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Biogeosciences Discussions

Interactive comment on "CO_2 flux determination by closed-chamber methods can be seriously biased by inappropriate application of linear regression" *by* L. Kutzbach et al.

L. Kutzbach et al.

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Thank you very much for the careful review, constructive critique, the hints to weak points and open questions in our study, and the many very useful suggestions to improve the manuscript. Sorry for not using the Interactive Discussion tool for more intense and quicker exchange of ideas. The substantial delay of this response is due to many unexpected organisational problems during our field campaigns in Russia this summer and unexpectedly long field stays of our first author Lars Kutzbach. In the following, we will answer all comments of reviewer #1. First, we will repeat the comment of the referee (shortened) and then we will give the respective answers. We will submit a considerably revised manuscript in which much of the reviewers' comments will be reflected.

Anonymous Referee #1

General comments

“This interdisciplinary manuscript demonstrates (...)as quickly as is reasonable.”

–>Answer: We plan to prepare a second paper where we divide the different situations regarding day or night conditions, soil and vegetation characteristics, soil hydrology, micrometeorological conditions and different chamber set-ups. For this paper, we would like to stick to a more general overview of the appropriateness of linear and nonlinear models looking at the large database as a whole.

Specific comments

“The proposed exponential model is (...) evaluation of the competing models.”

–>Answer: Regarding the modelling of soil diffusion, we absolutely agree that the NDFE model proposed by Livingston et al. (2006) is the better model compared to the soil diffusion approach implemented in our proposed model equation, which is based on early ideas of Matthias et al. (1978) and Hutchinson and Mosier (1981). However, we face the problem that the NDFE model is developed for a pure soil-atmosphere system without vegetation. Furthermore, the NDFE model is based on the assumption of homogenous soil pore space and only valid for trace gas sources. We think that it is practically impossible to develop a similar physically-based non-steady state diffusion model function for fitting to the c(t) data if the vertical soil structure is strongly heterogeneous and, particularly, if vegetation processes have to be considered in addition. As reviewer #3 stated in his comments, all the involved soil and vegetation processes are dynamic by nature and should ideally "be analyzed with a dynamic process model rather than with a statistical model”;. Anyway, such a dynamic process model would also have to incorporate many statistical regression components because many of the important parameters cannot be measured but must be estimated by “fitting” the dynamic process model to the data (inverse modelling). However, at the moment it seems

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unrealistic that all chamber experiments of the past and the future can be analysed by such an advanced dynamic process model. Therefore, we try to evaluate which form of nonlinearity could be expected using our conceptual modelling approach – which has to be significantly simplified to include soil and plant processes. From our admittedly strongly simplified modelling exercise, we conclude that the nonlinearity should be exponential or near-exponential. We are aware of these simplifications and that an exponential function would probably still underestimate the predeployment flux as was shown for the soil-atmosphere system by Livingston et al. (2005, 2006). How much it deviates from the NDFE model we can test only with our Linnansuo dataset which is non-vegetated. In the revised manuscript, we will compare the results of the the NDFE and the exponential regression for the Linnasuo dataset in an additional diagram. The major results of this comparison are:

- The NDFE function (parameters constrained to positive values as was done in Livingston et al. 2006) could be fitted successful for 349 of 399 experimental c(t) datasets. 50 datasets could not be fitted successful to the NDFE function mainly due to instable fitting calculations probably due to overparameterisation with respect to the data.

- 335 experiments remained after filtering the data with a noise filter (residual standard deviation of the exponential regression function must be < 2.2 ppm).

- From these 335 successful experiments, only 4 (1%) were significantly (p = 0.05) better fitted by the NDFE compared to the exponential regression. 39 of the 335 experiments (12%) were significantly better fitted by the NDFE function compared to a linear model.

- When considering only the fitted exponential regression with convex downwards curvature (as explainable by our exponential model and the NDFE model), the median ratio of the slopes of the NDFE and the exponential function is about 1.3. Thus, the exponential model yields systematically lower estimates of the initial c(t) curve slope than the NDFE approach as can be expected from theory. With increasing initial slopes the deviation between becomes very large, more than 2 ore 3fold. However, it is important to keep in mind that at Linnansuo no collars were used and thus the NDFE assumption of 1-dimesional flux could be seriously violated especially for great fluxes.

As we are not able to develop a non-steady state diffusion model for heterogeneous soils and vegetation and since there is none published yet, we think that the proposed exponential function is the best possible tool presently available for the chamber community working on vegetated surfaces. The main objectives of this study are to check 1) by means of residual analyses if the exponential model fits to the data, 2) if it fits better to the data than a quadratic or linear model, and 3) if the probable deviation is significant for short closure times. Although we are not able to develop a completely physically consistent model, we would argue that an exponential model is by far better suited to fit the data than the linear model. This was clearly shown by the residual analyses. We will add the statement to our manuscript that we have to expect the exponential model to likely still underestimate the predeployment fluxes but to approximate them much better than the linear model.

"The authors note that (...)as the mathematical model."

–> Answer: From our simplified considerations on diffusion and plant physiology theory, we derived an exponential form of the c-vs.-t curve in the chamber headspace. By using the Taylor power series expansion for curve fitting, we do not want to constrain the validity of this theoretical exponential curve form. Expanding the exponential to a power series of 17th order yields "exactly" the same curve as the exponential function for all observed datasets. Actually, the initial slopes of the exponential and the power series were checked and they never deviated more than 0.05 %. Our intention of using the power series is to keep the uncertainty estimates of the initial slopes small.

Physically or biologically meaningful models are often over-parameterized with respect to the available data. This has the consequence that some parameters cannot be estimated separately and estimations of the parameter uncertainty will yield very large values. By re-writing the exponential as the Taylor power series, we obtain three new parameters a, b, c which are much less dependent from each other than the parameters of the exponential p1, p2, p3. The main interest in this study is the initial slope of the c-vs.-t curve which is equal to b and also equal to p2 * p3). The advantage of the Taylor power series versus the original exponential function is obvious: b is directly determined by the power series expansion, is more independent from other parameters than the parameters of the exponential, and thus has a significantly lower relative uncertainty estimate than p2 and p3. Furthermore, using p2 * p3 for estimation of the initial slope, the resulting error by error propagation of two large errors will be even larger. If the focus would have been on the estimation of the physically-derived parameters p1, p2, p3, then we agree that the original exponential should be used as regression function. However, for this approach, the chamber closure time should have been longer to enforce nonlinearity which would decrease parameter dependency and thus decrease parameter uncertainty estimates.

We do not agree with the statement that “if Nature indeed demands an exponential”, then a true exponential must be fitted. In contrast, we would argue that when we are only interested in the initial slope of the exponential, then we should transform the exponential so that the curve form (as demanded by the theoretical model) is not changed but the uncertainty of the initial slope is minimised.

Nevertheless, we will remove the last part of chapter 2: from p. 2290, line 16 to p. 2291, line 18. We do this because (1.) the derived values for the initial slope by the exponential and the power series are virtually equal (deviation below 0.05%), and the error estimates of the initial slopes are not in the focus of this study, (2.) the manuscript has to be shortened somewhere, (3.) reviewer #3 suggested to remove this part as he felt that it confuses the message of the paper.

“The current analysis does (...) estimates will diverge.”

–>Answer: We absolutely agree with you here. This would be a very valuable study.

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However, we intended to perform such analyses in a following publication. For this study, we would like to limit our goals. We want to develop a conceptual model showing that nonlinearity of the c(t) curve is to be expected and linearity is not to be expected, what form of the nonlinear curve has to be expected, and to prove the nonlinearity by fitting linear and nonlinear regression functions to the data.

“The authors need (...) is also needed.”

–>Answer: We will provide such example graphs and parameter tables. Obviously, we can only select a small collection of the total of experiments (n=1764): We will choose typical c(t) series for which the expected curvature was found for night and day measurements and for the different sites. c(t) curves for which the expected curvature was not found will be presented in an additional graph as was requested by you below.

“p. 3, paragraph beginning: “The closed chamber method ...”. The authors list several potential (...) must be considered."

–>Answer: We will extend our list given in the text and include the pressure disturbance problem.

We tried to prevent any pressure disturbances by the following actions: At Salmisuo, Vaisjeäggi and Samoylov, we established permanent boardwalks at all sites. The boards rested on poles driven vertically into the soils. At Salmisuo and Vaisjeäggi, the chambers were installed 1.5-2 m away from the vertical poles to minimise possible compression when walking or standing on the boardwalk. At Samoylov, this distance was 0.5-1 m. At Linnasuo, no establishment of boardwalks was possible due to the ongoing peat excavation actions. The chambers were always put on the collars very carefully. During the placement of the chamber, one or two circular openings at the top wall of the chamber with a diameter of 2-4 cm were open to prevent pressure shocks on the surface. These openings were closed after chamber placement with rubber stoppers. During chamber placement no pressure changes more than 0.1 hPa could be observed at Salmisuo and Samoylov where pressure inside the chamber was

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measured.

“p. 5, paragraphs 1, 3: We agree (...) into the substrate.”

–>Answer: We agree again that leaks should be avoided if possible. However, there might be situations, in which leakage cannot be avoided. One example would be the measurement of CO2 exchange of a willow shrubbery. Willows have strong roots near the surface, which the researcher would have to cut to install a deep collar. This would disturb the ecophysiology of the micro-ecosystem very seriously by stressing the willows. We would argue that in this case, it would be better to allow for some leakage than to disturb the vegetation too strongly. In the exponential model which we propose, this moderate leakage, which must be limited to diffusion, can be integrated into the over-all model equation.

As also already explained above, we are aware of the strong simplification of our model but believe that fitting this exponential model can accurately derive the initial slope of the c(t) curve, particularly, if the measurement intervals are short and many data points are available over a short measurement period.

“p. 12, paragraph beginning: “The parameters (...) the theoretical model.”

–>Answer: We will add pressure perturbation of the soil pore space to the list. We will also add a sentence on our measures against potential pressure disturbances which we think is the maximum possible under field conditions. Indeed, we think that the changing turbulence due to the chamber deployment is very likely the main reason for the observed “unexplainable” curvatures. However, a pressure effect can not be ruled out. We think that more research is needed regarding this issue.

“p. 23, paragraph beginning: “Modelling of (...) in resultant flux estimates.”

–>Answer: See above. We think that we have as carefully as possible tried to prevent pressure perturbations. We think that the effect of changing headspace mixing as described by Hutchinson et al. (2000) is very likely a cause of serious error in al-most all chamber studies. It might also be a combination of a small pressure change and turbulence change effects. We consider writing a separate article on this issue. For this, the application of the numerical soil diffusion model as used by Healy et al. (1996), Hutchinson et al. (2000) and Livingston et al. (2006) would be very valuable. We absolutely agree with the reviewer about a more thorough quality control of flux data by using biophysical models as a reference. Without using biophysical models as a background and just using linear regression, the problems which likely occur when using closed chambers cannot be observed, understood and accounted for. Additionally, the usage of the correct statistical methodology would improve accuracy or at least realistic error estimates.

“p. 23, paragraph beginning: “Even if the (...) regulating chamber headspace concentrations.”

–>Answer: We will remove the complete paragraph and add instead the following sentences to the previous paragraph (page 2306, line 6): “The obvious violation of model assumptions indicates that the experiment design was sub-optimal and that the reason for it must be identified and accounted for. Otherwise, the calculated fluxes would be biased to an unknown extent.” Furthermore, we would add at page 2306, line 10, a sentence on the possible influence of pressure perturbations: “An additional reason for the unexplainable curvature could have been small positive pressure perturbations during chamber placement (Hutchinson and Livingston, 2001).”

“p. 24, paragraph beginning: “The measurement interval (...) resultant parameter estimates.”

–>Answer: We will add the recommendations of the reviewer to the manuscript to our list of practical recommendations, however, with some restrictions (page 2308, line 18-21): “When adopting a nonlinear approach, investigators should employ chambers with smaller headspace volumes and longer deployment times as warranted to emphasize the non-linearity of the c(t) response. For vegetated soils, however, the advantages of

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this approach must be carefully balanced with the risk of unpredictable plant responses due to strongly lowered CO2 concentrations or artificially high water vapour contents in the chamber headspace."

"p. 27, Conclusions. The developed (...) emissions studies."

–>; Answer: We will adopt your suggestion for rewording and change the text accordingly. Thank you.

Technical corrections

"p. 3, paragraph beginning: "The closed chamber (...) references as needed.)"

–>Answer: We will adopt all of your suggestions. We will cite (Hutchinson and Livingston, 2001; Livingston et al., 2006) for point (5.) and (Matthias et al., 1978; Hutchinson et al., 2000; Livingston et al., 2006) for point (6.).

"p. 4, paragraph continued from p.3: "Thus, for (...) and Hutchinson 1995)."

–>Answer: We will change the text according to your suggestion.

"Most of the recent studies ... for estimating CO2 fluxes"

–>Answer: "the" will be deleted.

"p. 17, paragraph (...)were also included."

–>Answer: The "also" will be moved.

"However, a substantial (...) curves would be of value.)"

–>Answer: We will adopt your text suggestions. We will provide some examples of such "unexplainable" curves.

"p. 19, paragraph (...)datasets (data not shown)."

–>Answer: We will move the "only".

“p. 23, paragraph (...) the theoretical model.”

–> Answer: We will adopt your suggestion for changing the text.

“p. 24, paragraph (...) autocorrelation and normality.”

–>Answer: We will adopt your suggestions.

“p. 24, paragraph (...) typically 0.95.”

–> Answer: We will adopt your suggestion.

“p. 24, paragraph (...) low measurement precision.”

–>Answer: We will adopt your suggestions.

“p. 25, paragraph (...) related recommendations.”

–>Answer: We will reorganise the entries.

“Considering the (...) follows:”

–>Answer: We will adopt your suggestion.

“Original: “Nonlinear (...) estimate the flux.”

–>Answer: We will adopt your suggestion.

“For closure times (...) regarding this issue)”

–>Answer: We will remove the recommendations about the Taylor power series here to prevent confusion. We will change the text as follows: “We recommend to fit an exponential function as given in Eq. (14) to the observed c(t) curves for experiments on vegetated soils. For experiments on non-vegetated soils, the NDFE model function proposed by Livingston et al. (2005, 2006) should be applied.”

“The slope of (...) needed here to provide context.”

–>Answer: We refer to the need to purge residual gases in the IRGA lines. Additionally, many chamber researchers discard the first 30 seconds of measurements because they observed a “higher noise level” at the experiment start (see comments of reviewer #3). We see such effects more often and to a stronger degree in the data from Linnansuo and Samoylov and less often and to a lesser degree in the Salmisuo and Vaisjeäggi datasets. For the Linnansuo dataset, the first 3 measurement points (30 s) were discarded. For Samoylov, the first concentration measurement point was discarded (45 s). For Salmisuo, the first 10 measurement points were discarded (10 s). For Vaisjeäggi, no measurement points were discarded. We will include this important information into Table 1. The approach of generally discarding some early measurement points and delaying the start point of the experiment t0 = 0 leads to lower estimates of the initial slope as the slope is greatest directly after chamber closure according to the exponential and the NDFE model. Therefore, the deviations between linear and exponential regression would be even greater without data discarding at the experiment start.

“The better the measurement (...) its significance demonstrated.”

–>Answer: We will adopt your suggestion.

“Original: When adopting the (...) non-linearity of the c(t) response.”

–>Answer: We will adopt your suggestion. However, we think that we will have to constrain the statement for experiments on vegetated soils. Therefore, we will add the sentence: “For vegetated soils, however, the advantages of this approach must be carefully balanced with the risk of unpredictable plant responses due to strongly lowered CO_2 concentrations or artificially high water vapour contents in the chamber headspace.”

“It is noted that (...) or remove it.”

–>Answer: As already noted above, a moderate leakage (which must be limited to diffusion) can be integrated into the over-all exponential model which we propose. As also already explained above, we are aware of the strong simplification of our model but

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believe that fitting this exponential model can accurately derive the initial slope of the c(t) curve, particularly, if the measurement intervals are short and many data points are available over a short measurement period. The nonlinear regression will always be better fitted to the initial, most nonlinear, part of the c(t) curve than a linear regression. This would also be true for nonlinearity due to leakage. Thus, the nonlinear regression approach would not be as susceptible to bias in the flux estimates due leakage as the linear regression approach.

“Additionally, in view of theoretical (...) title of this manuscript.”

–>Answer: We agree absolutely. We do not want to encourage linear regression; we just wanted to describe the reasoning of the linear regression users.

“Changing light, temperature and humidity conditions (...) the second assertion?”

–>Answer: We will adopt your text suggestion and also the suggestion for the additional reference. Furthermore, we retract the initial statement and will change the text block to: “Light, temperature and humidity conditions as well as wind speed and turbulence during chamber closure should be as similar as possible to the ambient conditions. Changes of light, temperature and humidity would change plant physiology and thus complicate the form of the c(t) curve whereas artificial changes of pressure, wind and turbulence may additionally impact transport processes and thus even compromise the assumption that the initial slope of the c(t) is the best estimator of the predeployment CO2 flux (Hutchinson et al., 2000, Hutchinson and Livingston, 2001).”

“p. 25, paragraph (...) would be smoothed.”

–>Answer: Will be changed.

“Here, the uneven underestimation (...) plant physiology differs.”

–>Answer: We will adopt your suggestions.

“p. 27, Conclusions: However, the curvature (...) due to soil compression)”

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–>Answer: We will adopt your text suggestion regarding the pressure problem, we will change the latter sentence to: “In particular, the effects of turbulence alteration and pressure disturbances across the soil-atmosphere interface by setting a closed chamber on the ecosystem should be investigated in more detail in the future.”

“p. 28: We developed (...) prior to publication.”

–>Answer: The URL is: http://biogeo.botanik.uni-greifswald.de/index.php?id=264 We will also indicate the URL in the manuscript.

“p. 41, Table 3: Significance (...) regression models f0 lin(t0).”

–>Answer: We adopted your suggestions.

“The null hypothesis H0 states (...) of the linear regression.”

–>Answer: Will be corrected.

Interactive comment on Biogeosciences Discuss., 4, 2279, 2007.