



Short communication

# Improved parameterization of the commonly used exponential equation for calculating soil-atmosphere exchange fluxes from closed-chamber measurements



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## ABSTRACT

The concentration change in a closed chamber derived from Fick's law for a steady flux leads to a differential equation which describes an exponential curve of limited growth. Here we introduce and compare an alternative parameterization with those commonly used in the chamber flux community when investigating soil-atmosphere exchange of N<sub>2</sub>O, CH<sub>4</sub>, or CO<sub>2</sub> using classical gas chromatography systems, infrared gas analyzers, or novel laser absorption spectrometers. This new parameterization has the advantages that the parameters are mathematically less dependent leading to a more stable regression and that all parameters are physically meaningful with one of them being the main quantity of interest, i.e. the initial flux at chamber closure.

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## 1. Introduction

Investigating the exchange of trace gases such as N<sub>2</sub>O, CH<sub>4</sub>, and CO<sub>2</sub> between soil and atmosphere has been in the focus of climatological and biogeochemical research for decades. Closed chamber measurements are the preferred method when studying the effects of different land use types or soil treatments on exchange fluxes over a variety of ecosystems at plot scale. While air samples of N<sub>2</sub>O and CH<sub>4</sub> were commonly analyzed by lab- or field-deployed gas chromatography systems (e.g. Brümmer et al., 2009; Castaldi et al., 2010; Christensen, 1983; Dannemann et al., 2006; Jassal et al., 2011; Livesley et al., 2011; Lohila et al., 2010; Pihlatie et al., 2013; Rosenkranz, 2006), more recent studies demonstrate the applicability of laser absorption spectrometers for all kinds of trace gases including N<sub>2</sub>O, CH<sub>4</sub>, and CO<sub>2</sub> (e.g. Brümmer et al., 2017; Cowan et al., 2014; Savage et al., 2014; Shurpali et al., 2016) with high temporal resolution.

There are different approaches to determine the soil-atmosphere flux from the change in gas concentration inside a closed chamber. While linear regression has been applied in many studies (e.g. Alm et al., 1997; Drösler, 2005; Laine et al., 2006), others have demonstrated the need for non-linear models (e.g.

Forbrich et al., 2010; Hutchinson and Mosier, 1981; Livingston et al., 2006; Pedersen et al., 2010; Pihlatie et al., 2013). Applying molecular diffusion theory for fluxes from the soil into the chamber with the simplification of a constant source concentration leads to a differential equation describing an exponential curve of limited growth (e.g. Hutchinson and Mosier, 1981; Nakano et al., 2004). More advanced non-linear models also account for chamber induced concentration changes in the soil (e.g. Conen and Smith, 2000; Livingston et al., 2005, 2006), altered atmospheric turbulence (Lai et al., 2012), or for chamber leakages (Kutzbach et al., 2007).

In this paper, we explore the differential equation for limited growth in more detail. This differential equation for the saturating gas concentration inside a closed chamber has multiple solutions, i.e. parameterizations. For the choice of the parameterization, it is usually advisable to have parameters that are physically meaningful and as independent from each other as possible. Here, we compare three parameter sets that have already been widely applied in environmental science with a new alternative set suggested in this study. This new parameterization has been used before in other fields of ecophysiology, for example for fitting light response curves (Falge et al., 2001; Moffat, 2012). A step-by-step derivation of all four parameterizations discloses differences in parameter meanings. To investigate the dependencies among each other, the method of bootstrapping will be applied to datasets of N<sub>2</sub>O, CH<sub>4</sub>, and CO<sub>2</sub>.

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**Table 1**  
List of variables.

Variable	Unit	Description
$t$	s	Time
$t_0$	s	Time of initial chamber closure
$t_\infty$	s	Time at infinity
$F(t)$	$\text{g m}^{-2} \text{s}^{-1}$	Flux (gas exchange rate) at time $t$
$F_0$	$\text{g m}^{-2} \text{s}^{-1}$	Initial flux
$C(t)$	$\text{g m}^{-3}$	Gas concentration inside chamber at time $t$
$C_S(t)$	$\text{g m}^{-3}$	Gas concentration at soil surface at time $t$
$C_d$	$\text{g m}^{-3}$	Constant source concentration
$C_0$	$\text{g m}^{-3}$	Initial gas concentration
$C_\infty$	$\text{g m}^{-3}$	Gas concentration at infinite time
$C_\ddagger$	$\text{g m}^{-3}$	Gas concentration range ( $C_\ddagger = C_\infty - C_0$ )
$z$	m	Vertical length
$z_d$	m	(Unknown) depth with constant $C_d$
$h$	m	Effective chamber height
$D$	$\text{m}^2 \text{s}^{-1}$	Gas diffusivity in the soil
$A$	$\text{g m}^{-3}$	Integration constant
$k$	$\text{s}^{-1}$	Exponential decay rate

## 2. Physical background

The gas exchange rate, flux  $F(t)$ , inside a closed-chamber is:

$$F(t) = h \frac{\partial C(t)}{\partial t} \quad (1)$$

where  $h$  is the effective chamber height and  $C(t)$  the gas concentration at time  $t$  inside the chamber. (All variables including their units are listed in Table 1).

The diffusion from the soil into the chamber can be described by Fick's law for the vertical gradient of the gas concentration:

$$F = -D \frac{\partial C}{\partial z} \quad (2)$$

where  $D$  is the gas diffusivity in the soil and  $z$  the vertical length. Considering a soil column with a gas concentration  $C_S(t)$  at the soil surface and with the simplification of a constant source concentration  $C_d$  at some unknown depth  $z_d$ , we can derive  $F(t)$  for a steady flux into the chamber:

$$F(t) = -D \frac{C_S(t) - C_d}{z_d} \quad (3)$$

Combining Eqs. (1) and (3) and assuming that the gas concentration inside the chamber  $C(t)$  is equal to the surface concentration  $C_S(t)$  leads to:

$$h \frac{\partial C(t)}{\partial t} = -D \frac{C(t) - C_d}{z_d} \quad (4)$$

Rearranging Eq. (4) yields the following differential equation with  $k = \frac{D}{hz_d}$ :

$$\frac{\partial C(t)}{C(t) - C_d} = -\frac{D}{hz_d} \partial t = -k \partial t \quad (5)$$

This differential equation describes the change of the gas concentration inside a closed chamber.

## 3. Derivation of the parameterizations

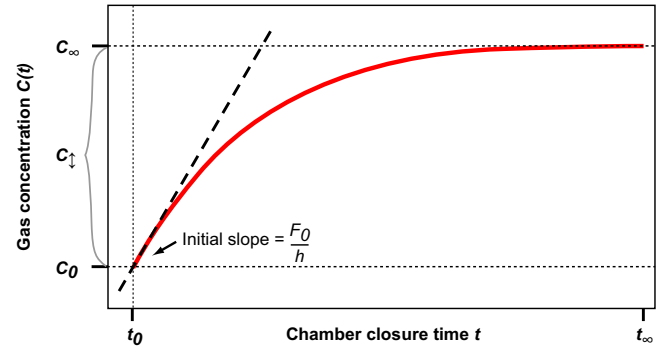
Integrating the differential Eq. (5) yields an exponential equation of limited growth:

$$C(t) - C_d = A \cdot e^{-kt} \quad (6)$$

where  $A$  is an integration constant and  $k$  the exponential decay rate.

Hence, the solution of the differential equation Eq. (5) is a saturating exponential curve:

$$C(t) = A \cdot e^{-kt} + C_d \quad (7)$$



**Fig. 1.** Sketch of the exponential curve for saturating gas concentrations (red line). For a description of the variables see Table 1.

with three parameters  $A$ ,  $C_d$ , and  $k$  which can be parameterized in different ways. In the following, all four presented parameterizations will be derived explicitly, with an overview provided in Table 2.

The parameters  $A$ ,  $k$ , and  $C_d$  of Eq. (7) can be defined using the three boundary conditions (see also Fig. 1). The 1st boundary condition is the initial concentration  $C_0$  at chamber closure  $t=0$ :

$$C(t=0) = C_0 = A + C_d \quad (8)$$

and 2nd boundary condition the concentration  $C_\infty$  at infinite time:

$$C(t=\infty) = C_\infty = C_d \quad (9)$$

Applying Fick's law, leads to the 3rd boundary condition, the initial flux  $F_0$  at  $t=0$ :

$$\left. \frac{\partial C(t)}{\partial t} \right|_{t=0} = \frac{F_0}{h} \quad (10)$$

which is the quantity of interest.

Replacing the parameters in Eq. (7) with boundary condition 1 (Eq. (8)) and 2 (Eq. (9)), yields parameterization I:

$$C(t) = C_\infty + (C_0 - C_\infty) \cdot e^{-kt} \quad (11)$$

Additionally substituting the range of the concentration as  $C_\ddagger = C_\infty - C_0$  leads to parameterization II:

$$C(t) = C_\ddagger(1 - e^{-kt}) + C_0 \quad (12)$$

Applying the 3rd boundary condition (Eq. (10)) to parameterization I (Eq. (11))

$$\left. \frac{\partial C(t)}{\partial t} \right|_{t=0} = -(C_0 - C_\infty)k = \frac{F_0}{h} \quad (13)$$

and substituting the rearranged Eq. (13) ( $C_0 - C_\infty$ ) =  $-\frac{F_0}{hk}$  in Eq. (11) yields parameterization III:

$$C(t) = C_\infty + \frac{F_0}{-hk} \cdot e^{-kt} \quad (14)$$

Applying the 3rd boundary condition (Eq. (10)) to parameterization II (Eq. (12)):

$$\left. \frac{\partial C(t)}{\partial t} \right|_{t=0} = C_\ddagger k = \frac{F_0}{h} \quad (15)$$

solving Eq. (15) for the decay rate  $k = \frac{F_0}{hC_\ddagger}$ , and substituting this in Eq. (12) yields the new alternative parameterization IV:

$$C(t) = C_\ddagger(1 - e^{-\frac{F_0}{hC_\ddagger}t}) + C_0 \quad (16)$$

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