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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.

Anonymous Referee #1

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General comments

This interdisciplinary manuscript demonstrates the potential of integrating biological and physical process models to aid the interpretation of chamber-based measures of net ecosystem exchange. As such, it represents an important step forward for the Earth Sciences community involved in measuring or interpreting ecosystem processes or trace gas exchange data. I therefore recommend publication but with the caveat that the concerns outlined below be formally addressed. The key issues noted are substantive and must be given careful consideration even at the possible expense of extensive revision of the current manuscript. Because the current manuscript is already relatively

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long, however, the authors should decide whether to pursue a companion manuscript or to refocus the current manuscript to eliminate redundancies and maintain reasonable length. Given the potential importance of this manuscript, the authors should be encouraged to submit an updated response as quickly as is reasonable.

Specific comments

- The proposed exponential model is a three-parameter model summarized by Eqns. 14 through 19:

  $$c(t) = p_1 + p_2 exp(p_3 t) + \epsilon(t)\ .$$

  As the authors correctly note, the fitted parameters "cannot directly be interpreted physiologically or physically since they represent a mathematical combination of several physiological and physical parameters ...". For example, under non-irradiation-limiting conditions, parameter p_1 is a function of 10 variables and p_3 is a function of four. The author's then assert, however, that "...the given derivation demonstrates that an exponential form of the regression model should be appropriate for describing the evolution of *c(t)* over time ...".

  In actuality, the derivation noted is based on solving a differential equation founded on assumptions. For example, Equation (3) which describes CO_2 efflux from soil, $F_{Soil}(t)$, is only an approximation for it assumes that Fick's Law is valid both before AND after chamber deployment. This assumption necessarily leads to an exponential model based on the hypothesis that the rate of change of concentration in the chamber headspace is proportional to the existing concentration. The validity of this assumption, however, has not been tested. In contrast, we note that the NDFE model recently proposed by *Livingston et al.* (2006) gets around this issue by matching boundary conditions at the air-soil interface before and after chamber deployment. The time-dependent diffusion model advanced by these authors therefore provides a physical argument that mathematically relates trace gas flux before chamber deployment to the parameters of the fitted model after chamber deployment. The physical argument is that the flux is proportional to the *concentration gradient* that is continuous through chamber deployment. Diffusion is necessary to relate mass transport (dm/dt) prior to chamber deployment (when dc/dt = 0 at the soil-air interface in the steady state) to mass transport after chamber deployment (when dc/dt $\neq$ 0 in the chamber).

The verdict on which model is more applicable should hinge on which one makes physical sense. If in nature, the source gas is continuously produced in the soil beneath the chamber and chamber deployment is executed to ensure a 1-dimensional system, then the resultant concentration gradient between the soil and the air in the chamber headspace should continuously drive the gas into the chamber as predicted by the NDFE model. The exponential model, in contrast, predicts that the chamber headspace concentration will asymptotically approach a saturation value.

Whichever model the authors choose, they need to justify their decision on *physical grounds* by presenting both theoretical and experimental justification. Outlined below is a suggested analysis using the author's extensive data that perhaps would allow evaluation of the competing models.

- The authors note that over parameterisation of the exponential model with respect to the number of *c(t)* observations in a typical deployment is a concern. To address the parameter dependency issue, the authors state that a Taylor power series expansion is "more stable and resistant against over parameterisation." We find the use of the power series to 17^{th} order disturbing. After all, digital computers determine the values of exponentials by summing the appropriate power series until a convergence criterion is met. Therefore, it is not clear what the authors achieve by doing the summation explicitly other than modifying the mathematical model. Although they present theoretical considerations that result in an exponential model, they end up using a hybrid function with a quadratic polynomial for the first three terms and an exponential "tail" for the rest. The key issues here are (a) why is this necessary, and (b) what does this imply about the underlying biophysical processes. If Nature does not demand an exponential model, then a different mathematical model is required; if Nature indeed demands an exponential, then the authors need to employ a fitting procedure that uses a true exponential as the mathematical model.

- The current analysis does not take full advantage of the tremendous data set (1764 chamber experiments) the authors collectively have at hand. As such, the current analysis does not address the validity of the underlying model components, i.e.

$$F_{net}(t) = F_{Soil}(t) + F_P(t) + F_R(t) + F_{Leak}(t)\ .$$

The question arises, therefore, whether the author's purpose would be better served by blocking (grouping) the data to evaluate the individual model components in a stepwise-like approach. This could be accomplished in effect by blocking the data on the basis of whether the surface was vegetated or not, whether photosynthesis was occurring or not, i.e. light vs. dark, and whether or not it can be assumed leakage $\rightarrow 0$ thus justifying modeling soil gas transport as a one-dimensional process. The latter could be readily assumed when the underlying peat/soil at the depth the chamber walls were inserted to was waterlogged. The authors, of course, must address whether there would be sufficient numbers of observations to make this approach feasible. If so, however, subsequent analyses could be focused to address each model component sequentially using the methodology outlined in the manuscript. For example, using only data for non-vegetated, waterlogged surfaces, the component model of CO_2 efflux from the soil ($F_{Soil}(t)$) could be addressed without being confounded by photosynthesis or leakage. Subsequent analysis of vegetated, dark and waterlogged blocked data could then focus on above-ground respiration ($F_{Soil}(t) + F_R(t)$), and so on. In this way, the performance of the individual components added individually or sequentially could be evaluated experimentally. The final analysis addressing all of the data is what is presented in the current manuscript.

Experimental evaluation of both the exponential and NDFE models is needed to assess which is most applicable to observed soil emissions. The residual evaluations outlined in the manuscript are appropriate for this purpose. It must be recognized, however, that when observed chamber concentration vs. time curves are nearly linear, the exponential and NDFE models are expected to yield very similar flux estimates. In contrast, the more nonlinear the curves, the more the respective estimates will diverge.

- The authors need to superimpose theoretical calculations with experimental data on the same plot to illustrate representative data and model fitting results. A table listing the fitted parameters for these plots is also needed.

- p. 3, paragraph beginning: "The closed chamber method ...". The authors list several potential sources of error in chamber-based flux density measurements, including: "(3.) suppression of the natural pressure fluctuations ...". We assume the authors are referring to fluctuations driven by barometric change or wind driven turbulence that can be communicated to the chamber headspace via an appropriately designed vent. Disturbance of pressure gradients across interface boundaries must also be avoided. Pressure disturbances across the soil-atmosphere interface can readily be induced, for example, by a poorly balanced circulating system or, particularly on waterlogged or low density soils, during initial chamber deployment or by the weight of the investigator compressing nearby soils. Given the susceptibility of chamber measurements from northern peatlands to such effects and because there is no reference in the present manuscript to precautions to minimize such error, such as the use of walkways, their potential impact on observed chamber concentrations must be considered.

- p. 5, paragraphs 1, 3: We agree with the statement (para. 3) that “leaks” either through the chamber components or through the underlying pore space “should be avoided” but are concerned that the authors have chosen to model this process on the argument that some loss “cannot be ruled out completely”. In fact, as was demonstrated by *Hutchinson and Livingston* (2001) and *Livingston et al.* (2006), even relatively small “leaks” can significantly impact the accuracy of resultant flux estimates when emissions into the chamber headspace are modeled as a one-dimensional process. Alternatively, lack of fit of a one-dimensional emissions model to observed chamber concentrations could greatly aid investigators in quality controlling observations compromised by leaks or by not sufficiently inserting the chamber walls into the substrate.

- p. 12, paragraph beginning: "The parameters *b* and *c* of the . . ." We suggest the authors add compression, and thus pressure perturbation of the soil pore space, to the list of potential violations of the basic assumptions of the theoretical model. Perhaps more readily than the factors already listed, such disturbance can lead to concentration vs. time curves (concave upwards) not explainable by the theoretical model.

- p. 23, paragraph beginning: “Modelling of the CO_2 . . . ”. Again, although the authors argue that the disturbing effects of altering turbulence within the chamber may result in fitted *c(t)* curves that do not conform to the proposed theoretical model, we strongly suggest that compression of nearby soils by the weight of one or more investigators be given serious consideration. Peats and organic-rich soils are highly susceptible to compression, particularly when waterlogged. We also urge the investigators to expand their discussion on the costs and benefits of introducing quality control measures based on the use of a theoretical model as a reference and to note how this may alter interpretation of net ecosystem exchange measurements. The fitting of observed chamber concentrations to biophysical models offers at least two major advantages over past approaches: (1) the ability to quality control observations and thus improve protocols, and (2) improved accuracy and lower uncertainty in resultant flux estimates.

- p. 23, paragraph beginning: “Even if the curvature . . . ”. “If the residual analyses show that the observed *c(t)* curve is nonlinear, then a nonlinear model should be favoured over the linear model even if the curvature is not explained by the theoretical model. ”

  We strongly recommend reconsideration/rewording of this conclusion. An appropriate biophysical model, however limited, offers far more value for data quality control, protocol development, and data interpretation than any empirical model. The theoretical and empirical evidence against the use of a linear model is rapidly building. Its continued application should be emphatically discouraged with only a few limited exceptions. An appropriate non-linear model, in turn, should adapt to experimental situations which yield nearly linear *c(t)* responses. Investigators should not arbitrarily apply one model or another based on the appearance of the data, but adopt and justify a specific (biophysical) model for all analyses. Because the factors controlling linearity in the *c(t)* response are, in part, experimentally determined (chamber height, deployment time), enhancement of the non-linear response should also be encouraged to improve the precision of non-linear regression parameter estimates. Additionally, the choice of which non-linear model to employ should ideally hinge on which model best represents the biological and physical processes regulating chamber headspace concentrations.

- p. 24, paragraph beginning: “The measurement interval length . . . ”. “The measurement interval length, the number of measurement points and the precision of the CO_2 concentration measurements determine whether the nonlinearity can be detected with sufficient statistical significance. ”

We fully agree but also strongly recommend that chamber heights be limited and deployment periods extended as is warranted to emphasize non-linearity in the *c(t)* response and improve the precision of resultant parameter estimates.

- p. 27, Conclusions. The developed exponential model is well suited for nonlinear regression of the *c(t)* evolution in the chamber headspace and estimation of the initial CO_2 fluxes at closure time for the majority of experiments.

  The question of whether or not the exponential model is most applicable was addressed above. We question here the apparent generalization of a conclusion to *all* experiments. Perhaps a rewording to the effect: the assumptions inherent in the proposed model fit the majority of the observations examined in this investigation, thus suggesting the potential value of biophysical models in future chamber-based emissions studies.

Technical corrections

Note text in **bold** represents suggested text or, in the least, sentences requiring reconsideration.

p. 3, paragraph beginning: "The closed chamber method . . . "

- "(5.) leakage directly at the chamber components or via the **underlying** soil pore space, and (6.) the concentration build-up or reduction **within** the chamber headspace that inherently disturbs the underlying **concentration gradient that was in effect prior to chamber deployment.** "
  (Cite references as needed.)

p. 4, paragraph continued from p.3:

- Thus, for assessing the CO_2 flux, **the rate of initial concentration change at the moment of deployment ($t = t_0 = 0$) should be used when the alteration of**

the headspace air is minimal, rather than the mean rate of the CO_2 concentration change over the chamber closure period (*Livingston and Hutchinson* 1995).

- Most of the recent studies . . . for estimating CO_2 fluxes

  p. 17, paragraph beginning: " summary of . . . "

- Thus, regression curves with curvatures not explainable by the developed theoretical model were **also** included.

- However, a substantial **fraction** (20% to 40%) of the **fitted** curves showed curvatures which **did** not conform **to** the theoretical model. (Given such a large proportion of observations did not meet expectations, a figure showing one or more "unexplainable" curves would be of value.)

  p. 19, paragraph beginning: "The F-test . . . "

- Furthermore, the residual variance of the exponential regression was **only** significantly smaller than the residual variance of the quadratic regression in less than 1 % of the experiments of all datasets (data not shown).

  p. 23, paragraph beginning: "Modeling of the CO_2 . . . "

- Original: Apparently, these assumptions were not valid for all experiments: Although the observed nonlinearity conformed with the theoretical exponential model for the majority of experiments, also significantly nonlinear *c(t)* curves were observed whose curvature was not explainable with the theoretical model. These unexplainable curvatures are considered to have been caused by violations of the basic assumptions of the theoretical model.

  Suggestion: Apparently, however, these assumptions were not valid for all experiments. Whereas the majority of fitted *c(t)* curves were consistent with the proposed theoretical model, a substantial fraction of the experiments were not.

These unexplainable curvatures are considered to have been caused by violations of the basic assumptions of the theoretical model.

p. 24, paragraph beginning: “For the evaluation . . . ”

- **To evaluate** the validity of **candidate** models, we recommend **the use of** residual analysis including tests for autocorrelation and normality.

  p. 24, paragraph beginning: “We note that . . . ”

- In extreme cases, the r^2 values were calculated for only three data points and were considered as **evidence of** linearity when greater than typically 0.95.

  p. 24, paragraph beginning: “The measurement interval length . . . ”

- It has to be stressed that strong nonlinearity can be present **even when** it **cannot** be detected **because of** long measurement intervals, few data points or low measurement precision.

  p. 25, paragraph beginning: “Considering the results . . . ”

- We suggest reorganizing entries to better group related recommendations.

- Considering the results of this study, a list of practical recommendations for closed chamber measurements **follows**:

  Original: “Nonlinear regression should be favoured over linear regression to fit the data and to estimate the initial slopes of the *c(t)* curves. ”

  Suggestion: A nonlinear model should be favoured over a linear model to reflect the various biophysical process in effect and thus to better estimate the flux.

- For closure times of two to ten minutes . . . (see comments above regarding this issue)

- The slope of the *c(t)* evolution curve is changing most pronouncedly at the start of the chamber closure time. Consequently, the interval length of discarding data at the beginning to avoid disturbances is critical and should not be too long.

  Clarification is needed. We assume the reference to discarding data refers to the need in using IRGA systems to purge residual gases in the lines accumulated prior to chamber deployment. Sufficient explanation is needed here to provide context.

- The better the measurement precision and the more data points are available for the regression, the better the nonlinearity can be detected and its significance **demonstrated**.

- Original: When adopting the nonlinear approach, closure times can be longer, headspaces can have smaller volumes, and leaks through the chamber or the soil are less critical compared to the linear regression approach, for which all experiment conditions must be optimised with regard to the best possible approximate linearity (short closure times, large headspace volumes, no leaks).

  Suggestion: 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.

  It is noted that "leaks . . . are less critical" for non-linear models than for a linear model. We know of no evidence to support this statement. The authors need to justify their statement or remove it. Additionally, in view of theoretical considerations (e.g. *Livingston et al.* 2006) it is evident that linearity in *c(t)* data will occur in application primarily only under conditions in which soil gas diffusion is much slower than in air, for example in waterlogged soils where the soil air porosity $\rightarrow 0$. Application of a linear model, therefore, would appear inappropriate unless the specific application justifies its use. Inability to detect non-linearity does not imply that it is unimportant as the authors themselves note. Do not loose the focus noted in the title of this manuscript.

- Changing light, temperature and humidity conditions during chamber closure are less critical when applying nonlinear regression compared to the use of linear regression as long as these changes are continuous and can be accounted for by relatively simple nonlinear functions. However, wind speed and turbulence in the chamber should be as similar as possible to the ambient conditions since abrupt turbulence changes **may impact transport processes and thus compromise** the assumption that the initial slope of *c(t)* is the best estimator of the undisturbed CO_2 flux before chamber closure (*Hutchinson et al.* 2000).

  What evidence is there to support the initial statement or is this speculation? Should *Hutchinson and Livingston* (2001) also be cited to support the second assertion?

  p. 25, paragraph beginning: “The underestimation effect . . . ”

- Thus, the underestimation of CO_2 fluxes by linear regression method not only disturbs the quantitative but also qualitative **evaluations** since differences between sites with strong and weak CO_2 exchange would be smoothed.

- Here, the uneven underestimation bias between sites can lead to the conclusion **that** CO_2 fluxes **differ greatly** between sites although, in fact, only the response to the chamber disturbance on **of soil gas** diffusion and **plant** physiology differs.

  p. 27, Conclusions:

- However, the curvature of the nonlinear *c(t)* curves is for a substantial percentage of the experiments not explainable with the **proposed** theoretical model. This is considered to be caused by violations of the basic assumptions of the theoretical model. In particular, the change of turbulence conditions by setting a closed

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chamber on the ecosystem should be investigated in more detail in the future. (see comments regarding pressure disturbance due to soil compression)

p. 28:

- “We developed a MATLAB routine . . . ” **A URL should be required prior to publication.**

p. 41, Table 3:

- Significance of deviations between the slope **estimates at *t* = 0 as yielded** by the exponential $f'_{exp}(t_0)$ and linear regression **models** $f'_{lin}(t_0)$.
- The null hypothesis H_0 states that the absolute value of the initial slope of the exponential regression is equal to **the absolute** value of the initial slope of the linear regression.

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