The carbon balance from an atmospheric perspective
*Inverse modeling of regional biospheric CO₂ fluxes*

**Summary and synthesis of the results**

### 1.1 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 (CO₂) 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 CO₂ in the atmosphere can be used to quantify surface fluxes, using numerical models of atmospheric transport as a key tool.

### 1.2 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.
1.3 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.

1.4 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.

1.4.1 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 CO₂ 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 CO₂ 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$_2$ 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$_2$ fluxes on the atmospheric CO$_2$ 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$_2$ fluxes on the atmospheric concentrations. This indicates the potential for inversions.

1.4.2 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$_2$ 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$_2$ 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).

1.4.3 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$_2$ 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).

1.4.4 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.

1.4.5 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.

1.5 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.
1.5.1 Reduction of the representation error

In low resolution inversions the use of observations near sharp changes in the CO\textsubscript{2} 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.

1.5.2 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 CO\textsubscript{2} 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 CO\textsubscript{2} 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 CO\textsubscript{2} 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 CO₂ 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.

1.6 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 CO₂ 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 CO₂ 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.


1.7 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 CO₂ 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 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.