxes (orange) and their mean (green-orange). The grey area gives an estimate of the RE\textsuperscript{2} due to CO\textsubscript{2} flux heterogeneity.

4.4 Discussion and conclusions

The RE of the atmospheric CO\textsubscript{2} mixing ratio at regional scales is found to be substantial. We concur with earlier studies (Gerbig et al. 2003a, b; Lin et al., 2004; Van der Molen and Dolman, 2007; Corbin et al. 2008) that it is a source of uncertainty that should be taken in account in inversion studies to avoid biased results. The order of magnitude of the RE above the continent appears to be comparable to other sources of uncertainties like transport and rectification errors (Gurney et al., 2002; Yang et al., 2007; Stephens et al., 2007; Denning et al., 1996; Perez-Landa et al., 2007; Ahmadov et al., 2007). The most important contribution to the RE in our small domain during the day comes from surface flux variability, convective atmospheric structures and mesoscale transport phenomena such as the land-sea breeze.

Our numbers are similar to the REs estimated in previous studies (figure 4.3). In the study by Gerbig et al. (2003a, b) the RE was estimated for many different areas within the US based on experimental and theoretical evidence. Our results for 6 June are slightly higher but comparable to these more general estimates of the RE. Coastal areas, like the Les Landes area studied here, are special because of the often occurring sea-breeze circulations as seen on 27 May. The higher domain averaged REs in that situation are more comparable with the REs found in the model study by Van der Molen and Dolman (2007) over Siberia, where mesoscale circulations also played an important role.

The results do not depend on the choice of the land cover map; simulations with the Pelcom and Modis land use maps (Table 4.1) give the same main sources of RE. The boundary layer height on 6 June was simulated correctly compared to the observations. On 27 May the boundary layer height was underestimated by the model at some locations (for details see Sarrat et al., 2007b). Since the strength of the
vertical mixing determines the dilution of the surface signal in the atmosphere, the occasional underestimation of the boundary layer depth may have led to a slight overestimation of the REs in this study. The assumption that the simulation at 2 km resolution captures all variability in the CO\textsubscript{2} mixing ratio may on the other hand lead to a small underestimation of the RE. Hence, the absolute values of the RE in this study must be handled with caution. The processes we found to cause the RE are robust and the difference of the RE between the two days is larger than the sensitivity to the model settings. Therefore, it seems justified to use the simulations as a basis for a qualitative analysis of the RE.

Because of the heterogeneity of the RE in time and space, we recommend to use a time and place dependent error estimate in inversions. Within the boundary layer, the RE is lowest during the day in the well mixed part. This is thus the best location and time to get a representative sample. Observations around the top of the boundary layer should be avoided as the RE is high there. Near land-sea and other surface cover contrasts the RE can be reduced substantially by the use of linear interpolation instead of a simple mean of the coarse grid results (figure 4.6).

During the day the largest REs in our simulations were associated with the sea breeze front caused by the sharp contrast between air masses with different flow histories. A correct interpretation of a CO\textsubscript{2} mixing ratio observation as representative for air with a terrestrial footprint or as representative for the sea breeze can reduce the RE. The measured wind direction and a possible change in the observed CO\textsubscript{2} mixing ratio as the sea breeze reaches the observation location may be used as indicators.

At night, unresolved topography is the main source of REs. The simulated accumulation of CO\textsubscript{2} in the valleys is in line with the findings of previous model (Nicholls et al., 2004; Van der Molen and Dolman, 2007) and observational studies (Eugster and Siegrist, 2000; Araújo et al., 2008; Goulden et al., 2006; Aubinet et al., 2003) which show that near surface cooling leads to katabatic drainage flow of CO\textsubscript{2} rich air. Nocturnal observations at high mountains may after data selection be taken as representative of the CO\textsubscript{2} mixing ratio at their height above sea level (e.g. Schmidt et al., 2003; Geels et al., 2007) with accompanying relatively low free tropospheric REs.

Katabatic drainage due to small scale topography of up to 100 m altitude leads to mixing ratio gradients within the nocturnal boundary layer. Mixing ratios in the valleys are enhanced by accumulation of respired CO\textsubscript{2}, while mixing ratios at higher parts are reduced. The signal may be advected and can also affect the observations downwind of the small scale topography. With moderate unresolved topography we therefore advice to be aware of a possible bias in the observations, and take a RE of \sim 3 ppm, depending on the flux intensity and the stability of the boundary layer, into account during the night.

Extra towers can give a better constraint on the average CO\textsubscript{2} mixing ratio and reduce the RE. Our simulations indicate that even at a relatively high resolution (10 km) the RE over the land exceeds the error introduced by the measurement accuracy aimed for at high accuracy stations. To reduce the RE an observation network with a number of clustered towers may be favourable over a regularly spaced network. The ring of towers around the WLEF tower is an example of such a tower cluster (Zupanski et al., 2007), which may be applied at smaller scales too.

Increasing the model resolution is the most straight forward manner of decreasing the RE. How much the resolution must be increased to resolve the main CO\textsubscript{2} mixing
ratio variability depends on the strength and the horizontal extent of the surface CO$_2$ flux variability and the meteorology. The results of this study suggest that much can be gained by increasing the resolution from relative coarse scales of 100 km toward finer resolutions (Figure 4.3), especially when relative large scale phenomena like the sea breeze cause contrasts in the CO$_2$ mixing ratio.

Although the simulations in this study resolve some formation of atmospheric eddies, it is difficult to simulate the location of the updrafts and downdrafts correctly. In the absence of mesoscale circulation, this means that increasing the resolution to scales below the size of convective structures does not necessarily reduce the RE. High resolution simulations may better simulate the formation of a mesoscale front like on 27 May. Therefore, when mesoscale circulations develop a further increase of the resolution may reduce the RE. This confirms the suggestions of previous studies to use a resolution of 30 km (Gerbig et al., 2003a, b) and a possible further refinement of the grid when mesoscale circulations develop, to reduce the error associated to mesoscale processes (Van der Molen and Dolman, 2007). If observations are associated with the proper influence history, our simulations suggest that the RE in the boundary layer during the afternoon can be limited to below 1 ppm up to at least 20 km resolution, or a coarser resolution when the circumstances are favourable like in this study at 6 June.

4.5 Acknowledgements

This work has been done in the framework of the Dutch project ‘Climate changes Spatial Planning’, BSIK-ME2 and the Carboeurope Regional Component (GOCE_CT2003_505572). We thank the CERES participants for discussions and making their observations available. Thanks to Peter Rayner and Scott Denning for their lessons and discussions on inverse CO$_2$ modelling. We gratefully acknowledge Christoph Gerbig for the constructive review.
Abstract

We have implemented six different inverse carbon flux estimation methods in a regional carbon dioxide (CO\textsubscript{2}) flux modelling system for the Netherlands. The system consists of the Regional Atmospheric Mesoscale Modelling System (RAMS) coupled to a simple carbon flux scheme which is run in a coupled fashion on relatively high resolution (10km). Using an Ensemble Kalman filter approach we try to estimate spatiotemporal carbon exchange patterns from atmospheric CO\textsubscript{2} mole fractions over the Netherlands for a two week period in spring 2008. The focus of this work is the different strategies that can be employed to turn first-guess fluxes into optimal ones, which is known as a fundamental design choice that can affect the outcome of an inversion significantly.

Different state-of-the-art approaches with respect to the estimation of net ecosystem exchange (NEE) are compared quantitatively: (1) where NEE is scaled by one linear multiplication factor per land-use type, (2) where the same is done for photosynthesis (GPP) and respiration (R) separately with varying assumptions for the correlation structure, (3) where we solve for those same multiplication factors but now for each grid box, and (4) where we optimize physical parameters of the underlying biosphere model for each land-use type. The pattern to be retrieved in this pseudo-data experiment is different in nearly all aspects from the first-guess fluxes, including the structure of the underlying flux model, reflecting the difference between the modeled fluxes and the fluxes in the real world. This makes our study a stringent test of the performance of these methods, which are currently widely used in carbon cycle inverse studies.

Our results show that all methods struggle to retrieve the spatiotemporal NEE distribution, and none of them succeeds in finding accurate domain averaged NEE with correct spatial and temporal behavior. The main cause is the difference between the structures of the first-guess and true CO\textsubscript{2} flux models used. Most methods display overconfidence in their estimate as a result. A commonly used daytime-only sampling scheme in the transport model leads to compensating biases in separate GPP and R scaling factors that are readily visible in the nighttime mixing ratio predictions of these systems.

Overall, we recommend that the estimate of NEE scaling factors should not be used in this regional setup, while estimating bias factors for GPP and R for every grid box works relatively well. The biosphere parameter inversion performs good compared to the other inversions at simultaneously producing space and time patterns of fluxes and CO\textsubscript{2} mixing ratios, but non-linearity may significantly reduce the information content in the inversion if true parameter values are far from the prior estimate. Our results suggest that a carefully designed biosphere model parameter inversion or a
pixel inversion of the respiration and GPP multiplication factors are from the tested inversions the most promising tools to optimize spatiotemporal patterns of NEE.

5.1 Introduction

Carbon cycle studies today rely on a wide range of methods with purely observation-based studies on one side of the spectrum and pure modelling on the other side. In between, there are many studies that use a combination of observations and modelling techniques. A special branch of these combined methods is inverse modelling, in which information is derived from observations using Bayesian statistical methods to minimize the difference between model predictions and observations. Recent inverse modelling studies include for instance efforts to derive the net carbon exchange across the globe or at smaller scales from mixing ratio observations of CO$_2$ (e.g., Bousquet et al. 2000; Gurney et al., 2003; Rödenbeck et al. 2003, Mueller et al., 2008; Lauvaux et al., 2009; Ciais et al., 2010, Göckede et al. 2010) or attempts to constrain biophysical parameters from eddy-covariance methods (Papale and Valentini, 2003; Carvalhais et al., 2008).

One recurring issue in inverse studies is the large number of choices to be made concerning amongst others, the selection and weighting of observations, the magnitude and correlations of the uncertainties, the treatment of the time and space domain, and even which unknowns to solve for in the application. As a result, no two inverse studies use the same assumptions and the outcome of inverse studies always needs to be evaluated within the limits of the modelling framework chosen.

Many authors have used atmospheric CO$_2$ mole fraction observations from around the globe to reconstruct the spatiotemporal patterns of net ecosystem exchange (NEE), each in a different way. Peters et al. (2007) used NEE multipliers across large areas of similar vegetation to scale calculated NEE from a biosphere model over each week over many years. Lokupitiya et al. (2008) estimated NEE for a similar time frame, but estimated separate multipliers for simulated gross photosynthetic production (GPP) and ecosystem respiration (R), and for each model grid box. Rayner et al. (2005) in contrast chose to modify a set of physical parameters in the underlying biosphere model directly, thus adjusting NEE to match with observed CO$_2$ mole fractions. That study however estimated only a limited number of regional parameters for separate parts of the globe. The large resulting NEE differences between these three estimates shows that methodology used is an important part of the final result. Clearly, the question which method is most appropriate to estimate NEE has not been yet been resolved (if it ever will) and remains one of the critical issues in estimating source and sink distributions from observations.

In this paper, we want to further investigate the impact of different methodological choices on estimated reanalysis of NEE. The application we chose for this purpose is a regional inversion of CO$_2$ mole fractions using a high-resolution transport model, and a realistic spatiotemporal distribution of NEE. We plan to use this framework for actual NEE inversions at a later stage, after determining the optimal approach through a set of pseudo-data inversions where the true answer is known. The regional character of this inversion allows us to disregard some of the issues related to carbon cycling on longer time scales, and from long-range atmospheric transport of CO$_2$. The four methods we want to test are related to the studies mentioned in the previous paragraph: (1) where we estimate NEE multipliers per vegetation type, (2) where we estimate GPP and R multipliers per vegetation type, (3) where we estimate GPP and R multipliers for each grid box, and (4) where we estimate biophysical model parameters for each vegetation type. The specific questions we want to address are:
What is the best strategy to determine the spatiotemporal pattern and magnitude of NEE in our domain? What are the strengths and weaknesses of each method?

Pseudodata studies always carry the danger of oversimplifying the real problem, or to be designed in a way to favor one outcome over another. We have tried to design our study to prevent this issue by using a “true” CO₂ exchange distribution from a different biosphere model (FACEM; Pieterse et al., 2007) than the one we use to retrieve the exchange patterns (5PM; Groenendijk et al., 2010). Differences exist between the models in physical formulations, plant functional types, driving parameter values, and in driving meteorological input data, minimizing the a-priori expected similarity. However, both models are based on similar principles and equations and even though they do not share the same land-use map for the domain, the prescribed land-use maps in each model are realistic and thus similar.

New in our approach is that we test all inversion approaches, each with different underlying assumptions, at a high resolution with the same meteorology, whereas in previous comparisons (e.g. Gurney et al. 2003) both the inversion method and the transport model could differ. This enables us to isolate the impact of the inversion methodology. We expect our results to be applicable to similar setups (short time periods, large flux heterogeneity, large CO₂ variations, small transport errors) but caution against extrapolation to the larger scales.

After describing the details of each of the methods included in our tests in section 5.2.1, we will describe the general characteristics of all inversions in section 5.2.2 to 5.2.5. We present our results next in section 5.3, using a set of five metrics applied to each solution. Special attention is given to the non-linearity of the biosphere model parameter inversion. The strengths and weaknesses revealed in the result sections are further discussed in Section 5.4. Finally, we revisit our research questions and we present general conclusions and recommendations in section 5.5.

5.2 Methods

5.2.1 Inversion methods

In this study we compare four different optimization methods that are used in current state-of-the-art inverse systems for CO₂. We will briefly describe their main characteristics, which are also summarized in table 5.1. For each inversion we applied the same methodology (Ensemble Kalman filter). This approach was necessary as the biosphere model parameter inversion is non-linear and could not be solved with typical linear Bayesian solution methods. A description of the Ensemble Kalman filter can be found in section 2.1. Further we refer to Peters et al., (2005) and references therein for a description of additional details of the inversion procedure.

The first inverse method is one where pre-calculated patterns of NEE from a biosphere model are linearly scaled across larger areas, similar to the CarbonTracker system (Peters et al., 2007, 2010). This can be denoted as:

\[ \text{NEE}_{\text{post}}(x, y, t) = \beta_{\text{NEE}}(e) \times \text{NEE}_{\text{prior}}(x, y, t), \]  

where \( \beta \) is a scaling factor for each land-use type \( (e) \), with an a-priori value of 1.0. \( \text{NEE}_{\text{prior}}(x, y, t) \) is a high resolution NEE field from a biosphere model. This method has as advantage that it is straightforward to implement and needs little extra
assumptions to stabilize the solution. Disadvantage is that the β factors offer little possibility to change sources into sinks (the sign of β then needs to change), or to scale small (near zero) fluxes to large fluxes (β needs to change a lot).

To overcome some of these disadvantages, systems were suggested that linearly scale gross fluxes instead (Zupanski et al., 2007, Lokupitiya et al., 2008, Schuh et al., 2009):

\[ NEE_{post}(x, y, t) = \beta_{\text{RESP}}(e)R_{\text{prior}}(x, y, t) - \beta_{\text{GPP}}(e)GPP_{\text{prior}}(x, y, t) \]  \hspace{1cm} (5.2)

R and GPP, which are large and stem from mostly independent processes at short time scales, then each carry a scaling factor β. An advantage is that this system does more justice to the actual processes in the carbon cycle, but a disadvantage is that the separation of the large and opposing fluxes using atmospheric CO₂ is very difficult, and might need extra regularization of the solution in the form of prescribed covariances. In addition to the uncorrelated version of this inversion, we therefore also test this option with correlations of 0.5 and 1.0 between βRESP and βGPP for each land-use type.

A final variant of the approach above is to make the βRESP and βGPP spatially explicit:

\[ NEE_{post}(x, y, t) = \beta_{\text{RESP}}(x, y)R_{\text{prior}}(x, y, t) - \beta_{\text{GPP}}(x, y)GPP_{\text{prior}}(x, y, t) \]  \hspace{1cm} (5.3)

This offers the advantage that the βR and βGPP spatial patterns are allowed to vary within each ecoregion. However, additional regularization is necessary because the number of unknown bias parameters is too large to estimate from the limited atmospheric observations. In this study, we apply a spatial covariation between all grid points in the same land-use type that decreases exponentially with distance, similar to methods used in Rodenbeck et al. (2003), Peylin et al (2005), Peters et al. (2005), Schuh et al. (2009), Chevallier et al. (2006) with a smaller length scale (L=100km) to fit with the more detailed regional setup of the inversion.

<table>
<thead>
<tr>
<th>Inversion name</th>
<th>Variables in state vector</th>
<th>Correlation</th>
<th>Optimization units</th>
<th>D.o.f.</th>
<th>( \chi^2 ) of innovations</th>
</tr>
</thead>
<tbody>
<tr>
<td>βNEE</td>
<td>βNEE</td>
<td>NA</td>
<td>ecoregions</td>
<td>6</td>
<td>0.4</td>
</tr>
<tr>
<td>βRG0.0</td>
<td>βRESP, βGPP</td>
<td>0.0</td>
<td>ecoregions</td>
<td>11</td>
<td>0.7</td>
</tr>
<tr>
<td>βRG0.5</td>
<td>βRESP, βGPP</td>
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<td>ecoregions</td>
<td>9</td>
<td>0.6</td>
</tr>
<tr>
<td>βRG1.0</td>
<td>βRESP, βGPP</td>
<td>1.0</td>
<td>ecoregions</td>
<td>6</td>
<td>0.3</td>
</tr>
<tr>
<td>βRGpixel</td>
<td>βRESP, βGPP</td>
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<td>pixels</td>
<td>62</td>
<td>0.3</td>
</tr>
<tr>
<td>Parameter</td>
<td>βE0, βRef, βV, βaj</td>
<td>0.0</td>
<td>ecoregions</td>
<td>22</td>
<td>0.6</td>
</tr>
</tbody>
</table>

*Table 5.1: Summary of the six inverse methods tested, indicating which variables are optimized in the inversions including their correlation and for which spatial unit they are optimized, the degrees of freedom (D.o.f.) as calculated from the a-priori covariance matrix of each system and the \( \chi^2 \) of innovations.*
Another class of inverse methods uses atmospheric CO$_2$ not to constrain the surface exchange patterns, but to directly optimize the parameters of the underlying biosphere model (Rayner et al., 2005, Scholze et al., 2007). The optimized parameters then control the new surface CO$_2$ exchange. An advantage of this approach is the seamless extrapolation of information across the space and time domain and the physical relevance of the optimized result (new biosphere model parameter values instead of scaling factors). Disadvantages come in the form of several pitfalls: limitations in the model structure are difficult to overcome, the model parameters are rarely directly constrained by atmospheric CO$_2$ and aliasing of information into the wrong parameter is possible. In addition, the biosphere model and often contains non-linearities that conflict with the inversion assumptions, as we will discuss elaborately in section 5.3.1. The biosphere model optimization can be written as:

$$\text{NEE}_{post}(x, y, t) = f(\beta_{E_0}(e)E_{0,\text{prior}}, \beta_{R_{\text{ref}}}(e)R_{\text{ref, prior}}, \beta_{V_m}(e)V_{m,\text{prior}}, \beta_{a_J}(e)a_{J,\text{prior}})$$

(5.4)

where we have selected to optimize 4 parameters for each land-use class: $\beta_{E_0}$ is a scaling factor for the respiration activation energy $E_0$, $\beta_{R_{\text{ref}}}$ is a scaling factor for the respiration rate at reference temperature, $\beta_{V_m}$ scales the carboxylation capacity, and $\beta_{a_J}$ scales the quantum yield for light limited assimilation. The first two parameters are used to adjust respiration while the latter two control photosynthesis (see next section).

The resulting six inverse methods described above will be referred to as the $\beta_{\text{NEE}}$ inversion, the $\beta_{\text{RG}0.0}$ inversion (no GPP and R correlations), the $\beta_{\text{RG}0.5}$ inversion (correlations of 0.5), the $\beta_{\text{RG}1.0}$ inversion (fully correlated GPP and R), the $\beta_{\text{RGpixel}}$ inversion (estimates for each pixel), and the parameter inversion. Note that the $\beta_{\text{RG}1.0}$ inversion is not the same as the $\beta_{\text{NEE}}$ inversion because the flux covariance is distributed differently in space and time.

For each inversion method the degrees of freedom are estimated with the simple formula from Patil et al., (2001) that considers the number of significant eigenvalues in the correlation matrix (normalized covariance matrix). For each of these inversions, the d.o.f. is relatively small compared to the number of observations (336). The estimated number of degrees of freedom is given in Table 5.1.

<table>
<thead>
<tr>
<th>Prior fluxes</th>
<th>‘True’ fluxes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resolution</td>
<td>10km</td>
</tr>
<tr>
<td>Landuse map</td>
<td>Corine2000</td>
</tr>
<tr>
<td>LAI</td>
<td>MODIS-2006</td>
</tr>
<tr>
<td>Soil map</td>
<td>UN-FAO*</td>
</tr>
<tr>
<td>Meteorology</td>
<td>RAMS</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of the differences between the FACEM biosphere model (‘true’) and the 5PM biosphere model (a-priori). In our pseudo-data study these differences mimic the expected structural differences between real CO$_2$ fluxes and those simulated with a biosphere model, and limit the performance of the inversions substantially.
5.2.2 Modelling system, simulation period and domain

All inversions are based on simulation with the same model setup in which the non-hydrostatic mesoscale model RAMS (Pielke et al., 1992) is used to simulate the atmospheric transport. The version used in this study is B-RAMS-3.2, including adaptations to ensure mass conservation (Meesters et al., 2008). The prior NEE flux estimates are calculated with the simple biosphere model 5PM (Groenendijk et al., 2010) in which photosynthesis is calculated following Farquhar et al. (1980) and respiration is calculated with the relationship by Lloyd and Taylor (1994). The input for the biosphere model is summarized in table 5.2. Further details on the transport and biosphere modelling system can be found in chapter 2 and 3.

The simulations are performed for an area of 400x400km at a relative high resolution of 10 km, centered in the Netherlands at 52.25°N and 5.2°E (Figure 5.1). The Corine 2000 land use maps are used (http://dataservice.eea.europa.eu). Most of the area consists of cultivated land, in which the most abundant land use type is ‘Agricultural areas with complex cultivation patterns’, which is further referred to as ‘crops 1’. Second most abundant is grassland, referred to as ‘grass’, and the third is ‘Agricultural land with significant areas of natural vegetation’, referred to as ‘crops2’. The simulation period 19 May 2008 – 2 June 2008 was selected to contain various weather types and thus flux regimes, including cloudy, rainy, and sunny days at the beginning of the growing season.

Figure 5.1: The domain of the study showing the distribution of six different land-use categories according to the Corinne database, as well as 4 locations where continuous, calibrated measurements of CO₂ are available (Cabauw, west; Lutjewad, north; Loobos, middle; Hengelman; east). The area displayed, shown as lat long on the x and y axis is used in the RAMS meso-scale transport model, and is resolved on 10x10km spatial resolution.
5.2.3 Control inversions

The simulations are performed in a pseudo-data environment, so that the ‘true’ fluxes are known and the results of the different inversion methods can be evaluated against them. As a check on the inversion system, and as a reference for the performance of the inversions with a perfect or near perfect structure of the NEE flux pattern, we performed two control simulations. In the first, pseudo data were created as a multiplication of the prior NEE fluxes. This pattern is within the solution capacity of each inversion option and it could be retrieved by all inversions, confirming that the inversion system worked correctly.

In addition, we created a flux field based on a simulation with 5PM with parameters that were a realization of the a-priori covariance of the parameters. The flux field is therefore fully within the statistical properties of each inversion method (see also section 5.2.5), and the spatial structure is represented perfectly in all methods. This is the control inversion referred to in the rest of the text and serves in our setup as a reference for the performance of the inversions in absence of spatial biosphere model structure differences.

Figure 5.2: The spatial distribution of the two-week average fluxes: top left: prior (from 5PM model); top right: ‘true’ flux (from FACEM model); the other pictures show the averaged posterior estimates of the different inversion methods. Both sets of fluxes are used with hourly temporal resolution.
5.2.4 **True fluxes and pseudo observations**

Usually, in pseudo-data studies true fluxes are chosen as some realization of the underlying biosphere model (Zupanski et al., 2007; Schuh et al., 2009), as done in our control inversions. This choice is not very realistic when the structure of the underlying biosphere model itself is part of the inverse problem, and different structures will work better with different optimization strategies. For example, a parameter inversion when the truth was created with perturbed parameters will perform better than a βNEE inversion against the same truth. To prevent this in our study, and also to make the pseudo-data study more realistic, we have used as “true” fluxes those from a different biosphere model.

Hourly biogenic respiration and photosynthesis flux fields from the FACEM model (Pieterse et al., 2007) were used. These were calculated at 6’ resolution and have a different underlying land-use description, different soil type and LAI map, and different meteorological driver data as summarized in Table 5. As a result, all six test inversions have to overcome a difference in model structure that causes the simulated pseudo-CO$_2$ time series to never perfectly match with the true NEE distribution (figure 5.2a, b). This situation mimics reality in which a biosphere model never grasps the full complexity nor heterogeneity of the true NEE distribution, which can be an important source of error (Kaminsky et al, 2001, Gerbig et al., 2006; Carvalhais et al., 2008).

To create pseudo CO$_2$ mixing ratio data, the true CO$_2$ fluxes are coupled to the atmospheric model RAMS. The simulated 3D atmospheric CO$_2$ field is sampled at the locations where also in reality CO$_2$ mixing ratios observations are available (figure 5.1), where the highest observation level at the towers is used (Cabauw, 200m; Lutjewad, 60m; Loobos, 24m; Hengelman; 18m). Real observations will be used in a companion paper to obtain a real flux estimate. The inversions use hourly CO$_2$ mixing ratios sampled from the well mixed PBL between 11:00 and 16:00 UTC. In the control inversion we applied a model-data-mismatch of 0.2 ppm and with the FACEM truth we assumed a standard deviation of 1.2 ppm to account for the possible differences in the biosphere structures. The observation selection and uncertainty are the same in all different inversion methods. The total number of observations assimilated is 4 towers times 14 days times 6 hours, equaling 336.

5.2.5 **Prior Flux Covariance**

A correct comparison between the different inversion options requires that the overall prior covariance of all options is equal. We require that the NEE, integrated over ecoregion and time, has the same ensemble-variance for all inversion options, and that the ratios between variance of ecoregion-time integrated respiration and GPP are also the same for the inversions. The standard is the parameter inversion, for which mean and variances are prescribed based on our previous work (Tolk et al., 2009; their table 5.2), which was in turn based on an eddy covariance study (Groenendijk et al., 2010). For the other inversions, the prior covariance is scaled such that the above-mentioned similarity between the inversions is satisfied (see 5.7 for details).
Figure 5.3: The distribution of calculated NEE from 5PM given a Gaussian distribution of values for four different parameters in the model. The figure shows the linear translation of for instance $V_m$ and $R_{ref}$ to a Gaussian shaped NEE distribution, and the non-linear response of $\alpha$ and $E_0$.

This approach is an important choice in our experiment design. It is interesting to note that equal variance of the time/ecoregion integrated NEE does not ensure the same uncertainty in the inversions at each point in space and time. Our choice of covariance treatment has ensured that (a) the inversions have equal covariance in the quantity that matters most to our CO$_2$ observations (NEE), (b) the spatial gradients in NEE variance between land-use types is conserved, and (c) the time integral covariance over the inversion are conserved suggesting that all inversions had an equal chance to find the mean NEE of the truth.

The $\chi^2$ metric compares the a-priori model performance to the specified error structure by dividing the squared forecast residuals $(y-Hx)^2$ by the total covariance $(HPH^T+R)$ of fluxes and measurements. It is thus a measure of the balance between expected skill and achieved skill. An innovation chi-squared of close to 1.0 indicates a correct balance, while smaller chi-squared values suggest that the model performed better than specified in the covariance structure and hence the inversion was conservative in its prescription of covariance (Michalak et al., 2005). The innovation $\chi^2$ statistics indicate that flux and observation uncertainties were well balanced. The $\chi^2$ values range from 0.34 to 0.78 (Table 5.1) indicating that the model skill was high relative to the assumed uncertainty. The inversions were thus conservative in their flux adjustments and not over-constrained.
5.3 Results

In this section we present our results according to the performance of all the different inversion methods against a set of different metrics that each highlight a particular aspect of the inverse results (section 5.3.2-5.3.6). Before the overview of the performance of all methods is presented, the special behavior of one of the methods which is partly non-linear (the parameter inversion) is highlighted in section 5.3.1. An overall assessment of each individual method is given in the discussion section.

5.3.1 Optimizations and non-linearity

Five out of six inversion systems used in this study are linear, in the sense that a Gaussian set of parameters will translate to a set of similar Gaussian set of CO$_2$ flux fields. The exception is the parameter inversion. Out of the four parameters chosen for optimization only the reference rate for respiration ($R_{ref}$) is linear, while the other ones are nonlinear. In addition, the model follows the Farquhar et al (1980) photosynthesis limitation principle, in which either light or carboxyl becomes limiting for photosynthesis. The transition from one regime to another presents an important nonlinear step in the simulation of NEE.

Figure 5.3 shows the distribution of fluxes resulting from a chosen distribution of parameter values. It shows that the activation energy parameter ($E_0$) in particular affects the fluxes in a nonlinear fashion when the chosen value approaches zero. The carboxylation capacity ($V_m$) and quantum yield ($\alpha_j$) parameters are weakly nonlinear across the chosen range, and the reference respiration rate ($R_{ref}$) is fully linear.

The nonlinearity in the parameter inversion should in principle be dealt with in the ensemble system as it implicitly linearizes over the full model ($H$). However, we could clearly see the effect of imperfect linearization in our results. When we fed the posterior parameter set back into our flux model, and consequently propagated the solution through the RAMS transport model ($H(x_a)$) we did not obtain the distribution of CO$_2$ mixing ratios that the linearized inverse solution ($Hx_a$) had predicted. Generally, the propagated mean was further away from the observations than the linearized mean, and the propagated standard deviation of the ensemble was larger than the linearized one.

We explored this further with an offline inverse system that had only three parameters, as is further shown in appendix A (section 5.6). A simple equation in which we varied the degree of non-linearity related the parameters to observations. The parameters were optimized against a truth obtained with one realization of the parameters, and some additional noise. We observed in our simple non-linear system that the propagated posterior parameter spread always correctly included the true parameter value. Additionally, the simplified model showed that introducing a non-linear parameter does not affect the ability of the inversion to return the correct values for the other, linear parameters in the model. Nonetheless, this simplified model showed the same behaviour with a poorer match to observations, and a larger spread in the concentration when using the propagated posterior parameters instead of the linearized model. This degraded performance of the linearized model is caused by the tails of the a-priori parameter probability density function (PDF), which do not follow the linearized propagation of the mean, or values close to that mean. This results in the observed larger spread in the non-linearly propagated CO$_2$, and also in the overconfidence of the posterior parameters (the linearized ensemble lacks spread). We found that this effect could be reduced in several ways: (1) by reducing
the degree of non-linearity in the model, (2) by starting with a good a-priori parameter value around which the model is linearized, or (3) by limiting the uncertainty of the non-linear parameter to a space where the effect is mostly linear. These three strategies may be generally applicable in future studies attempting non-linear inversions.

5.3.2 Metric 1: Domain integrated fluxes

One of the important metrics in evaluating the performance of the inversions is the ability to retrieve the NEE summed over time and space. This is a final goal of the inversions, but not the only one as more detail may be desired, and the summed values may hide opposing errors. These issues are addressed in the other metrics in the next sections. All except one of the inversions have managed to find an improved posterior time average flux for the whole domain (Figure 5.4). The two results closest to the truth are from the βRG inversions without correlations (βRG0.0), or with partial correlations (βRG0.5; not shown), followed by the βRGpixel inversion and the parameter inversion. The βNEE inversion was the only inversion that had a worse posterior time mean flux than prior time mean flux for the whole domain.

![Figure 5.4: True, prior and posterior NEE fluxes and its uncertainties for the different inversion methods integrated for the whole domain or per land use class [10⁻⁷ mol/s]. (a) Results of the control inversion, where the truth fits the biosphere model, (b) Results of the inversions with an imperfect biosphere model.](image-url)
If we consider the root-mean-square-difference (RMSD) of the true and estimated domain average flux over time, a similar picture emerges: all inversions show an improvement (table 5.3, first column). This agreement was expected under the current design of the study, in which many observations were available to constrain the hourly NEE. Again, the βRGpixel and βRG0.0/βRG0.5 perform best, but also the parameter inversion has captured the temporal structure of the domain total flux better than the prior. The βNEE inversion struggles not only to find an improved time mean flux, but also provides a poor match to the hourly domain averaged time series.

The degree of RMSD improvement is rather small, especially considering the large number of observations available. Further investigation showed that the main limitation to improving the flux estimate is the different structure of the a-priori model (5PM) and the truth (FACEM). In the control inversion, where this model structure difference was not present, all methods (including the βNEE inversion) gave much better time mean fluxes, and RMSD of the time series (Table 5.3). This suggests that synthetic studies using the same land surface model to generate and retrieve fluxes may overemphasize the ability of the model.

### 5.3.3 Metric 2: Fluxes per land-use type

We can further separate the results above into each individual land-use class considered. Figure 5.4 shows these results. The most striking feature is the lack of improvement in mean NEE for most land-use classes in most inversions. This suggests that overall, the inversions have failed to find a correct distribution of time mean NEE within the domain (see also figure 5.2). The discrepancy is relatively

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**Table 5.3: The performance of the six inverse methods expressed as the RMSD of the optimized NEE time series compared to the truth, for the total domain and for each separated land use class [µmol/m²/s]. The upper part of the table shows the results of the control inversions, the lower part shows the results of the inversions where the truth is generated with a different biosphere model than the priors.**

<table>
<thead>
<tr>
<th>Prior / Posterior</th>
<th>Inversion name</th>
<th>Domain total</th>
<th>Grass</th>
<th>Crops1</th>
<th>Crops2</th>
<th>ENF</th>
<th>DBF</th>
<th>Rest</th>
</tr>
</thead>
<tbody>
<tr>
<td>Truth fits biosphere</td>
<td>βNEE</td>
<td>0.9</td>
<td>3.7</td>
<td>5.5</td>
<td>6.9</td>
<td>6.9</td>
<td>6.3</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>βRG0.0</td>
<td>0.6</td>
<td>1.5</td>
<td>0.6</td>
<td>1.3</td>
<td>5.6</td>
<td>6.3</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>βRG0.5</td>
<td>0.5</td>
<td>1.5</td>
<td>0.6</td>
<td>1.4</td>
<td>5.8</td>
<td>6.3</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>βRG1.0</td>
<td>0.8</td>
<td>3.4</td>
<td>4.0</td>
<td>4.9</td>
<td>4.6</td>
<td>6.3</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>βRGpixel</td>
<td>0.7</td>
<td>1.6</td>
<td>2.4</td>
<td>3.5</td>
<td>6.1</td>
<td>6.7</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>Parameter</td>
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<td>0.6</td>
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<td>1.3</td>
<td>1.9</td>
<td>2.8</td>
<td>0.1</td>
</tr>
<tr>
<td>Imperfect biosphere</td>
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<td>2.9</td>
<td>2.9</td>
<td>3.1</td>
<td>3.7</td>
<td>4.0</td>
<td>3.4</td>
</tr>
<tr>
<td></td>
<td>βRG0.0</td>
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<td>2.8</td>
<td>2.6</td>
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<td>4.7</td>
<td>4.0</td>
<td>3.2</td>
</tr>
<tr>
<td></td>
<td>βRG0.5</td>
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<td>4.5</td>
<td>2.0</td>
<td>3.5</td>
<td>2.9</td>
<td>4.0</td>
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</tr>
<tr>
<td></td>
<td>βRG1.0</td>
<td>2.4</td>
<td>5.6</td>
<td>2.3</td>
<td>3.9</td>
<td>4.0</td>
<td>4.0</td>
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</tr>
<tr>
<td></td>
<td>βRGpixel</td>
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<td>2.7</td>
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<td>3.8</td>
<td>9.9</td>
<td>2.8</td>
</tr>
<tr>
<td></td>
<td>Parameter</td>
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<td>3.2</td>
<td>1.9</td>
<td>2.0</td>
<td>3.5</td>
<td>5.8</td>
<td>2.9</td>
</tr>
</tbody>
</table>
weak for the parameter inversion and the βRG1.0 inversion, which show improved posterior mean βNEE in 3 out of 6 land-use classes. The two inversions that did best on the total domain average NEE (βRG0.0 and βRG0.5) now reveal a lack of improvement within the dominant land-use classes, suggesting that they might have gotten domain total fluxes right for the wrong reason.

Assessing the RMSD of true and estimated flux time series per land-use type is consistent with the domain total picture of the previous paragraph: the parameter inversion and βRGpixel inversion generally show relatively low posterior RMSD and improve in 4 out of 6 land-use classes (Table 5.3). The other inversions improve substantially in RMSD in only 2 classes. An example of posterior flux performance for the largest land-use class (Crops1) is shown in Figure 5.5. It shows that poor RMSD is caused mostly by an inability to capture the difference in the daytime signal at the different days, and that nighttime NEE is poorly simulated in most of the inversions.

Considering that the instantaneous fluxes per land-use class are most closely connected to the CO2 mole fraction observations, the performance of the inversions is disappointing, and also alarming. Also in this metric the performance of the same inversion methods against the control fluxes is much better, and agrees with the expectation that domain total and land-use fluxes improve in time (both flux average and RMSD; figure 5.4 and table 5.3).

### 5.3.4 Metric 3: Uncertainty estimate

The contrasting performance of most inversions for individual land-use classes (bad) versus the domain integral (reasonable) suggests significant spatial correlations between classes, with canceling flux errors. Here we investigate the posterior uncertainties.

The inversions based on multiplication factors per land-use class (βNEE and βRG) all produce posterior uncertainties that are too small. This means they do at most locations not encompass the true flux within one or two standard deviations (figure 5.6). This might have been expected since the degrees of freedom in the inversion are much smaller (~6-62) than the number of observations assimilated (~336). However, the $\chi^2$ of innovations suggests a fair balance between CO2 residuals ($y-H(x_b)$) and prescribed uncertainty ($HP_bHT+R$) and the posterior uncertainty does not scale directly with the degrees of freedom in each inversion. Thus, the relatively large number of observations does not seem the main cause of too low posterior uncertainty.

In fact, when we reduced the number of assimilated observations to 1 per day we saw only minor effects on the posterior variances. Only if we reduced the number of observations and additionally increased the model-data mismatch did we see an increase in posterior variances for the individual land-use classes. But even then the domain total variance remained much too small to accommodate the large difference in flux mean. The small posterior uncertainty is thus not simply an artifact of the inverse method setup.

If we consider the control inversion, the posterior flux estimates are much better for all inversions, and 4 out of 6 inversions report ±1 sigma uncertainties that include the truth (figure 5.4). This again points at an important role of model structure in determining the outcome of an inversion, in this case leading to overconfidence that the true value is retrieved.
<table>
<thead>
<tr>
<th>Prior / Posterior</th>
<th>Inversion name</th>
<th>CO₂ mixing ratio RMSE</th>
<th>Truth fits biosphere model</th>
<th>Imperfect biosphere model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Daytime only</td>
<td>All hours</td>
</tr>
<tr>
<td>Prior</td>
<td></td>
<td>2.3</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td>Posterior</td>
<td>βNEE</td>
<td>1.1</td>
<td>5.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>βRG0.0</td>
<td>0.4</td>
<td>0.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>βRG0.5</td>
<td>0.4</td>
<td>0.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>βRG1.0</td>
<td>1.3</td>
<td>6.8</td>
<td></td>
</tr>
<tr>
<td></td>
<td>βRGpixel</td>
<td>0.5</td>
<td>1.0</td>
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</tr>
<tr>
<td></td>
<td>Parameter</td>
<td>0.4</td>
<td>0.5</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.4: The performance of the six inverse methods expressed as the RMSD of the time series of the atmospheric CO₂ mixing ratio related to the optimized NEE flux fields compared to the pseudo observations [ppm]. For the times the observations are used in the inversions (daytime only) and for the total time series (all hours). The left part of the table shows the results of the control inversions, the right part shows the results of the inversions where the truth is generated with a different biosphere model than the priors.

Figure 5.5: Time series of aggregated true, prior, and posterior fluxes for the dominant land use type in the domain, Crops1. The figure illustrates the different temporal behavior of each solution on hourly time scales, leading to differences in two-week aggregated RMSD.
The parameter and the βRGpixel inversions generally produce error estimates that are conservative and more realistic compared to the other inversions, in the sense that the posterior estimate (figure 5.6) is in large parts of the domain within 2 sigma of the truth and they encompass the truth within ±2.5 sigma in 5 out of 6 land use classes. Note that in the 6th land use class (rest) also the prior uncertainty is too low, and a realistic posterior uncertainty could therefore not be expected for this land use class.

Posterior covariances are large in all inversions. In the βRG inversions the covariances occur between β parameters for R and G. The covariances reveal an inability to separate the effect of photosynthesis and respiration based on CO2 alone. This was demonstrated in earlier work too (Ahmadov et al., 2009; Schuh et al., 2009). This type of covariances is more pronounced than those between β’s for different land-use classes.

Figure 5.6: Spatial maps of the posterior flux residuals (true-minus-optimized fluxes) scaled by the posterior standard deviation of the flux estimate. Green colors indicate that the true flux is within ±1 standard deviation of the estimated flux, yellow/light blue indicate within 2 or -2 standard deviation respectively and orange/blue colors are outside this range. The figure shows the general tendency of the inversions to be overconfident, because structural differences between 5PM and FACEM are not taken into account in the treatment of uncertainty.
5.3.5 Metric 4: Match to CO$_2$ mole fractions

All six inverse methods reduce the mismatch between pseudo-observations and simulated CO$_2$ mole fractions for those observations that were assimilated. This is expected from an inverse calculation. Not all methods obtain equal RMSD though, as each inversion adjusts fluxes differently. Table 5.4 shows that the posterior RMSD in CO$_2$ mole fractions is largest for the βNEE optimization and smallest for the βRGpixel optimization.

The $\chi^2$ of innovations (Table 5.1), which indicates the balance between a-priori mismatch and assumed uncertainties, is smaller for the βNEE and βRG1.0 inversion than for all other optimizations per ecoregion. This is because these two inversions had a much larger uncertainty in hourly NEE than the other inversions (necessary to maintain the same uncertainty over the full period, see section 5.2.5), translating to more simulated uncertainty in CO$_2$ mole fractions.

More interesting is the comparison to CO$_2$ mole fractions that were not assimilated as they show the performance against independent data. The second column of table 5.4 shows that only three inversions perform better when assessed against the full CO$_2$ time series, while for three others it deteriorates. This is an important result that suggests that the estimated NEE field reflects only a limited part of the CO$_2$ mole fraction time series, as a result of the daytime-only subsampling we used.

Moreover, the βNEE and βRG1.0 inversion -that improve RMSD of non-assimilated CO$_2$- show the opposite result in the control inversion, suggesting that the improvement in the real inversion was fortuitous. This leaves only the parameter inversion to improve the RMSD of assimilated and independent CO$_2$ observations, both in the control inversion and the real inversion.

For the RG inversions the good performance on the temporal structure of NEE (Tables 3 and 4) contrasts with the poor RMSD of the non-assimilated CO$_2$ observations. The reason is that the posterior nighttime flux is simulated poorly which does not affect the RMSD of fluxes much (the prior was also rather poor at night, and the nighttime NEE is relatively small compared to the daytime NEE), but is strongly amplified in CO$_2$ concentration space due to the shallow nighttime boundary layer. Now, the posterior variances in βR and βGPP mentioned in the previous paragraph really come to expression: they give an acceptable aggregated flux (NEE) but at the expense of incorrect nighttime CO$_2$ mixing ratios. The propagation of this incorrect nighttime CO$_2$ signal through the domain will likely result in compensating signals further downwind, or later in time. These effects are not visible yet in our short experiment though.

The results above suggest: (1) that nighttime CO$_2$ observations are needed to separate respiration from photosynthesis fluxes, and (2) that interpretation of these observations depends critically on the adequate simulation of the nocturnal boundary layer.

5.3.6 Limitations of the inversions

The NEE inversion is the most simple inversion method tested in this study, the number of degrees of freedom is with 6 the smallest compared to the other inversion methods (table 5.1). The results of this inversion did not correctly fit with the true fluxes and were overconfident. This inversion appeared to lack the flexibility to
capture the correct fluxes. In the other inversions tested in this study the flexibility is increased in a number of ways indicating the limitations of the inversion.

In the βRG inversions the flexibility is increased compared to the βNEE inversion as the respiration and GPP can be separately optimized. These βRG inversions provided a better estimate of the domain total fluxes than the βNEE inversion (figure 5.4). The different covariance strengths between βR and βGPP that were applied resulted in different d.o.f's. The performance of the inversions with 9 and 11 d.o.f. were comparable.

In the control inversions, where the truth fits the biosphere model inversions, the βRG inversion performed correctly improving the fluxes and the RMSE, for both the domain total fluxes and the fluxes per ecoregion, with a realistic uncertainty estimate (e.g. figure 5.4a). However, when the structure of the truth and the prior were non-similar, the flux distribution over space and time was not well captured. The flexibility of the system in time and/or space appeared to be limiting for the inversion. Below, first the temporal limitation of the βRG inversion is discussed based on an analysis of the results of the βRG inversion and the more flexible in time parameter inversion, and secondly the spatial limitations of the inversion are discussed based on the results of the pixel inversion.

The βRG inversion performed badly when looking at the CO₂ mixing ratio RMSE for all hours (table 5.4). This is caused by a difficulty in capturing the nighttime fluxes (figure 5.5). The CO₂ mixing ratios during the day, which are used to constrain the fluxes, contained a mixed signal of the respiration and GPP fluxes. The results suggest that the difference between the temporal structure of the truth and the prior caused the respiration fluxes to be altered by the inversion to overcome the difference in the flux structure during daytime, but thereby the nighttime flux estimate was worsened (figure 5.5). In an additional test, in which the inversions were performed for three days only instead of a 15 day period the effect on the nighttime fluxes was smaller. In these three days the weather was steady anticyclonic. This suggests that the structure mismatch of the fluxes between the prior and the truth over the 15 days time period due to differences in the response patterns to cyclonic and anti-cyclonic weather influences the estimate of the fluxes, next to the influence of the different diurnal pattern of the fluxes between the prior and the truth.

In the parameter inversion, the flexibility to change the fluxes in time is increased. In this inversion four instead of the previous one (in the βNEE inversion) or two (in the βRG inversion) parameters can be altered by the inversion for each ecoregion, which means a d.o.f. of 22. The additional temporal flexibility improved the results and was able to avoid the incorrect change in the nocturnal fluxes that was seen in the βRG inversions (figure 5.5, table 5.4).

In the inversions where the structure of the truth did not fit the structure of the prior, the βRG inversions showed a lack of improvement within the dominant land-use classes. This could be caused by the mismatch of variability of the fluxes within one land use type. Therefore, in the βRGpixel inversion, the flexibility of the system to alter the fluxes in space was increased. Instead of one adjustable βR and βGPP per landuse type, these parameters could be optimized for every pixel, with a correlation length scale of 100km, which increased the d.o.f. to 62. Despite the increased flexibility, the inversion still could not capture the fluxes per land use type. Nonetheless, the βRGpixel inversion provided acceptable results because it was
realistic in its uncertainty estimate, only changing the fluxes in a more limited part of the domain.

The fact that increasing the temporal flexibility in the parameter inversion and the spatial flexibility in the pixel inversion does not fully solve the problems faced in the inversions suggests that both temporal and spatial structure differences between the truth and the prior were limiting to obtain results at a smaller scales than a few hundred kilometer. For the coarser scale, which is in this inversion the full domain, the inversions performed well despite these limitations. The structure mismatch is thus limiting for the detailed analysis, and not so much for the aggregated results.

5.4 Discussion

With the steady expansion of (continuous) CO₂ observation sites comes a tendency to estimate carbon exchange patterns at increasingly higher resolutions. Inversion methods are thereto equipped with state-of-the-art meso-scale transport models and detailed ecosystem models. The methodology to optimize carbon exchange at regional scales is often transferred from existing global systems, thereby inheriting their known strengths and weaknesses. At these regional scales however, other considerations come into play that potentially turn weaknesses into strengths and vice versa. An example from this work is the scaling of the diurnal cycle amplitude in the NEE inversion. This was a rather robust way to maintain a balance between respiration and photosynthesis over long time periods in global inversions (Peters et al., 2010), but seems to fail on the smaller scales. We suspect that this is caused by the dominance of the CO₂ diurnal cycle as a source of information for the inversion, and the sensitivity of the inversions to changes in the response to short term weather influences, while in continental scale inversions the average CO₂ mixing ratios were more controlling.

In contrast, we see that at the regional scale the shortcomings of biosphere model structure is expressed more strongly than at continental scales. The potential to alias CO₂ signals onto the wrong parameter because they are simply not reproducible with the prescribed structure was demonstrated and discussed convincingly in Carvalhais et al (2008). Our study corroborates their conclusions, and shows that spatial mismatches in model structure can lead to incorrect mean flux estimates, with error bars that are overconfident. Since there is currently no metric, nor a place in the inversion for this type of error to be included, we suggest that model structure is assessed critically when optimizing biosphere model parameters or precalculated flux patterns on regional scales. Comparison of resulting fluxes and uncertainties against independent data (i.e., not used on the inversion) is one way to detect model structure errors for inversions using real data (e.g. Lavaux et al., 2009).

In our assessment of the inversions based on biosphere model parameter optimizations we have seen an important role of non-linearity in the model equations, similar to previous studies (Trudinger et al., 2007; Scholze et al., 2007; Rüdiger et al., 2010). In this regional optimization based on CO₂ mixing ratio observations, we noticed that the non-linear model parameters in particular were difficult to constrain. To use them correctly, they required a good first-guess, a small uncertainty, or a full non-linear model propagation of the solution (rather than a linearized one). These parameters were often also the ones least constrained by daytime atmospheric CO₂, and thus likely suffered from the specific setup of our experiment. Since the estimation of non-linear parameters did not affect the retrieval of the linear ones, we
suspect that a different setup (other observations, such as water, energy, and CO₂ fluxes and isotopes, more temporal constraints) might perform better.

In contrast, estimates of bias scaling factors on photosynthesis and respiration remains linear, depend less on model structure, and have more freedom to use the diurnal cycle information on regional scales. In our studies it also proves a good alternative to the NEE scaling and the biosphere model parameter optimization. Also here, the daytime CO₂ sampling scheme used makes it difficult to confidently separate the two processes. Simply including night time CO₂ mixing ratio observations is however not an option, because of the limited skill of transport models to simulate the stable boundary layer (Tolk et al., 2009; Gerbig et al., 2008; Law et al., 2008; Steeneveld et al., 2009). Also, there is a large potential for erroneous photosynthesis and respiration bias scaling factors to propagate in time, and destabilize the inversion after a few weeks. The short time window used in this study does not incorporate this complication.

Perhaps the most important result from our pseudo-data tests is that despite the relatively large number of observations, the high resolution of the (perfect) transport model, and the increased freedom to fit spatiotemporal flux patterns, we still have not achieved a correct estimate of carbon exchange at the local scale. Similar to previous studies (Carouge et al., 2010, Schuh et al., 2009, Gerbig et al., 2006, Ahmadov et al., 2009), we find that significant aggregation of results is needed to come to robust numbers. The aggregation scale is on the order of 100x100km as in previous work. This suggests that the simple translation of methods from the large scale to the small scale might not be sufficient. A re-evaluation of inversion methods might be needed, with an eye for nonlinear behavior, model structure, and multiple constraints. In that respect, recent work where model mean structure is relaxed in favor of extensive covariance structure based on multiple auxiliary datasets (Michalak et al., 2004; Gourdji et al., 2010; Yadav et al., 2010) is of great interest.

5.5 Conclusions

We started this paper asking which of six inversion approaches is the most suited for a regional inversion, and what the pitfalls are of each method. From our analysis we have learned that:

- With prior fluxes that have the same structure as the true fluxes, all inversion methods improved the estimate of the NEE, both for the domain total fluxes as for the fluxes per ecoregion.

- When the structure of the priors differed from that of the truth, the full domain estimates improved with all inversions except for the βNEE option, but all inversion approaches had difficulties in obtaining the fluxes per ecoregion.

- Model structure is therefore an important consideration for inverse estimates that can lead to incorrect spatiotemporal patterns of fluxes, and overconfidence in posterior results. An assessment of model structure error, and its inclusion in the quoted uncertainty would make any regional inversion more plausible.

- Inversions that scale NEE from prescribed spatiotemporal patterns are most susceptible to these errors (which include aggregation errors), and perform worst in the realistic tests presented. We do not recommend using this method for regional NEE estimates.
- Inversions that separately estimate photosynthesis and respiration perform better on NEE, at least on these short time scales, even though they cannot obtain realistic gross flux estimates, which might lead to problems later. We recommend to use them only if the realism of the gross fluxes can be assessed after the inversion, or maintained by other means such as through nighttime observations of fluxes or CO₂ mixing ratios.

- The results with the smallest deviations from the pseudo-truth over all metrics were obtained when the land-use class concept was applied least strictly by allowing spatial variations in bias corrections on gross fluxes (RGpixel), or when the bias parameter approach was abandoned altogether such as in the parameter inversion. Nonetheless, also these inversions had difficulties in estimating the specific fluxes per ecoregion.

- The parameter optimization approach has some appealing features. However, it can only be used if the non-linear behavior of the system is dealt with.

- When optimizing non-linear parameters we recommend to (a) start from a good a-priori mean estimate, (b) keep the uncertainty on the parameter small, and (c) check posterior results carefully using the full non-linear model.
5.6 Appendix A: Simple non-linear model

To test the impact of non-linearity on the inversions we applied simple forward models that calculate a series of observations from a triplet (a,b,c) of arbitrary parameters. Subsequently, several inversion methods were used to estimate (a,b,c) from the observations: a regular minimum least-squares without priors, a full Bayesian solution with a Kalman filter, a serial ensemble KF, and a matrix based ensemble KF. In the Bayesian solutions, the three parameters had prior values that varied between realistic and unrealistic relative to the truth. Also, we varied the degree of nonlinearity in the forecast model (from fully linear to strongly nonlinear).

We applied all methods to a fully linear problem first, and confirmed that each estimation method gave the same (correct) result as long as enough observations were available. Prior values that were reasonably chosen (i.e., with enough uncertainty to accommodate the truth) were thus correctly modified. The statistics of the posterior solution were also as expected: uncertainty on all 3 parameters was reduced in accordance with the specified noise, and the propagated posterior solution satisfied the observations to within the specified uncertainty.

Next, we applied the ensemble KF (the only system to handle nonlinear problems) to the nonlinear function $f(x) = a + \sin(b) \cdot x + c \cdot x^2$. We noticed here first that the mean of the linear parameters a, c was estimated correctly, but the mean of the nonlinear one (b) was not. Uncertainty on the non-linear parameter was also miscalculated: the truth was far outside the posterior error. Moreover, we noticed that if we placed the posterior parameter values back in the nonlinear model, the match to the observations was much worse than the statistics of the filter suggested. This was because the linearization that is contained in the ensemble method was not able to overcome the nonlinearity and therefore mispredicted the mixing ratios and their spread given a set of parameters.

![Figure 5.7](image_url)  
**Figure 5.7.** An illustration of the effect of non-linearity on the results of the inversion.
In figure 5.7 we show this feature for the typical nonlinear estimation problem as above. The yellow line is the true function, which. This we ‘observe’ at the 20 black dots, and then we add a little bit of noise. The noisy observations are fed to the ensemble KF to estimate the 3 parameters \((a,b,c)\) that underly the yellow curve. The red line \((± 1\) standard deviation\) is the match to the observations that the system thinks it will achieve given would correspond to the ensemble statistics and its posterior estimate. This coincides with the true curve in yellow. But when the posterior values \((a,b,c)\) are fed into the function \(f(x)\), the blue curve is the actual result. This is much less accurate than was predicted by the filter, and actually outside the specified uncertainty range.

The above problem could be remedied through the exact solutions we suggest in the main text: making the more problem more linear, starting from a better prior, or reducing uncertainty on the nonlinear parameter. The figure moreover led us to suggest to always use the full nonlinear model to check your the accuracy of the result, rather than the filter statistics.

5.7 Appendix B Applied Ensemble Kalman Filter Specifications

In the control inversions in this study the observation vector \((y)\) was created based on one realization of the parameter state vector by selecting one of the columns of ensemble \(X\). In the other inversions the observation vector \((y)\) was based on the hourly NEE flux fields created by the biosphere model FACEM (Pieterse et al., 2007). In both cases the corresponding CO\(_2\) mixing ratios were calculated with the atmospheric model RAMS in which the sea, the fossil fuel, and the boundary fluxes of CO\(_2\) were kept constant.

The size of the state vector differed in the different inversion methods, in the parameter inversion it had a dimension of 24 (4 parameters times 6 land use classes), in the \(\beta\)\(_{RG}\) inversions its dimension was 12 (twice the number of land use classes), in the \(\beta\)\(_{NEE}\) inversion its size was 6 (once the number of land use classes) and in the \(\beta\)\(_{RGpixel}\) inversion its size was 2218 (twice the number of land pixels). The dimension of the observation vector was the same in all inversions with 336.

For the parameter inversion, \(\beta\)\(_{RG0.0}\) and \(\beta\)\(_{NEE}\) inversions all off-diagonals in \(P_{prior}\) were zero. Additional inversions were performed with a correlation between \(\beta\)\(_{R}\) and \(\beta\)\(_{G}\) of 0.5 and 1.0. In this case all off-diagonals were zero except the ones denoting the correlations between \(\beta\)\(_{R}\) and \(\beta\)\(_{G}\) of the same land use type. Also in the pixel inversions only correlations within one land use type are applied with correlations calculated based on distance \((D)\) with a length scale \((L)\) of 100 km:

\[
P_{i,j} = \sigma_i \sigma_j \exp\left(-\frac{D}{L}\right)
\]

(A10)

By the way, a comparable correlation length (130 km) was found for the prior-truth residuals. The means and variances for the parameter inversion are prescribed based on Tolk et al. (2009). The other inversions use an ensemble of \(\beta\)’s with mean one and variances which are scaled to achieve the required similarity between the inversions (section 2.5). First the uncertainty related to the respiration fluxes on the one hand and to the GPP fluxes on the other hand were separated. This was done by running the biosphere model with two different ensembles: (1) containing only variations in the parameters determining respiration and (2) containing only variations in the parameters determining GPP. To convert this to the variance related with the \(\beta\) factors, each ensemble member is scaled with the flux per ecoregion, separately for
respiration and GPP in the $\beta_{RG}$ inversions and for NEE as a whole for the $\beta_{NEE}$ inversion. This ensures that the ratio between the uncertainty in respiration and GPP per ecoregion is the same in all inversion options. In the inversion where applicable correlations were added to $P$. The new variances were subsequently scaled with a multiplication factor per ecoregion, with the same multiplication factor for $\beta_{Resp}$ and $\beta_{GPP}$. These multiplication factors were chosen such that the uncertainty in NEE integrated over ecoregion and time became the same in all inversion options, taking into account the correlations between respiration and GPP in the $\beta_{RG0.5}$ and $\beta_{RG1.0}$ options and the reduced correlation within one ecoregion in the pixel inversion.

5.8 Acknowledgements

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Inverse carbon dioxide flux estimates for the Netherlands

Abstract

CO$_2$ fluxes for the Netherlands and surroundings are estimated for the year 2008, from concentration measurements at four towers, using an inverse model. The results are compared to direct CO$_2$ flux measurements by aircraft, for 6 flight tracks over the Netherlands, flown multiple times in each season. We applied the Regional Atmospheric Mesoscale Modelling system (RAMS) coupled to a simple carbon flux scheme (including fossil fuel), which was run at 10 km resolution, and inverted with an Ensemble Kalman Filter. The domain had 6 eco-regions, and inversions were performed for the four seasons separately. Inversion methods with pixel-dependent and -independent parameters for each eco-region were compared. The two inversion methods, in general, yield comparable flux averages for each eco-region and season, whereas the difference from the prior flux may be large. Posterior fluxes co-sampled along the aircraft flight tracks are usually much closer to the observations than the priors, with a comparable performance for both inversion methods, and with best performance for summer and autumn. The inversions showed more negative CO$_2$ fluxes than the priors, though the latter are obtained from a biosphere model optimized using the Fluxnet database, containing observations from more than 200 locations worldwide. The two different crop ecotypes showed very different CO$_2$ uptakes, which was unknown from the priors. The annual-average uptake is practically zero for the grassland class and for one of the cropland classes, whereas the other cropland class had a large net uptake, possibly because of the abundance of maize there.

6.1 Introduction

Knowledge of the surface atmosphere fluxes of CO$_2$ is important for our understanding of current and future climate change, and in particular the response of the carbon cycle to climate. The only existing direct observations of these fluxes consist of eddy-covariance measurements that provide information at scales of a few 100 of meters to a few kilometers (Baldocchi et al., 2001) at best, and in case of heterogeneous surfaces, need to be scaled up with land cover information and models, to obtain flux estimates at larger domains. However, recent research (Groenendijk et al. 2011a) shows that the vegetation parameters on which the CO$_2$ fluxes depend, are much more variable than assumed by current vegetation models, and this causes large uncertainties in upscaling. Another direct flux approach which has already been applied for the Netherlands is the $^{222}$Radon-tracer method (e.g. van der Laan, 2009a, van der Laan, 2010) which can be used for much larger scale (i.e. regional) surface flux estimates. However, its results are directly proportional to the assumed $^{222}$Radon soil emission rate, which is currently not well known. Inversion methods that derive fluxes from concentration measurements, a transport model and a priori guesses of the surface flux field, are arguably our current best method to obtain a more spatially integrated perspective.

There are, however, specific challenges with the application of inversion methods to determine fluxes at relatively high resolution. First, to apply an inversion to a limited area, it is necessary to use a high resolution transport model that resolves mesoscale circulations (size from a few km to a few hundreds of km), and the recycling of nocturnal CO$_2$ (e.g. Sarrat et al. 2007, Ahmadov et al. 2009, Schuh et al., 2010, Rivier et al., 2010; Broquet et al., 2011). Second, an a priori flux parameterization using surface maps at high resolutions is needed to resolve the heterogeneity of the surface fluxes. The third, while also common to more global inversions, is the large number of unknowns that have to be constrained by a limited number of observations. Finally, sufficient temporal resolution is required to obtain a good match with observed concentrations that exhibit large diurnal variability.

Until recently, most regional scale inversions have worked with “synthetic data” to test the performance of the inversion methods and the measurement network (e.g. Zupanski et al., 2007, Carouge et al., 2010, Gourdji et al., 2010, Tolk et al., 2011). Such work is obviously of considerable importance, but as synthetic flux fields form the basis of these methods it remains speculative to which extent the results can be generalized towards the real world. To test whether such regional methods produce credible results when applied to real observed data requires an independent comparison with observed flux data. The lack of appropriate data has unfortunately often presented a significant hurdle for such validation. For instance, the inversions by Göckede et al. (2010) use observed concentration data from two towers, but lack an independent validation of the calculated fluxes, while Rivier et al. (2010) evaluate their results against independent biosphere model calculations. Recently, as more appropriate flux data have become available, such data have been used for validation: Schuh et al. (2010), Broquet et al. (2011), and Lauvaux et al. (2012) evaluate fluxes against tower measurements, and Lauvaux et al. (2009) also employ additional aircraft measurements.

In this study, we extend that analysis further from the campaign scale to the seasonal scale by applying two state-of-the-art inversion methods to obtain the CO$_2$-fluxes for the Netherlands for the year 2008. The inversion schemes we use, are based on
previous theoretical and synthetic work by Tolk et al. (2009) and Tolk et al. (2011), i.e. chapter 3 and 5 of this thesis. A relatively dense and well-maintained network of four towers is used for the CO$_2$ concentration measurements. A large amount of flux measurements by aircraft (Vellinga et al., 2013) is available for all the seasons in 2008 to validate the calculated fluxes. This setup also offers the opportunity to test the usefulness of the existing concentration measurement network for regional inversions.

6.2 Methods

The set up of the modelling work is, to a large extent, similar to that in the previous studies: Tolk et al. (2009; chapter 3) for the forward modelling and Tolk et al. (2011; chapter 5) for the inversion modelling. A Bayesian inversion scheme that uses an ensemble Kalman filter with prior fluxes, is applied to estimate the surface CO$_2$ fluxes. Based on the comparison in chapter 5, the two best performing inversion setups (“parameter” and “pixel” inversion) were selected. In contrast to the previous synthetic data study, the inverse modelling is performed with real CO$_2$ concentration measurements. No “synthetic truth” is involved. Another difference with the studies in chapter 3 and 5 is that the calculations are performed with season-dependent model parameters, rather than stationary model parameters.

The next paragraphs present a summary of the modelling system used, and document the specific changes compared to the previous studies. The observation methods are also described.

6.2.1 Transport model and background fields

The transport model used in this study is the Regional Atmospheric Modelling System (RAMS), specifically version B-RAMS-3.2, with some adaptations described in chapter 3. The domain includes the Netherlands and some of its surroundings (figure 6.1). For this study, a single grid with 10 km resolution is used. Reanalysis data from ECMWF (which we imported at resolution 0.5°) are used for initialization and boundary conditions for the meteorological fields, where nudging is applied only close to the boundaries. Sea surface temperatures are also obtained from the ECMWF reanalysis.

The CO$_2$ transport is calculated simultaneously with the atmospheric modeling (Eulerian method). For initial and boundary conditions of the CO$_2$ mixing ratios, optimized fields at 1° × 1° resolution from CarbonTracker Europe (Peters et al. 2010) were used. Ensemble modelling is applied: One hundred three-dimensional CO$_2$ fields are simulated simultaneously, each of them driven by its own surface flux field (see hereafter).

6.2.2 Surface modelling

The surface model LEAF-3 is part of RAMS, and is used to calculate the meteorological fluxes from the land to the atmosphere. Land use is specified according to the Corine2000 database, and Leaf Area Index (LAI) according to MODIS data (monthly values). The domain contains six different land use classes, as shown in figure 6.1. The crop-covered pixels are classified according to the absence (“crops-1”) or presence (“crops-2”) of significant areas of natural vegetation. Subgrid patches of grassland and maize are more abundant in land use class crops-2 than in land use class crops-1. The latter is characterized by more large-scale farming
(potatoes, cereals) and locally by horticulture. The class “other” concerns several kinds of areas (urbanized areas, dunes).

CO$_2$ fluxes from fossil fuel burning are taken from the IER database at 10 km resolution (CarboEurope, 2003). These data are based on the year 2000. Since according to the national inventories (RIVM, see reference), the emissions grew from 178.2 Mton (2000) to 186.7 Mton (2008), the fossil fuel flux is multiplied with a constant scaling factor of 1.05 to obtain fluxes for 2008. Results appear rather insensitive to this scaling factor. To cope with the fact that fossil fuel emissions are lower in weekends, the emissions of 2000 were used with a shift of three days to get the days of the week matching those of 2008. The uncertainty of these fluxes is included in the “observation-representation” uncertainty (see below).

The calculation of the CO$_2$ surface fluxes is performed, simultaneously with the atmospheric transport calculations, for a random ensemble of parameter combinations, each ensemble member generating its own CO$_2$ field. CO$_2$ assimilation and autotrophic respiration are calculated with a scheme derived from Farquhar (1980), and heterotrophic respiration according to Lloyd and Taylor (1994). More details can be found in chapter 2.

![Figure 6.1 Dominant land use class per pixel (crops-2 has more natural vegetation mixed with the crops than crops-1). Triangles indicate concentration measurements: Lutjewad (north), Cabauw (west), Loobos (center), and Hengelman (east). Region shown is longitude 2.56E–8.44E, latitude 50.45N–54.05N.](image)
6.2.3 Modelling periods

Four separate model simulations have been performed:

1) Spring: March-May 2008;
2) Summer: June-August 2008;

To obtain a comparable winter season, winter data have been combined for the winter 2007-2008 (January-February 2008) and that of 2008-2009 (December 2008). These periods are run separately for their meteorology but with a single set of vegetation parameters. The results are combined afterwards, so that effectively one season is obtained.

In the modelling domain, the first four months in 2008 were climatologically mild or very mild, except for March that was relatively cold. May 2008 was the hottest May in 100 years. The summer was rather wet, but warm. The autumn was average. December was cold compared to 2000-2010 average (KNMI 2008).

6.2.4 Parameter inversion

For each of the six land use classes, two parameters are estimated: carboxylation capacity \((V_{c_{\text{max}}})\) to control photosynthesis (and indirectly autotrophic respiration), and reference respiration rate \((R_{10})\) which controls heterotrophic respiration. Hence, for this method, 12 unknowns have to be solved per season. In contrast to chapter 5, the values of quantum yield \((\alpha)\) and activation energy \((E_0)\) were kept fixed everywhere, to prevent the aliasing effects as discussed in chapter 5. For \(E_0/R\) a value of 200 K is used (\(R\) denotes the gas constant). The parameters \(V_{c_{\text{max}}}\) and \(R_{10}\) are assumed to be stationary within each season. The prior parameter values used in the inversions are identical for each season, and given in chapter 5. Due to the imperfectness of observed LAI-values and of the vegetation model, \(V_{c_{\text{max}}}\) and \(R_{10}\) have the character of tuning parameters, whose best fits may be season-dependent (Groenendijk et al. 2011b). For this reason we allow their posterior values to depend on season.

With the reduction in number of parameters to solve for each land-use class, the inversion method resembles the so-called \(\betaRG0.0\) – method of chapter 5, since the unknown parameters are essentially linear or close to linear scaling factors. In setting up the ensemble (100 members), the parameters are assumed to be uncorrelated, and to have standard deviations of 30 \(\mu\text{mol} \text{ m}^{-2} \text{ s}^{-1}\) \((V_{c_{\text{max}}})\) and 2 \(\mu\text{mol} \text{ m}^{-2} \text{ s}^{-1}\) \((R_{10})\).

As in chapter 5, to suppress the influence of random noise in the updating of the parameters we prescribe that a parameter is updated on inversion, only if after processing of all the observations, \(\sigma_{\text{prior}}/\sigma_{\text{post}}\) for that parameter is at least 1.05 times the smallest \(\sigma_{\text{prior}}/\sigma_{\text{post}}\) of all the parameters (Zupanski et al. 2007).

6.2.5 Pixel inversion

The inversion procedure is extensively described in chapter 5, and is summarized here briefly. The domain contains 1109 land pixels of 10 km \(\times\) 10 km. For each pixel, the surface \(\text{CO}_2\)-flux is:

\[
\text{NEE}(t) = \beta_{\text{resp}}R_{\text{prior}}(t) - \beta_{\text{GPP}}GPP_{\text{prior}}(t)
\]
with the scaling factors $\beta$ depending on pixel but not on the time within a specific season. The prior fluxes are calculated from the prior parameter values in the forward run, and for the two $\beta$’s an ensemble is set up with the following properties. The means are equal to one, and there is no correlation between $\beta_{\text{GPP}}$ and $\beta_{\text{resp}}$, nor between the $\beta$’s of different land use types. Within a land use class, the $\beta_{\text{GPP}}$-values are correlated with an e-folding length of 100 km, as was found appropriate in section 5.7. The standard deviation of $\beta_{\text{GPP}}$ is constant within a land use class, and is tuned so that the variance of the time series of each land-use-class-averaged flux is the same as for the ensemble that was used for the parameter run. To reach this, first an initial run has to be executed; from that run we calculate how the $\beta$’s have to be rescaled to meet the variance requirement. For $\beta_{\text{resp}}$, the same remarks apply as for $\beta_{\text{GPP}}$. The number of unknowns to be solved amounts to 2218 for each season. The rule for suppressing the influence of random noise is applied in the same way as for the parameter inversion (see above).

6.2.6 Overview of the inversions

All runs are performed for each season separately. First, runs were executed with an ensemble of parameters (for the parameter inversion) or $\beta$-coefficients (for the pixel inversion). Then the inversions were performed, and new runs were performed with an ensemble of posterior parameters or $\beta$-coefficients, respectively. The CO$_2$ mixing ratio fields generated by the (ensemble of) fluxes is propagated through the domain from day-to-day, and constrained on the larger scales by the CarbonTracker boundary conditions. Each new seasonal inversion starts with a new initial CO$_2$ field from CarbonTracker.

6.2.7 Concentrations from atmospheric observations

Hourly atmospheric CO$_2$ concentrations from four observation sites for the year 2008 are used. The measurement locations are also shown in figure 6.1. The Cabauw mixing ratio observations are described in Vermeulen et al. 2011. At Loobos, concentrations were measured using a single infrared gas analyzer and a solenoid switching system. An AIRCOA system was used (http://www.col.ucar.edu/~stephens/RACCOON). The uncertainty (standard error) of the CO$_2$ concentration measurements with the AIRCOA system is 0.2 ppm. See for further information Elbers et al. 2011. At Lutjewad, concentrations are measured with a modified Agilent 6890 N Gas Chromatograph. The obtained measurement uncertainty is usually <0.1 ppm. For details see Van der Laan 2009a. At Hengelman, concentrations were measured at one level using a single infrared gas analyzer CIRAS-SC (PP Systems, Amesbury, USA), which was calibrated twice daily. The uncertainty of the CO$_2$ concentration measurements with the CIRAS systems was 2 ppm. The measurement heights above ground level used for this paper are 200, 24, 60 and 18 m for Cabauw, Loobos, Lutjewad and Hengelman, respectively, and all measurements are reported on the WMO2007x scale. Only hourly values (average over last 5 minutes), from 11 to 16 UT (6 values) are used for each day, since transport errors are likely to be larger for other hours (chapter 3).

An “observation representation uncertainty” (standard error) has to be assigned to the concentrations, but its quantification is difficult. In chapter 5 we found that for synthetic inversions with the present model and network, a hourly uncertainty of 1.2 ppm worked well. This translates to an uncertainty of $1.2/\sqrt{6} = 0.5$ ppm for the daily average over 6 values. Since the present work with real observations has also to cope
with (large but unknown) transport errors, we have enhanced the estimated uncertainty to 2 ppm. This explains why our uncertainty is somewhat larger than the instrument uncertainties. This value is multiplied with \( \sqrt{6} \) to obtain the hourly observation representation uncertainty. For the autumn (SON), the data from Hengelman have been omitted because of known calibration issues. For the winter, there were no data from Hengelman available.

6.2.8  Surface fluxes from atmospheric observations

Flux observations were carried out by a small, low altitude and at low speed flying Sky Arrow 650 TCNS aircraft (O.S. Vellinga, R.J. Dobosy, E.J. Dumas, B. Gioli, J.A. Elbers, and R.W.A. Hutjes, Calibration and quality assurance of flux observations from a small research aircraft, submitted to Journal of Atmospheric and Oceanic Technology 2012). There are data from flights available for 6 trajectories (figure 6.1), which were flown 2 by 2 on a weekly schedule throughout 2008 and early 2009. The measurement height was usually around 70 m above the surface. The surface fluxes have been derived using the eddy covariance method based on 50 Hz raw data of wind fields, temperature, and CO\(_2\) and H\(_2\)O concentrations, all measured with fast response sensors (Vellinga et al., 2010). Covariance and fluxes were computed for 2 km windows, representing the spatial resolution of this type of airborne flux measurement. The instruments and aircraft configuration were calibrated following procedures described elsewhere (Vellinga et al. submitted to Journal of Atmospheric and Oceanic Technology 2012). That publication also documents further details of data processing and quality assessment.

Data were available from 64 flights. The uncertainty (standard error) in the flux measurements was estimated based on twin flights, and varies from 10 to 20 % for the flight averages (uncertainties in averages over shorter distances are much larger). These fluxes are used for validating our posterior fluxes. Flux divergence occurs between the surface and the measurement level, but generally the resulting flux-loss at these flight levels is smaller than other errors (Vellinga, et al. 2010, supplementary material) and neglected in the current comparison. Rather than aggregating the flux observations to prescribed parts of the model domain, as is often done (e.g. Lauvaux et al. 2009), we chose an alternative approach: A routine was added to the model to import the locations and times of the observations, and to export the calculated fluxes exactly for these locations and times.

6.3  Results

6.3.1  Goodness-of-fits for the concentrations

Figure 6.2 shows a comparison of observed and modeled CO\(_2\) concentration series for Cabauw in summer. Averages of the “daytime” (11, 12, ..., 16 UT) values which are used for the inversion and the distribution of the residuals are shown. The unrealistically high concentrations of the prior simulation, and the reduction of the error on inversion (both kinds) are typical for most stations and seasons. The residual distributions are close to Gaussian, as expected. Similar results are found for Loobos (not shown). For Hengelman (not shown) and in particular for Lutjewad (figure 6.3), the Gaussian shape is less well approximated, which is caused by the frequent occurrence of unexpectedly high observed concentrations. It is likely that the discrepancy for Lutjewad is caused by transport errors which are not yet fully understood, but probably related to the coastal character of the station. It is unlikely

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that the observations are erroneous, as these have been well scrutinized (Van der Laan 2009a).

To find out whether this behavior could cause a bias in the resulting fluxes, a test inversion has been performed for summer in which the high-concentration outliers were discarded. Though this obviously improved the fit for the concentrations, it did not lead to a substantial change in the fluxes, which appear less sensitive to the concentrations at Lutjewad than to other stations. This will be further considered below. For this reason, only results obtained using data that included the outliers are presented in this paper.

Figure 6.2 Example of observed and modeled CO₂ concentration time series: Cabauw, summer. Left panel: daytime average, with root-mean-square values for the differences between observed and modeled values. Right panel: Distribution of residuals (hourly daytime values), with means and standard deviations.

Figure 6.3 The same as figure 6.2, but now for station Lutjewad.
Table 6.1. Difference between observed, prior and posterior CO$_2$ concentrations (daytime averaged) for all stations and seasons. Values are in ppm. Stations: CBW = Cabauw, LOO = Loobos, LUT = Lutjewad, HEN = Hengelman.

Table 6.1 lists the differences between the modeled and observed CO$_2$ concentrations for the various stations and seasons, based on the daily-averages of the “daytime” (11, 12, ..., 16 UT) values which are used for the inversion. The prior concentrations show a significant bias (too high), especially in summer and autumn, for some but not all of the stations. In the posterior results, this bias has been strongly reduced. It will be shown below that the bias in the prior concentrations is most likely due to a too small modeled net uptake of CO$_2$, rather than to an assumed high background concentration. Both Cabauw and Loobos have a strong RMS error reduction (except in winter) while Lutjewad and Hengelman have less. Our results suggest that with the present observation network, for spring, summer and autumn, the inversion scheme is able to produce concentration series which are, in general, significantly improved. They also suggest, however, a lower sensitivity specifically for the coastal station Lutjewad. A further observation is that the fit of the CO$_2$ mixing ratios is practically always better for the pixel inversion than for the parameter inversion. This is to be expected, as the pixel inversion has much more degrees of freedom.

Nevertheless, the posterior concentrations still differ considerably from the observations. The main contributions to this difference stem from (1) transport errors, and (2) errors in the flux model. The synthetic runs of chapter 5 for the same network had much smaller RMS of the concentration difference. Since these runs used the same transport model, but strongly different flux models, for the forward run (creating synthetic concentrations) and the inversion, they show that the
inversion can correct the errors caused by a wrong flux model, provided the transport model is accurate. Hence, it is likely that the decreased performance with real data is not due in the first place to errors in the flux model, but to the difference between the real and modeled transport. It is well known (e.g. Gurney et al. 2002, Stephens et al., 2007) that current schemes for transport modelling have imperfect treatment of vertical transport in the atmospheric boundary layer.

6.3.2 Flux estimates and uncertainty

We now turn to the comparison of the best estimates of the fluxes for both inversion methods. Figure 6.4 gives an overview of the flux-averages (terrestrial biogenic part) for each season and eco-region. Flux-averages for the whole year are also shown. Figure 6.5 shows the prior and the two posterior fields for all seasons. In interpreting the results, it should be kept in mind that the error bars depict random standard errors, as represented by the ensemble, but that they do not account for other types of errors. One such an error source is the following: with the parameter inversion, vegetation parameters etc. are changed so as to produce concentrations that better fit with the observations; but by the rigidness of the base functions, this also affects unmonitored areas which may have in reality other values for the vegetation parameters, causing a systematic (but unknown) bias there. On the other hand, for the pixel inversion, regions outside the footprint are hardly affected by the inversion, and there the posterior fluxes will tend to stay close the prior values. In both cases, errors arise locally which are not encompassed by the random spread of the ensemble. These errors are of a systematic nature, but they are very hard to quantify, because of lacking information about such things as the spatial variation of the vegetation parameters etc..systematic errors caused by the spatial rigidness of the base functions for the parameter inversion, nor for the lack of adaptation outside the footprints for the pixel inversion (to mention the most obvious error sources). Problems in transport modeling are also a source of systematic errors. Hence, real uncertainties may be larger than indicated, and results of the two methods should not always be expected to correspond within the error bars.

<table>
<thead>
<tr>
<th></th>
<th>NE</th>
<th>SE</th>
<th>SW</th>
<th>NW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spring</td>
<td>32</td>
<td>15</td>
<td>27</td>
<td>18</td>
</tr>
<tr>
<td>Summer</td>
<td>8</td>
<td>12</td>
<td>51</td>
<td>21</td>
</tr>
<tr>
<td>Autumn</td>
<td>23</td>
<td>13</td>
<td>49</td>
<td>6</td>
</tr>
<tr>
<td>Winter</td>
<td>14</td>
<td>15</td>
<td>55</td>
<td>7</td>
</tr>
</tbody>
</table>

**Table 6.2. Wind direction frequencies (days per season per 90 degree sector) in 2008 according to the daily vector-averages of station De Bilt, in the center of the Netherlands. Data obtained from Royal Netherlands Meteorological Institute (KNMI).**

<table>
<thead>
<tr>
<th></th>
<th>Spring</th>
<th>Summer</th>
<th>Autumn</th>
<th>Winter</th>
</tr>
</thead>
<tbody>
<tr>
<td>East</td>
<td>5</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>North</td>
<td>5</td>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>West</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>South</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Center</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Polder</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>2</td>
</tr>
</tbody>
</table>

**Table 6.3. Number of days with observations for each flight trajectory, per season**
The averages (figure 6.4) for the dominant land use classes (grass, crops-1 and crops-2) contain the most important information. For both inversion methods, there is on average a tendency towards larger posterior net uptake in the posterior fluxes, with the exception of the winter for all eco-regions, and the summer for crops-1. The two inversion approaches, although strongly different, yield the same direction for the shifts, though the magnitudes differ sometimes more than indicated by the error bars (for the reasons explained above). A second conclusion is that crops-2 has a much larger uptake than crops-1, at least for spring and summer (the two methods disagree for autumn).

The small summer uptake of crops-1 contrasts not only with the crops-2 but also with the grasslands uptake, which appears large in summer, as expected in the growing season. Whether this small uptake of crops-1 is real or not needs further investigation.

An odd result is the large error bar for the crops-1 class in winter for the parameter inversion. Common Bayesian inversion cannot increase errors. However, for the parameter inversion, we used a model in which the fluxes are functions of the vegetation parameters with nonlinear dependence for some of them, and this can cause posterior errors to become even larger than the prior errors. This phenomenon has been elaborately discussed in chapter 5 (section 5.3.1 and 5.6).

Averaged over the whole year (see figure 6.4), the mean flux is not significantly different from zero for three classes (Grassland, crops-1, other), but does show large net uptake for crops-2. For this class, the average uptake is $6.5 \pm 0.9$ and $3.5 \pm 1.0 \mu\text{mol m}^{-2}\ \text{s}^{-1}$ (standard errors), according to the parameter- and pixel-inversion, respectively. Both methods lead to a small though significant net uptake for the needle leaf forest and the deciduous broadleaf forest. The calculated uncertainties in
the annual averages are small, but as discussed above they do not include the possible effect of systematic errors (of various origins) which could lead to relatively large shifts of these small averages.

The sub-ecoregion distribution within one land use class often differs strongly between the inversion methods. As expected, for the parameter inversion the spatial distribution is rather homogeneous, while more spatial structure is present in the pixel inversion results. Figure 6.5 illustrates how the distribution of observation towers, together with the chosen structure of the unknowns and assumed covariances, spreads information across the domain to yield such differing regional fluxes. Whereas the pixel inversion focuses most of its parameter adjustments in a region around the towers, the ecoregion based method spreads information over a larger domain, and much more homogeneously. This result is consistent with earlier inverse studies employing such “regularization” methods (Carouge et al. 2010, Schuh et al. 2010).

![Figure 6.5 Mean biogenic flux (μmol m$^{-2}$ s$^{-1}$). Left to right: Prior, posterior parameter inversion, posterior pixel inversion.](image-url)
Concerning the smaller classes, there is often (summer, autumn) a difference in the results of the two inversion methods for the needle leaf forest, in spite of the fact that the class is monitored at Loobos. For this class, the uncertainty in the posterior fluxes was found to be usually greater than for the classes with a larger surface area (figure 6.4). Little information seems to be retrieved by the network for the deciduous broadleaf forest class (no direct observations in the area), and the “other” class (very small fluxes).

Figure 6.6 shows the relative improvement of the standard error, as calculated by the Kalman filter. Note that the results for autumn and winter were obtained with a reduced network (no Hengelman data). Since the parameters are spatially constant for each region, the error reduction map reflects the land use map. For the same reason, the error reduction is for most ecoregions much stronger than for the pixel inversion (for which there are much more unknowns to constrain). This strong reduction of the error per pixel is an artifact of the parameter method. The error reduction is primarily calculated for the vegetation parameters, and causes an appropriate error reduction for the average fluxes over the ecoregions to which these parameters apply. However, owing to the low number of basis functions, the small spread of the averages is automatically translated to a small spread per pixel, causing an unrealistically low uncertainty in the flux per pixel. The other (pixel) inversion method, on the other hand, does not suffer from this artifact.

Figure 6.6 Improvement of the flux: \((\sigma_{\text{prior}} - \sigma_{\text{post}})/\sigma_{\text{prior}}\). Top: parameter, bottom: pixel inversion.
The finer structure of the error reduction close to the observation sites shows details which are not always obvious to explain. Cabauw and Loobos have an overlapping region of influence, which is mainly restricted to grassland, which limits the effective radius. For Hengelman the region of influence is larger, because of the extensive crops-1 region there. It is remarkable that the influence of Hengelman is most conspicuous on the eastern side, whereas the prevailing wind direction is from the west.

From figure 6.6 Lutjewad is seen to have the smallest influence on the error reduction. The impact of the coastal station Lutjewad on error reduction depends on the frequency of southerly wind, which is locally on average about 30% of the time (Van der Laan et al., 2009b). The southerly winds are less prevalent in spring than in summer and autumn 2008 (see table 6.2).

Figure 6.7 Example of one day of flux measurements by aircraft, compared to the simulated total flux (prior and two posteriors), for the same points of the trajectory.

<table>
<thead>
<tr>
<th></th>
<th>Parameter inversion</th>
<th>Pixel inversion</th>
<th>Fossil fuel emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spring (2008)</td>
<td>-7.54 ± 0.95</td>
<td>-9.63 ± 0.91</td>
<td>13.43</td>
</tr>
<tr>
<td>Autumn (2008)</td>
<td>-6.51 ± 0.53</td>
<td>-5.23 ± 0.89</td>
<td>13.94</td>
</tr>
<tr>
<td>Winter (2008)</td>
<td>5.68 ± 3.36</td>
<td>5.88 ± 0.85</td>
<td>13.49</td>
</tr>
<tr>
<td>Year (2008)</td>
<td>-17.59 ± 3.80</td>
<td>-17.23 ± 1.87</td>
<td>53.12</td>
</tr>
</tbody>
</table>

Table 6.4. Calculated carbon budget of the Netherlands, according to the two methods (unit: TgC season-1). The fossil fuel emission for the same region has been added for comparison.
6.3.3 Comparison with CO$_2$ flux measurements by aircraft

The aircraft flux measurements are summarized in table 6.3. The winter measurements were restricted to December 2008, as the flights started in March 2008, and the inversion results are confined to 2008. The error in the observed fluxes is estimated as 15% based on comparison of simultaneous flights over SW France in 2007 (Vellinga, unpublished). Figure 6.7 shows an example of one day of flux measurements by aircraft, compared to modeled posterior total fluxes, found by both parameter and pixel inversion. Note that the simulated fluxes pertain to the same places and times as the observations, so that unnecessary aggregation uncertainties are avoided.

Figure 6.7 illustrates the problems pertaining to the comparison of calculated and observed fluxes on the short term. First, continuous observations exist only for brief intervals. Second, the simulated and observed time series have different shapes, because the observations are strongly influenced, on the short term, by random effects like turbulence and intermittent clouds, which are in the simulations either averaged out, or not well timed. As a consequence of this randomness, it is practically impossible to assess the flux difference between ecoregions by looking at data from single days.

Since it appears rather meaningless to compare observed fluxes, averaged over 2 km, with our posterior fluxes, we compare in the following only averaged flux values which belong to the same trajectory and season. Figure 6.8 shows these average flux values for the observations, priors and the two posteriors. As indicated earlier (at the start of the discussion of figure 6.4), the standard errors which are given for the posterior fluxes may underestimate the uncertainty, as they do not account for systematic errors which are inherent to the inversion methods. Within the enhanced uncertainty of both our estimates and the aircraft data, the observations confirm, in most cases, the shift towards much larger uptake (for spring to autumn) that is produced by the inversions. This increases the confidence in the ability of the inversion system to improve on prior estimates, and also demonstrates the value of our assimilation approach in integrating different types of information of the regional carbon cycle.

Figure 6.9a shows the root-mean-square differences between the simulated (prior and both posteriors) and the observed average fluxes, for all seasons. The employed averages are taken immediately from figure 6.8. In the comparison to independent flux data we find a remarkable improvement of estimated fluxes over prior fluxes for summer and autumn, but not for winter and spring. The bad result for winter is related to the existence of small fluxes overall with the coupling between observed concentrations and nearby fluxes being weak, so that the posterior values do not move far away from the priors. A likely cause for the spring mismatch is the representation of the LAI, which changes faster in spring than in other seasons. The monthly LAI maps (used to calculate both prior and posterior fluxes) cannot well resolve these changes. The LAI maps were according to MODIS data for 2006, but have not been adjusted to 2008. However, an inspection of the meteorological data (source: KNMI) shows no reason for a great difference. Chapter 3 also suggests that regional scale inversions appear to be quite sensitive to the precise specification of the land surface properties. The difference in performance between the parameter- and pixel inversion is small.
Figure 6.8 Average CO₂ flux over aircraft flight trajectory for each season, unit: μmol m⁻² s⁻¹. From left to right: prior of simulated total flux, simulated total flux from parameter-inversion and from pixel inversion, and observed flux from aircraft.

Figure 6.9b shows root-mean-square differences between the average fluxes of figure 6.8, this time for each trajectory. In the computation, the winter data were not used. There are large differences in performance between the trajectories: when considering the parameter inversion, a quite large error reduction is noted for the West and South and, to a lesser extent, Center and East trajectory. For the others, the error reduction is modest or even (for north) absent. There is no clear link to the presence or absence of concentration measurements close to the trajectory: The North trajectory has the worst performance, although it is covered by the Lutjewad site. This might again be because Lutjewad is a coastal station, and concentrations are insensitive to land based CO₂ fluxes when the wind is onshore (which occurs for March-November 2008 for about 40 % of the time, and maybe more often due to local sea breezes (e.g. Ahmadov et al., 2009). Strong horizontal flux gradients may also be a source of errors, as the aircraft roughly follows the coastline for the North trajectory. The strongest error reduction and the best posterior fluxes are obtained for the South trajectory, though there are no concentration measurements performed there. This trajectory largely runs through the crops-2 eco-region, which was seen earlier (in the section on fluxes: best estimates) to have strong and consistent flux shifts produced by the inversion scheme. The strongest observed uptake (see figure 6.8) occur in summer for trajectories South (largest) and East (second largest), which happen to be the trajectories for which the crops-2 class is dominant respectively substantial (figure 6.1). These flux measurements confirm the large uptake for crops-2 which was found by the inversion (figure 6.4).
6.3.4 Calculated national carbon budget of the Netherlands for 2008

Table 6.4 shows the calculated biotic uptake integrated over the Netherlands, for the seasons and for the whole year (the land area, calculated on model resolution, is about 35000 km²). For comparison, the integrated fossil fuel emission (as assumed for the modeling) has been added. As elsewhere in this paper, the winter contribution is the sum of the months January, February and December 2008. For spring to autumn, the calculated uncertainties of the biotic fluxes are in agreement with the differences between the methods. For winter, an unusually large relative uncertainty is calculated for the parameter inversion. This is related to the nonlinearity of the parameter inversion, which seems to cause specific problems when winter data are used, as remarked earlier when discussing figure 6.4.

The two year sums are in close agreement, but as the differences are larger for the contributions of the seasons, this seems to be coincidental. The estimated uncertainty for the year sum is much larger for the parameter than for the pixel inversion, which is caused by the uncertainty in the winter contribution.

6.4 Discussion and conclusions

The results of the paper have to be interpreted carefully, because the flux values resulting from the inversions may have biases (dependent on the inversion method and the region) which are difficult to characterize and estimate, and which cause results from different inversion methods to be differ more than expected from the random errors. Important factors contributing to this are, besides transport errors, also erroneous assumptions concerning spatially constancy or smooth spatial
correlations of vegetation parameters etc., and there will be more research needed to mitigate such problems.

An important observation is that the prior fluxes for the net uptake are in general too small. This follows both from the comparison with concentration measurements (using inversion) and from the flux measurements (performed by aircraft). The reason however is not entirely clear. There are uncertainties in both the biotic component and the heterotrophic respiration. The first is based on a rather well-founded vegetation model combined with LAI-maps based on observations. On the other hand, for the heterotrophic component there is a lack of data, and we had to base the estimates on preliminary research (Chapter 3). The present results suggest that the prior heterotrophic respiration is too large for the dominating land use types.

The inversion produces posterior fluxes which are, on average more reliable than the priors. The comparison with independent flux estimates from aircraft confirms this. This pertains primarily to the flux averages as observed by aircraft flights. On a finer scale, the scatter between observations and simulations remains quite large, owing to the noisy nature of the real turbulent fluxes, as illustrated by figure 6.7. Further, there is no improvement for winter. The small fluxes in winter and the lack of convection (causing larger transport errors) are likely to be the main reasons why improvement by inversion is difficult for the winter season. The larger impact of errors in the assumed fossil fuel emissions in winter may also play a role.

The present results also bear on the relation of the results to spatial and temporal resolution. We had to average the aircraft measurements over trajectories to obtain useful results. The bars in figure 6.8 actually represent averages over observations of, on average, 2.7 days (of the about 91 days in a season). In spite of this rather sparse temporal coverage, the inversion produces a considerable improvement of the RMS difference between simulation and observation (for most of the trajectories and seasons). This shows that the inversion with the present setup produces already a considerable improvement of averages even over periods of no more than a few days. Note that these results primarily refer to daytime values.

The improvement for spring is less than for summer and autumn. We suggest this is caused by errors in the modelling of the timing of LAI changes. This parameter changes faster in spring than in the other seasons.

A simple experiment was performed to estimate the sensitivity of posterior fluxes to CO₂ boundary conditions, for the summer season only: the inversion was repeated with one ppm subtracted from the background field (the response to bigger shifts can be estimated using linearity). For the parameter inversion, this caused a shift of the posterior fluxes of + 0.8 to + 1.0 μmol m⁻² s⁻¹ for grassland and crops-2, but 0.0 for crops-1. For the pixel inversion, the shifts were quite evenly distributed for the dominant classes: + 0.7 to + 0.8 μmol m⁻² s⁻¹ for grassland, crops-1 and crops-2. These shifts preserve the flux pattern (for the assumed 1 ppm), but cause the overall flux average to become less negative. Nonetheless, a substantial bias is not expected. The use of the results of European scale CO₂ inversions, and the various meteorological circumstances and wind directions over which the results for a season are averaged are expected to prevent a large bias.

It is difficult to draw conclusions concerning the performance of the inversion in recovering flux field structures smaller than the eco-region scale. There are sometimes strong differences between the outcomes of the two inversion methods, but it remains in general difficult to say which one performs best. Whereas the
parameter inversion assumes an unproven homogeneity of vegetation and heterotrophic respiration parameters, the pixel inversion is more flexible, but its results reflect to some extent the stochastic properties (mean field as well as noise) of the prior ensemble. Eddy correlation (EC) measurements, from surface sites and by aircraft, lack the required spatial and temporal averaging to settle the question.

The inversions showed a large and unexpected difference in the behavior of the two crops regions. The large uptake of the second crops class cannot be explained from the higher sub-pixel abundance of natural vegetation, as such vegetations tend to have a small uptake (also in our results). The difference must thus be caused by a difference in crops species. We suggest that the higher abundance of maize in the second crops class contributes much to its large uptake. Maize is known to have a very large uptake (Verma et al. 2005). However, the dataset of Fluxnet measurements within the modelling domain, which was used to tune the model (Chapter 3), contained no sites with maize (Groenendijk et al. 2011a) and the present results suggest that this has caused a bias in the prior flux calculations. The annual carbon balance according to the inversions is practically zero for both grassland and the first crop class, whereas for the second class there is a significant uptake.

A negative feature of the results, which was found to a weaker extent in the synthetic inversions of chapter 5, is the “aliasing” in the two terms in the net flux, biotic flux and heterotrophic respiration. The aliasing is evident from the occurrence of cases with negative (hence certainly spurious) posterior heterotrophic respiration. This is worrying because it causes difficulties in accurately identifying errors in the flux modelling, such as those, which cause the bias in the prior fluxes. An improvement would require in the first place an improved transport modelling for the inversions, in particular better modelling of nocturnal transport. This is a rather long-lasting problem, though some advances have been made (Steeneveld et al. 2008).

This study presents the first regional scale inversion of CO₂ fluxes for the Netherlands using an inverse model. The posterior fluxes were compared with aircraft measurements of seasonal and flight-leg averaged fluxes. For most regions, there is a significant and sometimes strong improvement of the posterior fluxes. The improvement is greatest for summer and autumn, whereas for winter, no improvement occurs. For spring, it will be important to have reliable data for the development of the LAI in time. For extended eco-regions, there was significant improvement of the average fluxes, also if no homogeneity of the unknown parameters within the eco-region was assumed. On the other hand, it is difficult to monitor small eco-regions, even if they have a nearby site for concentration measurements, and to monitor urbanized regions, which have small fluxes. Though improvements with respect to the prior fluxes are clear, the posterior results still depend on assumptions that remain difficult to validate, such as homogeneity of parameters for vegetation and heterotrophic respiration within an eco-region. The results reveal a large and unexpected difference between the fluxes for crops eco-regions without and with significant natural vegetation, especially in summer (much smaller net uptake for the first class). This is most likely caused by a very large uptake of one or more crop types that are more abundant in the second class (potentially maize).
6.5 Acknowledgements

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Summary and synthesis of the results

7.1 Background
The climate system is warming, and a key factor in this change of the climate system is the increase of atmospheric concentrations of greenhouse gases, which alter the balance of incoming and outgoing energy at the surface (Solomon et al., 2007). The most important anthropogenic greenhouse gas is carbon dioxide (CO$_2$) and the uptake of carbon by the biosphere is a substantial component affecting, and mitigating, climate change (e.g. Canadell et al., 2007, Dolman et al., 2010).

Inverse methods provide an independent top-down approach to verify greenhouse gas emissions based on observations of atmospheric concentrations of greenhouse gases. Through inverse modelling the distribution and temporal evolution of CO$_2$ in the atmosphere can be used to quantify surface fluxes, using numerical models of atmospheric transport as a key tool.

7.2 This thesis
In this thesis the development and the performance of a regional scale inverse modelling system is addressed to show to what extent we can constrain the regional carbon fluxes with a high resolution atmospheric observation and modelling system. The performance of this regional atmospheric carbon modelling system is tested in forward and inverse mode. In this chapter the research performed in this thesis will be summarized and aggregated into the answers at the research questions formulated in the introduction. As a recap, this thesis addresses the following parts of inverse modelling:

1. **the practical considerations**, i.e. is it possible to develop a stable and robust nested modelling framework at the required high resolution;

2. **the performance** of a high resolution inverse modelling system, i.e. what can be gained and what are the limitations when moving towards higher resolutions, and

3. **the application** of the high resolution inverse modelling system to constrain the carbon balance, i.e. what can be learned about the carbon balance, in this study for the Netherlands as a pilot area.

7.3 Overall conclusions
The overall answer to these questions is that the high resolution inverse modelling system is a good, appropriate and useful tool to verify our understanding of the behavior of the land carbon fluxes. For example, for the Netherlands we showed that the carbon balance based on a state-of-the-art biospheric model underestimated the carbon uptake. Additionally we showed that the application of the modelling system combined with different complementary observations is not only capable of
validating the carbon balance, but also has the capacity to reveal errors within the meteorological modelling. As such, the regional inverse modelling system and the use of various complementary atmospheric and flux observations at high resolutions as developed in this thesis, can be used as a prototype verification system for regional biospheric carbon exchange.

The inverse modelling system can validate the a priori fluxes at the scale of about a hundred kilometer. We showed that at a more detailed level the distinction between the fluxes of for example different land use types is generally not realistic. Therefore, the system can demonstrate that errors in e.g. the carbon balance are present, but it cannot locate and correct the error. The regional scale inverse modelling system is thus not a tool that provides direct information about the processes controlling the carbon fluxes. It does however provide the opportunity to check whether the current knowledge about the carbon system is to a certain degree correct, and to verify the emissions reported by different countries within certain limits of uncertainty.

Below, the results of the studies in this thesis are summarized in more detail to answer the sub-questions.

7.4 Practical possibilities for a high resolution modelling system

The first sub-question concerns the practical considerations, i.e. is it possible to develop a stable and robust nested modelling framework at the required high resolution? The answer to this sub-question is in general positive. In this project we developed and applied a modelling framework that was able to provide a full-year high resolution inversion. We tested this framework throughout and the results are in general quite encouraging.

7.4.1 Non-stop modelling at the appropriate scale with a good signal-to-noise ratio

When modelling at this detailed scale, the resolution did not permit modelling for the full globe, nor with a very long spin-up at this resolution. One of the research questions was therefore to use such a limited area model without a divergence of the simulation results from the observations. We found that non-stop, nested simulations without restart are indeed possible. The regional atmospheric model is off-line coupled to the reanalyzed meteorological variables and the CO$_2$ concentration of the ECMWF and Carbontracker continental scale models. This avoids a run-away and thus provides and instrument for dynamic non-stop modelling (see Chapter 3). For this approach reliable background values are necessary to prescribe CO$_2$ inflow and outflow at high temporal resolutions at the edges of the regional model. In Europe these are provided by e.g. Carbon tracker (as used in this study; Peters et al., 2010) and LMDZ (Chevallier et al., 2010).

The regional scale in the order of 10-100km is an appropriate scale to constrain the terrestrial carbon fluxes (Chapter 3, 5 and 6). We showed that the influence of the variability (diurnal and synoptic) of the background fluxes does not overwhelm the signal of the fluxes within the limited area domain. Additionally, we showed that the simulated signal at the observation location is not only influenced by the fluxes of the land use type nearest to the observation location, but also by the signal of the fluxes of other land use types in the region. This confirms the findings of e.g. Gerbig et al. (2003), Lauvaux et al. (2009) who also showed that the local scale is an important scale contributing to the variations seen in the atmosphere. The
atmospheric observations can thus indeed be applied to constrain the fluxes at the scale where this study focuses on.

Also the signal-to-noise was investigated to establish whether the variations in the atmospheric CO\textsubscript{2} concentration could be used to constrain the biospheric fluxes. First we found that even in a very heterogeneous area like the Netherlands, with a substantial fossil fuel flux that is scattered across the area, the variability due to biogenic fluxes exceeds the variability due to the fossil fuel fluxes (Chapter 3). Further we compared the ratio of the impact of the uncertainty of the CO\textsubscript{2} fluxes on the atmospheric CO\textsubscript{2} concentration (i.e. the signal) to the model-data mismatch due to uncertainties in the modelling system (i.e. the noise). The signal was found to be on average 11.7 ppm. The noise due to errors in the simulation of the diurnal boundary layer was in this study found to be in the order of 1.7 ppm (Chapter 3). The representation error was found to be in the order of 0.2 ppm at 10 km resolution, in the study performed for southern France (Chapter 4). Even though transport errors are in the order of a few ppm, the signal-to-noise ratio is substantial during the day, due to the rather large impact from the uncertainty in the CO\textsubscript{2} fluxes on the atmospheric concentrations. This indicates the potential for inversions.

7.4.2 Difficulties with stable boundary layers

However, the nocturnal boundary is very difficult to simulate. This difficulty is not overcome by moving towards smaller scales. We found that in the simulation for May and June 2008, the nocturnal boundary layer height was systematically underestimated (Chapter 3). Because the CO\textsubscript{2} gradient in the stable boundary layer is strong, the inversion is very sensitive to incorrect modelling of the nocturnal boundary layer. Up till now no reliable correction for the bias in the nocturnal boundary layer calculations is available (e.g. Steeneveld et al., 2008; Gerbig et al., 2008; Law et al., 2008). Therefore, we had to exclude the nocturnal CO\textsubscript{2} observations from the inversions. Because of more often occurring stable conditions during the day in wintertime, this may also make the inversions during wintertime less reliable (Chapter 6).

7.4.3 Effective use of high resolution, complementary observations

Further, the use of complementary high resolution observations is made possible within this modelling framework. Most importantly we included in the inversions the time series of the afternoon atmospheric CO\textsubscript{2} concentration observations, by which we could use the inter-daily variability to constrain the carbon fluxes (Chapter 6). To incorporate observations within the boundary layer over the land at this level of detail, the variations caused by for example meso-scale circulations should be resolved (e.g. Perez-Landa et al., 2007; Ahmadov et al., 2007; Rivier et al., 2010; Broquet et al., 2011). This is done in this study by the application of the high resolution modelling system, which we thoroughly tested in the studies presented in this thesis and in the model intercomparison study of Sarrat et al. (2007).

Additionally, we used the data from aircraft observations, scintillometers, eddy correlation measurements, radiosondes and the atmospheric towers with observations at different altitudes to further constrain the system (Chapter 3). Because of the high resolution of the modelling system it was possible to link directly the results of the inversion to observed fluxes by the aircraft (Chapter 6). This provided a strong validation for the inversion technique (e.g., Lauvaux et al., 2009), which is only possible when the scale of the inversions is detailed enough.
The combination of the detailed meteorological data and atmospheric model revealed a mismatch between either the simulated and observed energy fluxes or between the simulated and observed boundary layer depth (Chapter 3). We found that this discrepancy was not limited to the modelling system RAMS-Leaf3, but that it was also present in the atmospheric model WRF. We explored this mismatch further and published it in Steeneveld et al. (2011). The mismatch could not be solved yet, but this did reveal the strength of the modelling system to reveal earlier unseen errors, and thus proves its validation opportunities. Further an error specific for RAMS was found by detailed analysis of the atmospheric model. We published this flaw in the model, which should be repaired to avoid mass-balance errors, in Meesters et al. (2008).

7.4.4 Inversions applicable at the regional scale
To perform inversions at the regional scale, we successfully implemented the Ensemble Kalman Filter. We applied it with different inverse carbon flux estimation approaches and tested it thoroughly in a pseudo-data environment. The majority of the state-of-the-art approaches were able to constrain the domain total carbon balance satisfactorily (Chapter 5). The exception was the inversion where NEE is scaled by one linear multiplication factor per land-use type which did not perform well. The inversion approaches in which either parameters of the biosphere model are optimized per land use class (i.e. the parameter inversion), or in which respiration and GPP are optimized per pixel (i.e. the βRGpixel inversion) performed best and are selected to apply in our prototype simulation for the Netherlands.

7.4.5 Final practical considerations
Concluding, we developed in this project a stable and robust nested modelling framework for the regional scale. It has an acceptable signal-to-noise ratio for atmospheric CO₂ mixing ratios and the atmospheric signal can be used at a high spatial and temporal resolution to constrain the carbon fluxes. The performance of the nocturnal atmospheric simulations is not yet good enough to include the full time series in the inversions. Therefore, the modelling framework provides the opportunity to use the inter-daily variation to constrain the carbon fluxes. We showed that a number of selected inversion methods work correctly when applied at the regional scale and that the direct comparison with observations of various surface flux and atmospheric parameters is possible.

7.5 Advantages and limitations of high resolution modelling
Secondly, the performance of the high-resolution inverse modelling system is systematically assessed. Here we summarize what can be gained and what are the limitations when moving towards higher resolution inversions.

7.5.1 Reduction of the representation error
In low resolution inversions the use of observations near sharp changes in the CO₂ field, for example due to the edge of the sea breeze is not recommended, because at lower resolutions the representation error may be substantial (e.g. Gerbig et al. 2003a, b; Lin et al., 2004; Van der Molen and Dolman, 2007; Corbin et al., 2008; Patra et al., 2008). At higher resolutions the mesoscale circulations such as a sea breeze can be simulated better. Also the differences in the boundary layer height, caused by contrasts in the land use, can be captured when modelling at the high
resolution. Therefore, high resolution modelling makes it possible to use observations within the boundary layer close to sharp land cover contrasts at the surface in a much more reliable manner (Chapter 4). Also further away from mesoscale circulations, the representation error can be substantially reduced from about 1.5 ppm at 100km resolution to just about 0.4 ppm at 10km resolution.

7.5.2 Performance of the regional inversions

The performance of the inversions is assessed both with pseudo-data as with real data. In the latter with independent CO₂ flux estimates which were available to check the results of the inversions. Two inversion approaches, the parameter inversion and the βRGpixel inversion, showed the best performance in the pseudo data study (Chapter 5) and were selected for the real data study. The results of the pseudo data study suggest that these two approaches are best suited for the use at the regional scale.

Also in the real world study these two methods performed well and provided consistent results. Even though the absolute values of the fluxes are different between the parameter inversion and the βRGpixel inversion, the correction from the prior to the posterior was always in the same direction for almost all land use classes and seasons. Moreover, for the major part of the year, the posterior estimate is much closer to the CO₂ fluxes independently observed with the aircraft than the prior estimate (Chapter 6). This direct comparison with aircraft data is a gain of the high resolution modelling, and it confirms that also under real circumstances the inversion are capable to provide improvements of the integrated CO₂ flux over a domain of a few hundred kilometres compared to the prior estimate. This is comparable to the scale found in most inverse models (e.g. Carouge et al., 2010; Schuh et al., 2009; Gerbig et al., 2006; Ahmadov et al., 2009).

However, the work done in this thesis also showed some important limitations, and sometimes challenging preconditions for the inversions to work well. The inversion requires a certain amount of knowledge of the structure of the fluxes. For example, in the real data study we found that the inversion performed not as good in the spring as in the summer or autumn (Chapter 6). This was probably due to the fast changes in the LAI during the spring, which were not adequately resolved by the monthly LAI data. The pseudo-data study (Chapter 5) showed that if the prior structure is incorrect, the inversion has difficulties to incorporate this source of error, and the results of the inversion are too confident. In this study, the difference in the structure of the respiration field in the priors (based on 5PM; Groenendijk et al., 2009) and pseudotruth (based on FACEM; Pieterse et al., 2007), did not coincide with the land use classes, which is a realistic situation (e.g. Chevallier et al., 2011). The aggregation error found to be important in large scale inversions (e.g. Kaminski et al., 2001), thus still plays a role in the high-resolution inversions, even though it is now related to errors in the prior structure at much smaller scales (Chapter 5).

Despite errors in structure of the prior fields, the selected inversions performed well to constrain the averaged flux over the limited area. This could even be accomplished in the pseudo-data study where we gave the inversion the difficult task to solve for the fluxes in an environment where the structure of the prior was substantially different from the pseudo-truth (Chapter 5). Both the prior and the truth were based on state-of-the-art, though different models, indicating that such a structure mismatch is rather realistic and may occur often. Integrated over a few hundred kilometre, it is
thus possible to constrain the fluxes, even with a difficult structure difference. This integrated scale is already much more detailed than the continental scale.

At a smaller level of aggregation the information that can be obtained from the regional scale inversions was found to be very limited. The estimates at the scale of land use types appeared in general not reliable (Chapter 5). This is, besides the difficulties due to incorrect prior structures, caused by the high correlation between the atmospheric CO$_2$ signal from different land use types. Additionally, a good division between respiration and GPP by the inversion is difficult to obtain because of the strong anti-correlation of the two signals during the day (Chapter 3). This aliasing is a well known problem (e.g. Carvalhais et al., 2008). Because during the night respiration is the only biospheric carbon flux and photosynthesis is absent, future possible improvements in atmospheric modelling of the nocturnal boundary layer could resolve this problem. However, currently these improvements are not available yet.

7.6 **Application of the inverse model for the Netherlands**

Finally, we performed in this thesis the application of the high resolution inverse modelling system to constrain the carbon balance. In this study the Netherlands is taken as a pilot area for which the carbon balance is constrained. This provides a nice test bed to determine the carbon balance for the region compared to the prior flux estimate. Throughout spring, summer and autumn the Netherlands is a net sink according to the inversion. The inversions showed that the CO$_2$ fluxes are more negative (larger uptake) than suggested by the priors (Chapter 6). This pilot provides an example of the strength of the inversion framework developed in this study to validate the biospheric component of the carbon balance.

Another remarkable result is the strong difference between the posterior uptake in two separate agricultural land use categories. In the first the net carbon flux is relatively modest, while in the second the uptake is relatively high. Even though this result should be handled with caution, because this is a division at a more detailed level than the level at which the inversions are always reliable, this result might help explain the underestimation of the net carbon uptake by the biospheric model. The second crop class has a large abundance of maize, which is known to have a high carbon uptake (e.g. Verma et al. 2005). The dataset used to optimize the parameters of the biospheric model 5PM for the temperate zone did not contain data from maize sites, which may be the reason why the biospheric model underestimates the carbon uptake. Either way, this confrontation of the biospheric fluxes with the complementary atmospheric CO$_2$ observations in the regional inverse modelling system has identified a difference in the estimate of the carbon fluxes, and thus puts an important constraint on the carbon flux estimate.

7.7 **Recommendations and future work**

Based on the studies in this thesis, a number of recommendations are provided. Concerning the practical considerations, we showed that basically the modelling system is well applicable. Nonetheless, it has an important shortcoming in correctly modelling the nocturnal boundary layer. An improvement in the simulation of the stable boundary layer would strongly increase the possibilities to constrain the surface fluxes. An unbiased estimate of the nocturnal atmospheric transport would
allow for the use of atmospheric CO$_2$ concentrations throughout the full diurnal cycle. This would strongly improve the separated constrain on respiration and GPP.

However, the problem of modelling the nocturnal boundary layer was in previous studies found to be very difficult to fix. As we showed in chapter 3, the approach with complementary surface and atmospheric data is not only applicable for CO$_2$ fluxes, but also for the other modelled surface fluxes, the energy balance and the boundary layer processes. Within this PhD-project already two substantial shortcomings of the current meteorological models were revealed: a flaw in the mass balance (Meesters et al., 2008), and a mismatch between the modelled and observed surface energy flux - boundary layer depth relation (Steeneveld et al., 2011). A further systematic verification of meteorological models, based on surface flux and boundary layer observations is highly recommended, including an analysis of the impact of e.g. clouds and aerosols on the boundary layer development. An intensive check of currently used high resolution meteorological models for the Netherlands, with the available observations from this project in the Dutch area, may help to identify incorrect parameterizations. This may provide important clues on how to solve the difficulties with the (stable) boundary layer modelling.

Concerning the performance of the high resolution inverse modelling system, the parameter inversion and the βRGpixel inversion showed the best performance in the pseudo data study. These two inversion methods appear, based on these results, most suitable to use at the regional scale. The use of high resolution models is especially recommended at locations with a high spatial variability in the landscape, and near atmospheric mesoscale circulations. By increasing the resolution the representation error can be strongly reduced, and atmospheric observations close to mesoscale circulations can be more reliably used to constrain the carbon fluxes. These kinds of inversions are recommended to be employed as a zoom of a coarser scale model, like in this thesis the continental scale model Carbontracker Europe. The prototype modelling system developed in this thesis can in future research be applied to further verify the carbon fluxes.

However, it is recommended to keep the limitations of the inversions in mind. The first limitation is that in inversions the carbon fluxes are optimized based on an aggregated atmospheric signal, which inherently reduces the ability of the inversion to separate between two flux signals, especially if their observed signal has a comparable temporal pattern. Therefore, some sort of aggregation will be required over the posterior results. The studies in this thesis showed that at scale coarser than 100km the results of the inversions were reliable, however the posterior detail at smaller scales was not always reliable. This was, at least partly, due to aliasing. Further increasing the spatial resolution of observations than in this study is, because of the aggregation of the signal in the atmosphere, currently not expected to strongly improve the details of the results.

The second limitation is that the ability of the inversion to correctly optimize the fluxes depends on the choice of the unknowns and the underlying prior flux structures. If the unknowns do not cover the reasons for the mismatch between the observed and simulated CO$_2$ concentration, the inversion lacks the flexibility to correctly adjust the flux estimates, which may result in overconfident posterior results. Therefore, a reasonable good prior structure, both temporal and spatial, is required for a trustworthy posterior result. Where the prior structure in not accurate, it should theoretically be included in the unknowns, so that it can be altered by the
inversion. This is an extra challenge at the high resolution, because of the extra small scale variability that is included at this scale.

When the (structure of the) prior is far from the truth, the inversions were found to be able to indicate that adjustments in the flux field were necessary, but could not provide reliable detailed information about the adjustment. As was shown most pronounced for non-linear inversions, the inversions perform best in tuning the prior towards the truth when the truth is not too far from the prior.

Therefore, an iterative use of the inversion approach is recommended. First it can be used to indicate whether and where large adjustments of the flux estimates are needed, i.e. identification of the areas with a bad understanding of the carbon fluxes. Second, a manual improvement of the prior, and its error covariance matrix, is recommended, with a focus on the characteristics of the areas where the previous prior ill-performed. One can think of improvements of the biospheric and heterotrophic formulas, improvements of the structure of the flux field and its covariance structure with for example extra satellite data and geo-statistical methods, and improvement of the empirical relations based on extra bottom-up, non-atmospheric data. It is important that the additional information used to adjust the prior and its error covariance matrix is independent of the atmospheric observations, to avoid a linkage of observation errors and prior errors. Third, it is recommended to repeat the inversion with the new prior. This iterative process may be needed to be repeat several times. It must be stressed, that the data used within the manual step should be independent from and complementary to the atmospheric data used for the inversions.

A hybrid of automatic optimization and focussed manual optimization, based on complementary information, allows the inversion to perform to its full strength: (1) as indicator where improvements are required and (2) as fine-tuner to further constrain the fluxes which are already rather well known at a high resolution. Moreover, in this manner, the processes behind the carbon fluxes can be improved in the manual step, with more flexibility than if they are automatically optimized. This provides the opportunity to improve the understanding of the carbon balance, which finally can lead to improvement in climate change predictions.

In case the adjustment from the prior to the posterior is relatively small, and importantly- in line with the prior uncertainty, it might indicate that the posterior flux estimate has reliably converged towards the truth. To check this, it is recommended to perform an additional inversion with a different temporal and/or spatial window, or to use complementary, previously unused data, like aircraft observations.

To get a better understanding of the carbon balance, in my view, investments in top down and bottom up studies should not be seen separately, but should reinforce each other. To verify the fluxes reported for example under the Kyoto protocol, an inversion which only states that the reported fluxes are correct or incorrect (within a certain margin) may be enough. Then just the first step of the iteration described above is required. For improving our knowledge of the carbon cycle though, the use of a full hybrid of automatic optimization and focussed manual optimization is recommended.

The application of the high resolution inverse modelling system in the Netherlands can be seen as an example of the important first step in the iteration. It provided a clear means to verify the prior calculated carbon emissions. It showed that the net carbon uptake in the region is probably higher than prior calculated. Nonetheless, it
appeared that the modelling system could not provide direct reliable information about the processes driving the carbon cycle (e.g. the posteriors were sometimes far outside prior uncertainty, which indicates the flux system is not properly understood yet). The inversion suggested that the net uptake of the crops was much higher than expected. Therefore, it is recommended to work on improvement of the prior estimate, in particular on the crop scheme for the biospheric uptake and the heterotrophic respiration, and make a more detailed separation between the different kinds of crops / crop-rotations in this region.

Summarizing, the regional inverse modelling system developed and tested in this thesis, is an independent check to validate our knowledge about the carbon fluxes. For a better use of the small scale variability contained in regional inversions it is recommended to invest in improvement of the description of the carbon flux processes, the structure of the priors and the formulation of the unknowns. Finally, it is recommended to use inversions either as indicators where improvements are required or as fine-tuners to better constrain the fluxes, depending on the quality of the prior structure and the unknowns.
8 Samenvatting

8.1 Achtergrond

Het klimaat warmt op, en een van de belangrijkste factoren daarin is de toename van de hoeveelheid CO₂ in de atmosfeer (Solomon et al., 2007). Dit komt bijvoorbeeld vrij wanneer fossiele brandstoffen, zoals olie en gas, worden verbrand. Gelukkig komt niet alle CO₂ die daarbij wordt uitgestoten in de lucht terecht, waar het zorgt voor het broeikaseffect. Een substantieel deel van de CO₂ wordt namelijk opgenomen in de oceanen en door de vegetatie op het land. Het systeem aarde zorgt op deze manier voor een bufferfunctie waardoor het tempo van klimaatverandering wordt afgeremd (bijvoorbeeld Canadell et al., 2007, Dolman et al., 2010). Om een goede voorspelling van de veranderingen in het klimaat te kunnen doen is het belangrijk om een goed begrip te hebben van deze opname van CO₂. In het promotieonderzoek dat in dit proefschrift wordt beschreven hebben we een methode ontwikkeld en onderzocht om de locatie van de CO₂ uitstoot en opname op het land beter te kunnen bepalen. Met deze methode kan onze kennis over de invloed van vegetatie op de CO₂ concentratie in de lucht (en daarmee op de snelheid van klimaatverandering) worden gecontroleerd en verbeterd.

De methode die in dit proefschrift wordt toegepast maakte gebruik van de reden waarom de opname en uitstoot van CO₂ door de vegetatie belangrijk zijn, namelijk omdat ze de CO₂ hoeveelheid in de lucht beïnvloeden. Ruimtelijke verschillen in de opname en uitstoot van CO₂ veroorzaken variaties in de atmosferische CO₂ concentraties. Waarnemingen van deze variaties kunnen worden gebruikt om de fluxen van de biosfeer aan het aardoppervlak te bepalen. Deze methode, waarbij het gevolg (variaties in de CO₂ concentratie in de atmosfeer) gebruikt wordt om de oorzaak (de opname en uitstoot van CO₂ aan het landoppervlak) te bepalen, wordt invers modelleren genoemd. Om de waarnemingen in de atmosfeer aan de processen op het landoppervlak te koppelen wordt gebruik gemaakt van een atmosferisch transportmodel, waarmee de verandering in de concentratie en het transport daarvan door de lucht wordt gemodelleerd. Met andere woorden, met invers modelleren kan de verdeling van de hoeveelheid CO₂ in de atmosfeer, en de verandering daarvan in de tijd, worden gebruikt om de oppervlakte fluxen te kwantificeren, door het gebruik van numerieke transport modellen. Inverse modellen verschaffen een onafhankelijke, zogenaamde top-down methode om de emissies van broeikasgassen te verifiëren op basis van atmosferische waarnemingen van broeikasgasconcentraties.

8.2 Dit proefschrift

In dit proefschrift wordt de ontwikkeling van een invers modelleersysteem op regionale schaal beschreven en wordt de werking ervan onderzocht. Daarbij laten we zien tot op welk niveau de regionale CO₂ fluxen kunnen worden bepaald met een atmosferisch observatie- en modelleringsysteem op hoge resolutie. De hoofdonderzoeksvraag van dit proefschrift is: “Tot op welk niveau kunnen we de regionale CO₂-fluxen bepalen met een atmosferisch observatie- en
modelleersysteem op hoge resolutie?”. Deze vraag kan worden onderverdeeld in de volgende drie onderdelen:

1) **de praktische aspecten**, is het mogelijk om een stabiel en robuust modelleersysteem te ontwikkelen op de gewenste hoge resolutie;

2) **de prestatie** van een invers modelleersysteem op hoge resolutie. Wat kan worden bereikt en wat zijn de beperkingen bij het verhogen van de resolutie van een dergelijk systeem;

3) **de toepassing** van een invers modelleringsysteem op hoge resolutie om de koolstofbalans te bepalen. In deze studie wordt gefocust op Nederland als een proefgebied om deze vraag te beantwoorden.

**8.3 Algemene conclusies**

Over het algemeen kan worden geconcludeerd dat het inverse modelleersysteem op hoge resolutie een goede, toepasselijke en bruikbare methode is om ons begrip van het gedrag van de CO₂ fluxen te verifiëren. Voor bijvoorbeeld de Nederlandse situatie hebben we aangetoond dat met een state-of-the-art biosfeer model de opname van CO₂ wordt onderschat. Verder hebben we aangetoond dat wanneer in het modelleersysteem verschillende complementaire waarnemingen worden gecombineerd dit niet alleen de CO₂ fluxen kan bepalen, maar dat het ook kan helpen om fouten in de meteorologische modellen op te sporen. Het regionale modelleersysteem op hoge resolutie zoals ontwikkeld in dit project, en het gebruik van verschillende complementaire waarnemingen van atmosferische eigenschappen en van de energiestromen van het oppervlak naar de atmosfeer, kan worden gebruikt als een prototype verificatiesysteem voor de regionale biosferische CO₂ uitwisseling.

Het inverse modelleersysteem kan de a priori CO₂ fluxen bepalen op het niveau van ongeveer 100 kilometer. We hebben laten zien dat op een fijner niveau het onderscheid tussen de fluxen van bijvoorbeeld verschillende landgebruiksklassen niet realistisch meer is. Het systeem is daarom in staat om aan te geven dat er fouten zitten in onze a priori schattingen, maar het kan niet de exacte locatie van de foute schatting aangeven noch deze verbeteren. Het regionale modelleersysteem geeft dus geen directe informatie over de processen die de CO₂ fluxen bepalen. Wel geeft het de mogelijkheid om te checken of de huidige kennis tot op een bepaald niveau correct is, en of de emissies zoals gerapporteerd door verschillende landen binnen bepaalde grenzen kloppen.

**8.4 De praktische mogelijkheden van een modelleersysteem op hoge resolutie**

De eerste deelvraag behelst de **praktische aspecten** en de vraag of het mogelijk is om een stabiel en robuust modelleersysteem te maken op de gewenste hoge resolutie. Over het algemeen is het antwoord op deze deelvraag positief. In dit project hebben we een modelleersysteem ontwikkeld en toegepast dat in staat was om een inversie te doen voor een gehele jaar op hoge resolutie. We hebben dit systeem intensief getest en de resultaten zijn over het algemeen vrij bemoedigend.
8.4.1 Continue modelleren op de gewenste schaal met een goede signaal-ruis verhouding

Door het hoge detailniveau van de modellering was het niet mogelijk om het model voor de gehele wereld, noch om het met een lange inslingertijd te draaien. Daarom was een van de onderzoeksvragen of het mogelijk was om een dergelijk begrensd model voor langere tijd te laten lopen zonder divergentie van de simulatie resultaten van de waarnemingen. Onze bevinding was dat continue, geneste simulaties zonder herstart inderdaad mogelijk zijn. De randvoorwaarden van het model worden bepaald door de resultaten van grootschaliger modellen (ECMWF voor de meteorologie en Carbontracker voor de CO₂), hierdoor wordt voorkomen dat de resultaten gaan divergeren (zie hoofdstuk 3). Voor deze aanpak zijn betrouwbare achtergrondwaardes nodig om de CO₂ in- en uitvoer op hoge temporele resolutie aan de randen van het regionale model voor te schrijven. In Europa zijn deze beschikbaar vanuit bijvoorbeeld Carbon Tracker (zoals gebruikt in deze studie; Peters et al., 2010) en LMDZ (Chevallier et al., 2010).

De regionale schaal in de orde van grootte van 10-100km is een geschikte schaal om de CO₂ fluxen te bepalen (hoofdstuk 3, 5 en 6). De invloed van de variatie (dagelijks en synoptisch) van het achtergrond signaal bleek niet groter te zijn dan het signaal van de fluxen in het domein waarvoor de optimalisatie wordt gedaan. Daarnaast hebben we aangetoond dat het gesimuleerde signaal op de observatie locatie niet alleen wordt beïnvloed door de fluxen van de landgebruiktypes nabij deze locatie, maar ook door het signaal van fluxen van andere landgebruiktypes in de regio. Hiermee worden de bevindingen van bijvoorbeeld Gerbig et al. (2003) en Lauvaux et al. (2009) bevestigd, die ook aantoonden dat de locale schaal een belangrijke invloed heeft op de variaties die worden waargenomen in de atmosfeer. Geconcludeerd kan worden dat de atmosferische observaties inderdaad kunnen worden gebruikt om de fluxen te bepalen op de schaal waar deze studie zich op richt.

De signaal-ruis verhouding is tevens onderzocht om vast te stellen of variatie in de atmosferische CO₂ concentratie kan worden gebruikt om de biosferische fluxen te bepalen. Zelfs in een heterogene omgeving zoals in Nederland, met een substantiële fossiele brandstofflux die is verspreid over het gebied, vonden we dat de variatie veroorzaakt door biosferische fluxen groter is dan de variatie door fossiele brandstof fluxen (hoofdstuk 3). Verder hebben we de verhouding bestudeerd tussen de invloed van de onzekerheid van de CO₂ fluxen op de atmosferische CO₂ concentratie (oftewel het signaal) en de afwijking tussen model en data als gevolg van onzekerheden in het modelleersysteem (oftewel de ruis). Het signaal bleek gemiddeld 11,7 ppm te zijn. We hebben vastgesteld dat de ruis veroorzaakt door fouten in de simulatie van de dagelijkse grenslaag in deze studie ongeveer 1,7 ppm is (hoofdstuk 3). De onderzochte representatiefout bleek in de orde van 0,2 ppm op 10km resolutie in de studie voor zuid Frankrijk (hoofdstuk 4). Ondanks de transport fouten in de orde van enkele ppm’s, is de signaal-ruis verhouding substantieel gedurende de dag, door de relatief grote invloed van de onzekerheid in de CO₂ fluxen op de atmosferische concentraties. Dit geeft aan dat er potentie bestaat voor inversies.

8.4.2 Moeilijkheden met stabiele grenslagen

De nachtelijke grenslaag is zeer moeilijk te simuleren. Deze moeilijkheid wordt niet opgelost door op een kleinere schaal te modelleren. In de simulatie voor mei en juni 2008 vonden we dat de nachtelijke grenslaaghoogte systematisch wordt onderschat
Omdat de CO\textsubscript{2} gradiënt in de stabiele grenslaag sterk is, is de inversie erg gevoelig voor een incorrecte modellering van de nachtelijke grenslaag. Tot nu toe is er geen betrouwbare correctie voor de bias in de nachtelijke grenslaagberekeningen beschikbaar (bijvoorbeeld Steeneveld et al., 2008; Gerbig et al., 2008; Law et al., 2008). Daarom moesten de nachtelijke CO\textsubscript{2} observaties worden uitgesloten van de inversies. Omdat in de winter stabiele condities vaker gedurende de dag voorkomen, maakt dit de inversies voor de winterperiode mogelijk minder betrouwbaar (hoofdstuk 6).

8.4.3 Effectief gebruik van complementaire observaties op hoge resolutie

Het gebruik van complementaire observaties op hoge resolutie wordt met het modelleringsysteem mogelijk gemaakt. Het belangrijkste hierin is dat in de inversies tijdseries van de middag atmosferische CO\textsubscript{2} concentratie observaties zijn opgenomen. Hierdoor kan gebruik worden gemaakt van de inter-dagelijkse variabiliteit om de CO\textsubscript{2} fluxen te bepalen (hoofdstuk 6). Om het mogelijk te maken om de observaties in de grenslaag boven het land met dit detailniveau op te nemen is het essentieel om de variaties die worden veroorzaakt door mesoschaal circulaties te resoveren (e.g. Perez-Landa et al., 2007; Ahmadov et al., 2007; Rivier et al., 2010; Broquet et al., 2011). Dit is in deze studie gedaan door de toepassing van een modelleringsysteem op hoge resolutie. Dit systeem hebben we grondig getest in de studies die in dit proefschrift worden gepresenteerd, en in de modelvergelijkingsstudie van Sarrat et al. (2007).

Verder hebben we data van vliegtuigobservaties, scintillometers, eddy correlatie metingen, radiosondes en van torens met metingen op verschillende hoogtes gebruikt om het systeem verder te bepalen (hoofdstuk 3). Door het gebruik van het hoge resolutie modelleringsysteem was het mogelijk de resultaten van de inversies en de waargenomen fluxen met het vliegtuig direct met elkaar te vergelijken (hoofdstuk 6). Dit verschafte een sterke validatie voor de inversietechniek (bijvoorbeeld Lauvaux et al., 2009), die alleen mogelijk is wanneer de schaal van de inversie gedetailleerd genoeg is.

De combinatie van de gedetailleerde meteorologische data en het atmosferische model onthulde een mismatch tussen de gesimuleerde en geobserveerde energie fluxen of tussen de gesimuleerde en geobserveerde grenslaagdiepte (hoofdstuk 3). We vonden dat deze discrepantie niet was beperkt tot het modelleringsysteem RAMS-Leaf3, maar dat het ook aanwezig was in het atmosferische model WRF. We hebben deze mismatch verder onderzocht en het gepubliceerd als Steeneveld et al. (2011). Het was nog niet mogelijk om de mismatch te verhelpen, maar we zijn succesvol met de aanpak van deze mismatch gevonden door de gedetailleerde analyse van het atmosferische model. We hebben de oplossing voor deze onjuistheid in het model, die moet worden gerepareerd om massa balans fouten te voorkomen, gepubliceerd als Meesters et al. (2008).

8.4.4 Inversies toepasbaar op de regionale schaal

Om inversies op de regionale schaal uit te voeren, hebben we het Ensemble Kalman Filter succesvol geïmplementeerd. We hebben hierin verschillende state-of-the-art inverse methodes om de CO\textsubscript{2} flux te bepalen toegepast, en deze intensief getest in een pseudo-data omgeving. Het grootste deel van deze methodes voldeed om de CO\textsubscript{2}
balans geïntegreerd over het totale domein vast te stellen. Uitzondering hierop was de inversie waarbij NEE werd geschaald met een lineaire vermenigvuldigingsfactor per landgebruik type, die niet goed presteerde. De inversies waarbij de parameters van het biosfeer model worden geoptimaliseerd per land gebruikt klasse (de parameter inversie), en de inversies waarbij respiratie en GPP worden geoptimaliseerd per pixel (de βRGpixel inversie) gaven de beste resultaten. Deze twee methodes zijn geselecteerd voor de toepassing in onze prototype simulatie voor Nederland.

8.4.5 Concluderende praktische overwegingen

Concluderend, hebben we in dit project een stabiel en robuust genest modelleringsysteem ontwikkeld voor de regionale schaal. Het heeft een acceptabele signaal-ruis verhouding voor atmosferische CO₂ concentraties en het atmosferische signaal kan worden gebruikt om de CO₂ fluxen op een hoge ruimtelijke en tijdelijke resolutie te bepalen. De prestatie van de nachtelijke atmosferisch simulaties is nog niet goed genoeg om volledige tijdsseries van CO₂ observaties te kunnen gebruiken in de inversies. Daarom geeft het modelleringsysteem de mogelijkheid om interdagelijkse variatie te gebruiken om de CO₂ fluxen te bepalen. We hebben aangetoond dat een aantal van de geselecteerde inversiemethodes correct werken wanneer ze worden toegepast op de regionale schaal, en dat een directe vergelijking met observaties van verschillende oppervlaktefluxen en atmosferische parameters mogelijk is.

8.5 Voordelen en beperkingen van modelleren op hoge resolutie

Ten tweede is de prestatie van het invers modelleringsysteem op hoge resolutie systematisch onderzocht. Hier geven we een samenvatting van wat kan worden bereikt en wat de beperkingen zijn wanneer naar inversies op een hogere resolutie wordt gegaan.

8.5.1 Reductie van de representatiefout

Bij inversies op lage resoluties wordt het afgeraden om gebruik te maken van observaties in de buurt van sterke veranderingen van het CO₂ veld, bijvoorbeeld veroorzaakt door de rand van de circulatie van de zeebries, omdat op lage resoluties de representatiefout aanzienlijk kan zijn (bijvoorbeeld Gerbig et al. 2003a; Lin et al., 2004; Van der Molen and Dolman, 2007; Corbin et al., 2008; Patra et al., 2008). Op hoge resoluties kunnen mesoschaal circulaties, zoals die van de zeebries, beter worden gesimuleerd. Ook de verschillen in de hoogte van de grenslaag, veroorzaakt door contrasten in het landgebruik, kunnen worden weergegeven wanneer op een hoge resolutie wordt gemodelleerd. Daarom maakt hoge resolutie modellering het mogelijk om observaties in de grenslaag, dicht bij scherpe overgangen in de landbedekking op een betrouwbare manier te gebruiken (hoofdstuk 4). Ook verder van mesoschaal circulaties kan de representatiefout substantieel worden verkleind van ongeveer 1,5 ppm op 100km resolutie naar slechts 0,4 ppm op 10 km resolutie.

8.5.2 Prestaties van de regionale inversies

De prestaties van de inversies zijn bestudeerd met zowel pseudo-data als met echte data. Bij het laatste is gebruik gemaakt van onafhankelijke CO₂ flux schattingen die beschikbaar waren om de resultaten van de inversies mee te controleren. Twee inversiemethodes, de parameterinversie en de βRGpixel inversie, gaven de beste
prestaties in de pseudo-data studie (hoofdstuk 5) en zijn geselecteerd voor de echte data studie. De resultaten van de pseudo-data studie suggereerden dat deze twee methodes het beste passen bij het gebruik op de regionale schaal.

Ook in de studie met echte data presteerden deze twee methodes goed, en gaven consistente resultaten. Hoewel de absolute waardes van de fluxen geoptimaliseerd met de parameter inversie en de βRGpixel inversie verschillen, was de correctie van prior naar posterior altijd in dezelfde richting voor vrijwel alle landgebruikklassen en seizoenen. Daarbij komt dat voor het grootste deel van het jaar, de posterior schattingen veel dichter bij de onafhankelijk met vliegtuigen waargenomen CO₂ fluxen liggen (hoofdstuk 6). Dit bevestigt dat de inversies ook onder echte omstandigheden in staat zijn om verbeteringen aan te brengen in de schattingen van de geïntegreerde CO₂ flux over een gebied van enkele honderden kilometers vergeleken met de prior schattingen. Dit is vergelijkbaar met de schaal die in de meeste inversie modellen gevonden als geschikt (bijvoorbeeld Carouge et al., 2010; Schuh et al., 2009; Gerbig et al., 2006; Ahmadov et al., 2009).

Het onderzoek in dit proefschrift toont ook een aantal belangrijke beperkingen van de inversies, en gaf aan dat er soms uitdagende vereisten bestaan om de inversies goed te laten werken. De inverse vereist een zekere hoeveelheid kennis over de structuur van de fluxen. Bijvoorbeeld, in de echte data studie hebben we gevonden dat de inverse slechter presteerde in het voorjaar, dan in de zomer en de herfst (hoofdstuk 6). Dit was waarschijnlijk te wijten aan de snelle veranderingen van de LAI (Leaf Area Index; maat voor dichtheid van de vegetatie) tijdens het voorjaar, die niet adequaat zijn weergegeven door de maandelijkse LAI data. De pseudo-data studie (hoofdstuk 5) liet zien dat als de prior structuur niet correct is, de inverse moeilijkheden heeft om correct met deze foutenbron om te gaan en dat de onzekerheden weergegeven in de resultaten van de inverse onrealistisch klein zijn. In deze studie, komt het verschil in de structuur van de respiratie tussen de prior (gebaseerd op 5PM; Groenendijk et al., 2009) en de pseudo-voorwaarde (gebaseerd op FACEM; Pieterse et al., 2007) niet overeen met de landgebruiklassen, wat een realistische situatie is (bijvoorbeeld Chevallier et al., 2011). De aggregatiefout die in grootschalige inversies belangrijk was gevonden (bijvoorbeeld Kaminski et al., 2001), speelt dus ook in hoge resolutie inversies een rol, al is hij nu gerelateerd aan fouten in de prior structuur op veel kleinere schalen (hoofdstuk 5).

Ondanks fouten in de structuur van de prior velden, presteerden de geselecteerde inversies goed om de gemiddelde flux over het inversegebied te bepalen. Dit kon zelfs worden bereikt in de pseudo-data studie waar we de inverse de moeilijke taak hadden gegeven om de fluxen te bepalen in een omgeving waar de structuur van de prior heel anders was dan die van de pseudo-voorwaarde (hoofdstuk 5). Zowel de prior als de pseudo-voorwaarde waren in deze studie gebaseerd op state-of-the-art, maar verschillende modellen, wat aangeeft dat een dergelijke mismatch in de structuur realistisch is en geregeld kan voorkomen. Geïntegreerd over een paar honderd kilometer is het dus mogelijk om de schatting van de fluxen te verbeteren, zelfs met een moeilijk structuurverschil. Opgevat moet worden dat deze geïntegreerde schaal veel gedetailleerder is dan de continentale schaal.

Op een kleiner aggregatieniveau bleek de informatie die met de inverse op regionale schaal kon worden verkregen, zeer beperkt. De schattingen op het niveau van landgebruiktypes bleken over het algemeen niet betrouwbaar (hoofdstuk 5). Dit wordt, behalve door de moeilijkheden veroorzaakt door de incorrecte prior
structuren, ook veroorzaakt door de hoge correlatie tussen het atmosferische CO₂ signaal van de verschillende landgebruiktypes. Ook een goede scheiding tussen respiratie en GPP door de inversie is moeilijk te verkrijgen vanwege de sterke anticorrelatie van de twee signalen gedurende de dag (hoofdstuk 3). Dit ‘aliassten’ is een bekend probleem (bijvoorbeeld Carvalhais et al., 2008). Aangezien tijdens de nacht respiratie de enige biosfeer CO₂ flux is en fotosynthese dan afwezig is, kan een mogelijke verbetering in de nachtelijke atmosferische modellering helpen om dit probleem op te lossen. Op dit moment zijn dergelijke verbeteringen echter nog niet beschikbaar.

8.6 Toepassing van het inversie model voor Nederland

Tot slot hebben we het modelleersysteem op hoge resolutie toegepast om de biosfeer component van de CO₂ balans beter te bepalen. In deze studie is Nederland als testregio gebruikt, om de schatting van de CO₂ balans te verbeteren in vergelijking met de prior schatting. De inversies lieten dat gedurende het voorjaar, de zomer en de herfst Nederland een netto opnamegebied is voor CO₂. De CO₂ fluxen zijn negatiever (meer opname) volgens de inversies dan door de priors werd gesuggereerd (hoofdstuk 6). Deze proef levert een voorbeeld van de kracht van het inversie systeem dat is in deze studie is ontwikkeld om de CO₂ balans te valideren.

Een ander opmerkelijk resultaat is het grote verschil tussen de posterior opname in twee verschillende landbouw landgebruik categorieën. In de eerst is de netto CO₂ opname relatief beperkt, terwijl dit in de tweede de opname relatief hoog is. Dit resultaat moet wel voorzichtig behandeld worden, omdat het dit onderscheid op een gedetailleerder niveau is dan het niveau waarop de inversies betrouwbaar zijn gebleken. Dit resultaat kan mogelijk wel helpen om de prior onderschatte CO₂ flux te verklaren. De tweede klasse met landbouw bevat veel maïs, waarvan bekend is dat deze een hoge CO₂ opname heeft (e.g. Verma et al. 2005). De dataset die is gebruikt op de parameters van 5PM te optimaliseren voor de gematigde breedtegraden bevatte geen data voor maïs. Dit kan een verklaring zijn waarom de biosfeer model de opname onderschatte. In ieder geval heeft de confrontatie van de biosfeer fluxen met complementaire atmosferische CO₂ observaties in het regionale inverse modelleersysteem een verschil in de schatting van de CO₂ flux geïdentificeerd, en zorgt dit daarmee voor een verfijning van de CO₂ flux schatting.

8.7 Aanbevelingen en toekomstig werk

Op basis van de onderzoeken die zijn gepresenteerd in dit proefschrift kan een aantal aanbevelingen worden gedaan. Op het gebied van de praktische overwegingen hebben we laten zien dat het modelleersysteem in principe goed toepasbaar is. Desondanks heeft het een belangrijke tekortkoming, aangezien het niet in staat is om de nachtelijke grenslaag goed te simuleren. Een verbetering van de simulatie van de stabiele grenslaag zou de mogelijkheden om de oppervlaktefluxen te bepalen sterk verbeteren, aangezien het daarmee mogelijk zou worden om CO₂ concentratiemetingen van de volledige dagelijkse cyclus te gebruiken. Hiermee zal de scheiding tussen respiratie en GPP sterk verbeteren.

Helaas is uit eerdere studies duidelijk geworden dat de problemen met het modelleren van de grenslaag erg moeilijk te verhelpen zijn. Zoals we in hoofdstuk 3 hebben laten zien, is de methode om complementaire oppervlakte en atmosferische
data te combineren niet alleen mogelijk voor CO₂, maar kan ze ook worden toegepast voor andere gesimuleerde oppervlakte fluxen, de energiebalans en de processen in de grenslaag. In dit promotieonderzoek zijn reeds twee substantiële tekortkomingen van de huidige meteorologische modellen onthult: een fout in de massa balans in RAMS (Meesters et al., 2008) en een mismatch tussen de gemodelleerde en geobserveerde oppervlakte energieflux - grenslaagdiepte relatie (Steeneveld et al., 2011). Een verdere systematische verificatie van meteorologische modellen, gebaseerd op oppervlakte flux en grens laag observaties wordt dan ook sterk aangeraden. Een intensieve check op de hoge resolutie meteorologische modellen die in gebruik zijn voor Nederland met de grote dataset die vanuit het BSIK project hier beschikbaar is, kan helpen om incorrecte parametrisatie te identificeren. Dit kan belangrijke aanwijzingen opleveren om de moeilijkheden met het modelleren van de (stabiele) grens laag op te lossen.

Wat betreft de prestatie van het inverse modelleersysteem op hoge resolutie, hebben de parameter inversie en de βRGpixel de beste resultaten geleverd in de pseudodata studie. Op basis van deze resultaten lijken deze twee inversiemethodes het meest geschikt voor deze regionale schaal. Het gebruik van hoge resolutie modellering wordt vooral aanbevolen voor gebieden met een sterke ruimtelijke variatie in het landschap, en nabij atmosferische mesoschaal circulaties. Door de resolutie te vergroten kan de representatiefout sterk worden gereduceerd, en zijn de atmosferische observaties nabij mesoschaal circulaties te gebruiken met een grotere betrouwbaarheid voor het schatten van de CO₂-fluxen. Het wordt aangeraden om dit soort inversies te gebruiken als een zoom van de grootschalige modellen, zoals in dit project Carbontracker Europe. Het prototype-modelleersysteem ontwikkeld in dit proefschrift kan in toekomstig onderzoek worden toegepast om CO₂-fluxen verder te verifiëren.

Het wordt echter aanbevolen om de beperkingen van de inversies in gedachten te houden. De eerste beperking is dat in de inversies de CO₂ fluxen worden geoptimaliseerd op basis van een geaggregeerd atmosferische signaal, waardoor het vermogen van de inversie wordt verminderd om een onderscheid te maken tussen twee flux signalen, met name als hun geobserveerde signalen een vergelijkbare patroon hebben in de tijd. Daarom zal een vorm van aggregatietrategie vereist zijn om de posterior resultaten. De studies in dit proefschrift laten zien dat de resultaten op een grovere schaal dan 100km betrouwbaar zijn, maar dat het posterior detail op een kleiner niveau niet altijd betrouwbaar is. Dit kwam in ieder geval deels door het aliasseren. Van het verder verhogen van de ruimtelijke resolutie van de observaties dan in de voorliggende studie is gebruikt, wordt vanwege de aggregatie van het signaal in de atmosfeer op dit moment niet verwacht dat het voor een sterke verbetering van het detail in de resultaten zal zorgen.

De tweede beperking is dat het vermogen van de inversie om fluxen correct te optimaliseren bepaald wordt door de keuze van de onbekenden en de achterliggende prior flux structuren. Indien de onbekenden de redenen voor de mismatch tussen de observaties en de simulaties niet correct dekken, ontbreekt het de inversie aan flexibiliteit om de flux schattingen correct aan te passen. Dit kan resulteren in een te lage posterior onzekerheid. Daarom is een redelijk goede prior schatting van de temporele en ruimtelijke structuur van de fluxen vereist om tot betrouwbare resultaten te komen. Wanneer de prior structuur niet accuraat is zou dit theoretisch in de keuze van de onbekenden moeten zijn opgenomen, zodat het kan worden
aangepast in de inversie. Dit is een extra uitdaging aan de hoge resolutie, door de extra kleinschalige variabiliteit die op dit schaalniveau wordt toegevoegd.

Wanneer de (structuur van de) prior sterk afwijkt van de waarheid, bleken de inversies in staat om aan te geven dat er aanpassingen in het fluxveld nodig waren, maar ze waren niet in staat om betrouwbare gedetailleerde informatie over de aanpassing te geven. De inversies, en vooral de niet-lineaire, presteren het beste om de prior te verbeteren wanneer de waarheid niet te ver van de prior is verwijderd.

Daarom wordt een iteratief gebruik van de inversie methode aangeraden. Als eerste stap kan ze gebruikt worden om een indicatie te geven of een grote aanpassing van de flux schattingen nodig is, oftewel, het kan gebieden met een slecht begrip van de CO₂ fluxen identificeren. Als tweede stap is een handmatige aanpassing van de prior, en van zijn fout-covariantiemaat matrix aan te raden, waarbij de focus ligt op de eigenschappen in de gebieden waar de vorige prior slecht presteerde. Hierbij kan gedacht worden aan verbeteringen in de formules die de biosfeer en heterotrofe processen beschrijven, verbeteringen in structuur van het flux veld en zijn covariantie structuur met bijvoorbeeld extra satelliet data en geo-statistische methoden, en aan verbeteringen van de empirische relaties gebaseerd op extra bottom-up (niet atmosferische data). Als derde stap is het aan te raden om de inversie te herhalen met de nieuwe prior. Dit iteratieve proces moet mogelijk meerdere keren herhaald worden. Het moet worden benadrukt dat de data die in de handmatige stap worden gebruikt totaal onafhankelijk en complementair moeten zijn van de atmosferische data die in de inversies worden gebruikt.

Een dergelijke hybride van geautomatiseerde optimalisatie en gefocuste handmatige optimalisatie, gebaseerd op complementaire informatie, geeft de inversie de kans om zijn volledige kracht te benutten: (1) als indicatiemiddel om aan te geven waar verbeteringen nodig zijn en (2) als fine-tuner om de fluxen die reeds vrij goed bekend zijn op hoge resolutie nog verder te bepalen. Op deze manier kunnen de processen achter de CO₂ fluxen worden verbeterd in de handmatige stap, met meer flexibiliteit dan als ze automatisch zouden worden geoptimaliseerd. Dit geeft de mogelijkheid om het begrip van de koolstofbalans beter te begrijpen, wat uiteindelijk tot verbeteringen in het voorspellen van klimaatverandering kan leiden.

Wanneer de aanpassingen van de prior naar de posterior relatief klein zijn, en -belangrijk- in lijn met de prior onzekerheden, kan dit aangeven dat de posterior flux schattingen geconfereerde manier naar de waarheid zijn geconvergeerd. Om dit te controleren, is het aan te raden om een additionele inversie uit te voeren voor een ander moment en/of een ander gebied, of om complementaire, eerder ongebruikte data te gebruiken, zoals vliegtuig metingen. Om een beter begrip van de koolstofbalans te ontwikkelen, moeten in mijn ogen investeringen in top-down en bottom-up studies niet afzonderlijk worden gedaan, maar zouden ze elkaar moeten versterken. Om slechts fluxen te controleren, en te kunnen aangeven of ze correct of incorrect zijn (binnen een bepaalde marge) is de eerste stap van de bovenstaande iteratie voldoende. Echter, om ons begrip te vergroten van de koolstofbalans, is de toepassing van de volledige hybride van geautomatiseerde en gefocuste handmatige optimalisatie aan te raden.

**De toepassing** van een invers modelleersysteem op hoge resolutie in Nederland kan worden beschouwd als een voorbeeld van de eerste stap van de iteratie. Hiermee werd aangetoond dat de netto CO₂ opname in de regio waarschijnlijk hoger is dan prior is berekend. Desalniettemin bleek het modelleersysteem niet in staat om directe
betrouwbare informatie over de processen die de koolstofcyclus bepalen te kunnen leveren. De posterior resultaten waren soms ver buiten de prior onzekerheid, wat aangeeft dat het fluxsysteem nog niet goed begrepen is. De inversie suggereerde een veel hogere opname door de landbouwgewassen dan oorspronkelijk was verwacht. Daarom is het aan te raden om aan een verbetering van de prior schatting te werken, met name aan het schema voor de landbouwgewassen, en om een gedetailleerder onderscheid te maken tussen verschillende soorten van gewassen en gewas rotaties in deze regio.

Samenvattend, het regionale inverse modelleersysteem ontwikkeld en getest in dit promotieonderzoek verschafte een onafhankelijke check op onze kennis over de CO₂ fluxen. Voor een beter gebruik van de kleinschalige variatie in de regionale inversies wordt aangeraden om te investeren in een verbetering van de beschrijving van de CO₂ flux processen, de structuur van de priors en de formulering van de onbekenden. Tot slot, wordt aangeraden om de inversie te gebruiken als indicatie waar verbeteringen nodig zijn, of als fine-tuner om de fluxen beter te bepalen, afhankelijk van de kwaliteit van de prior structuur en de onbekenden.


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