# Testing Daisy's new approach to modelling $N_2O$ emissions

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**Daisy lunch**

UNIVERSITY OF COPENHAGEN

## Projects

*KlimaGødning* & SmartField Science Policy Practice

## Collaborators

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*Simon Fiil Svane (KU)*
*Lars Stoumann Jensen (KU)*

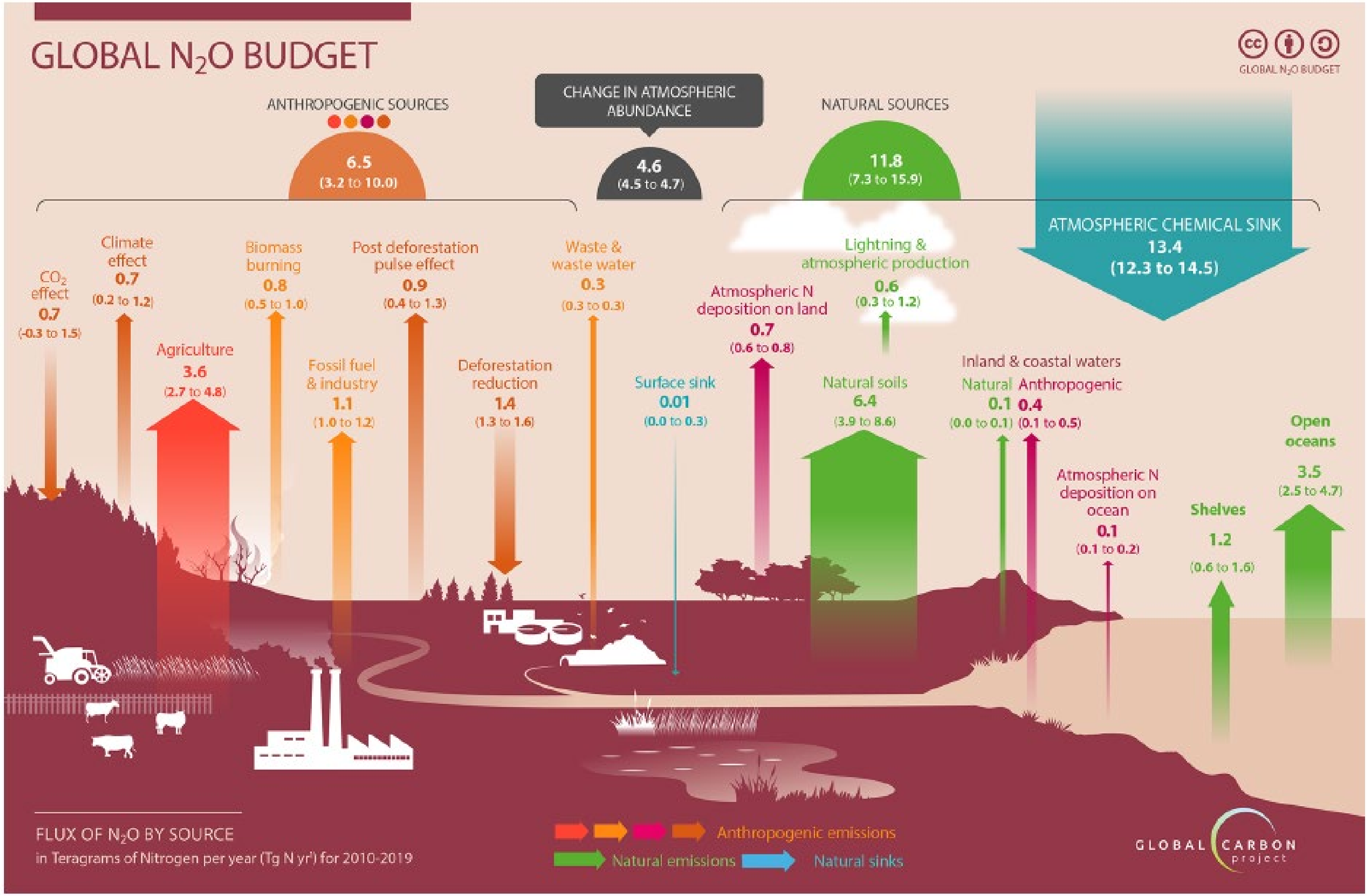
# Motivation

$N_2O$ is a **highly potent greenhouse gas** (265 $CO_2$ eqv.)

$N_2O$ contributes **7-8% to the effective anthropogenic radiative forcing**.

$N_2O$ is the dominant **ozone-depleting** substance.

~32 % of total anthropogenic $N_2O$ emissions come **directly from soils**.




Tian et al. (2020). *Nature;* Tian et al. (2024). *Earth Syst. Sci. Data*

# Why modelling $N_2O$ emissions is a challenge

- $N_2O$ is a **multisource gas** and created through different pathways, most of which are **microbial** (e.g., nitrification, denitrification).
- Each pathway is driven by several **different soil state variables** (e.g., soil moisture, soil temperature, soil organic matter), which are themselves affected by **environmental and anthropogenic drivers**.
- $N_2O$ is an **intermediate product** in the reaction chain of nitrification and denitrification, which makes it dependent of the kinetics of production, consumption and diffusion.

Li et al. (2000). *J. of Geophy. Res.*

# Specific aims (*KlimaGødning*)

1. Calibrate and test Daisy's **current $N_2O$ functions** in the context of different **environmental and soil (fertility) management settings**.

2. Implement and compare **other $N_2O$ models** in Daisy using Daisy's **Python interface**.

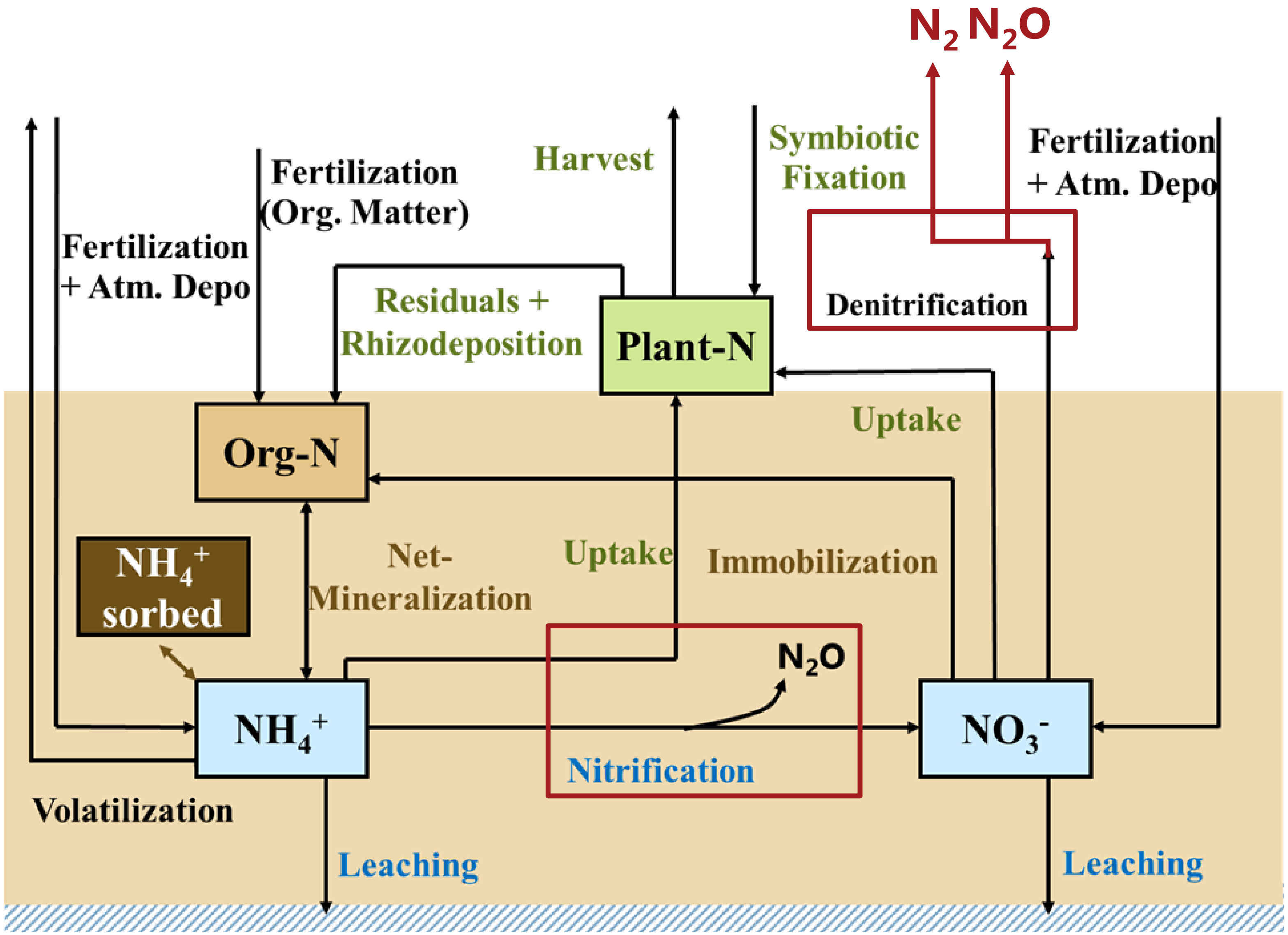
3. Test Daisy's ability to model **$N_2O$ emissions from organic hotspots**.

4. Develop and implement potential **improvements in describing $N_2O$ dynamics** in Daisy.

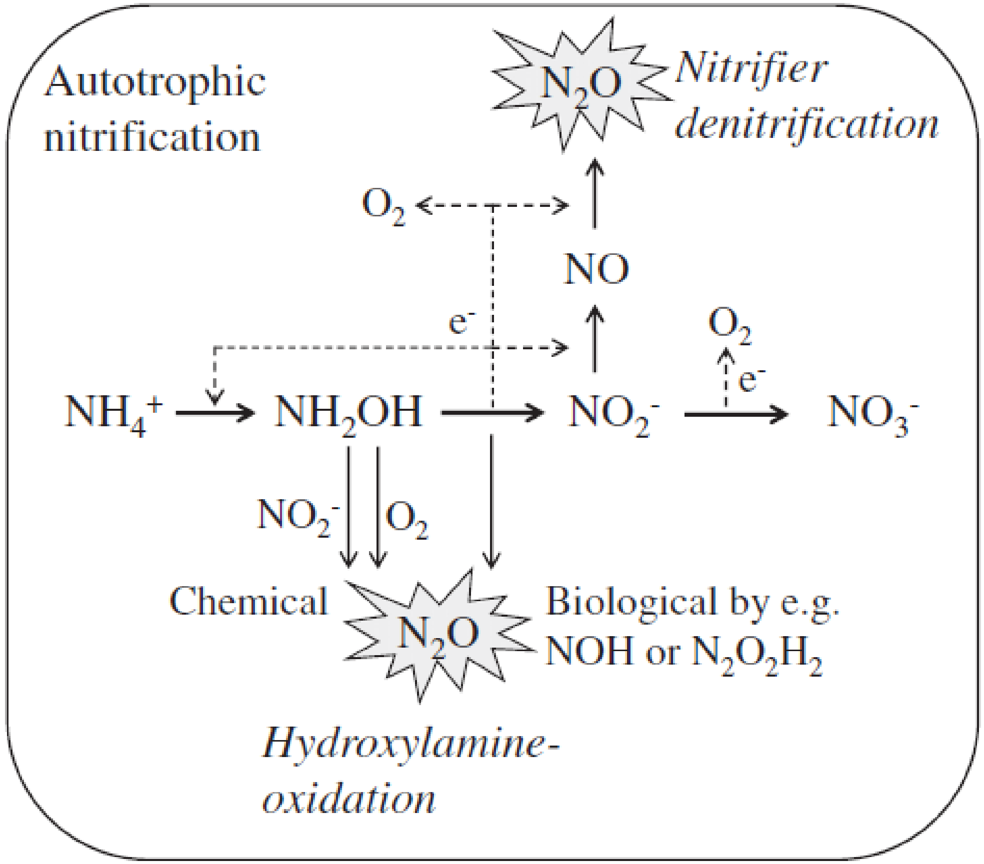
# PREDICTING $N_2O$ EMISSIONS WITH DAISY

## THE MODELLED PROCESSES

# Nitrogen cycling in Daisy



# $N_2O$ production from nitrification – a “leaky” pipe approach




Adapted from Wunderlin et al. (2012). *Water research*

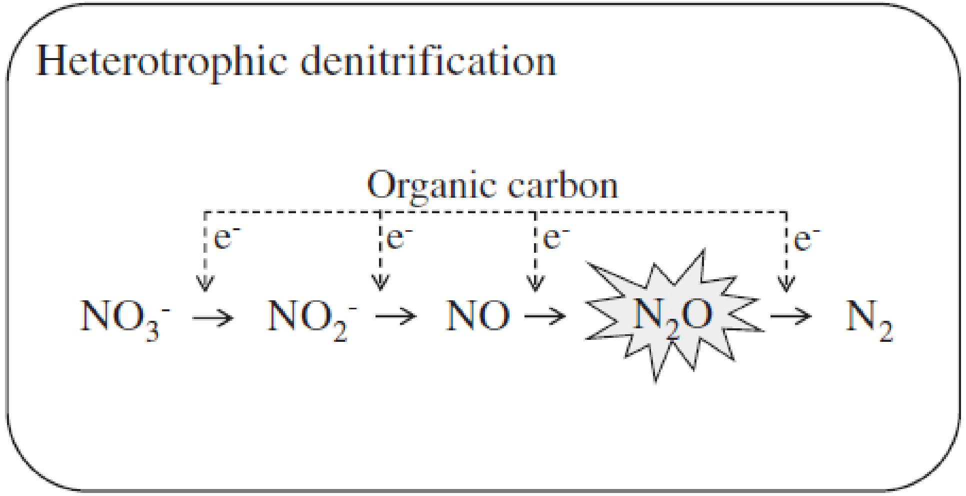
In Daisy, a **constant fraction ($K_n$)** of nitrified N is converted to $N_2O$:

$$N_2O_{nit} = K_n \cdot N_{nitrified}$$

→ default: $K_n$ **= 2%**

| $K_n$ [%] | Study |
|---|---|
| **[0.1; 0.2]** | Goodroad and Keeney (1984) |
| **[0.008; 0.053]** | Ingwersen et al. (1999) |
| **0.06** | Li et al. (2000) → *DNDC* model |
| **0.16** | Khalil et al. (2004) → *STICS* model |

# Potential denitrification in Daisy




Adapted from Wunderlin et al. (2012). *Water research*

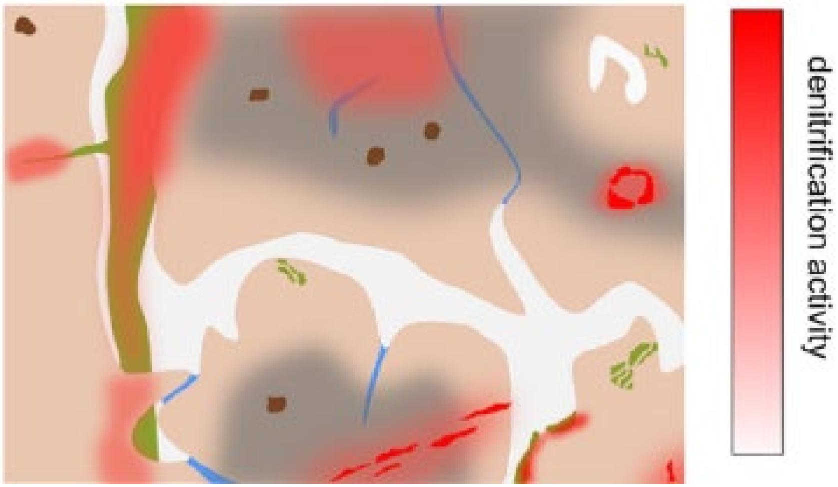
Calculating **potential denitrification** ($\xi_d^*$):

$$\xi_d^* = \xi_{CO_2} \cdot f^T(T) \cdot \alpha$$

**$\alpha$ :** proportionality factor [($N_2O$ + $N_2$)-N / $CO_2$-C respired]

→ can be defined **separately for fast and slow SOM pool**

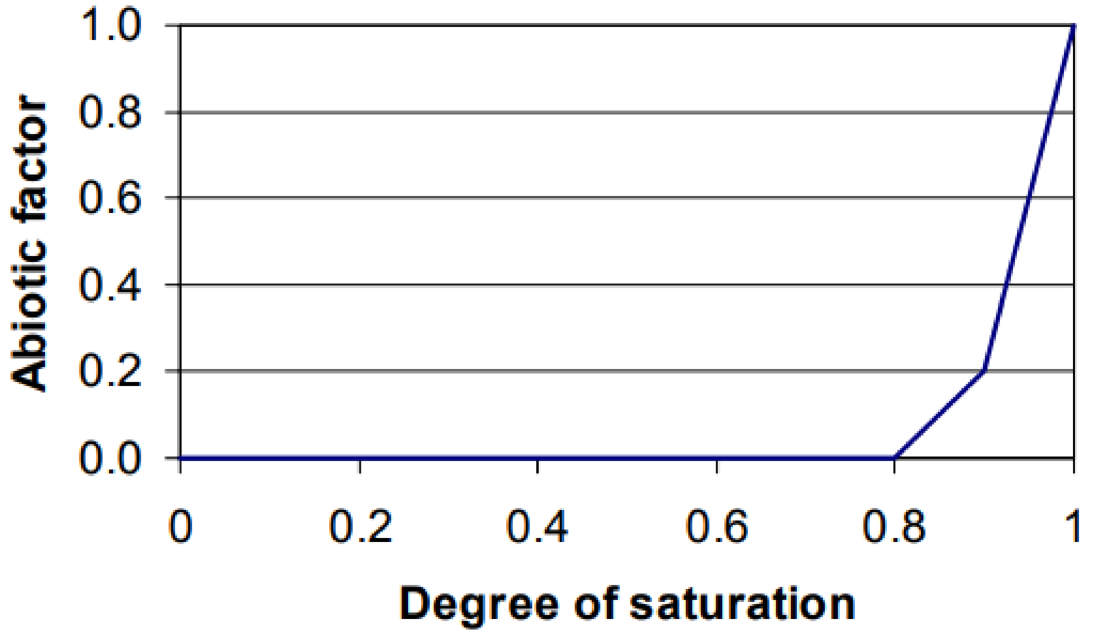
→ default: **0.1 g/g**




Schlüter et al. (2024). *Biol. Fert. of Soils*

| **Organic substrate** (experiment duration) | α | Study |
|---|---|---|
| **POM/MAOM** (2-24 h) | [**0.08; 0.45**] | Surey et al. (2021) |
| **Organic residues** (124 h) | **0.03** | Senbayram et al. (2012) |
| **Digestate manure** (21 d) | **0.03** | Petersen et al. (1996) |
| **Fresh manure** (21 d) | **0.15** | Petersen et al. (1996) |

# Actual denitrification in Daisy




Calculating **actual denitrification** ($\xi_d$):

$$\xi_d = min\{f^W(\theta) \cdot \xi_d^*, K_d \cdot N_{NO_3^-}\}$$

$\boldsymbol{K_d}$ : proportionality factor [$h^{-1}$]

→ default: **0.020833 $h^{-1}$**

**No nitrate function, only the proportionality factor $K_d$.**

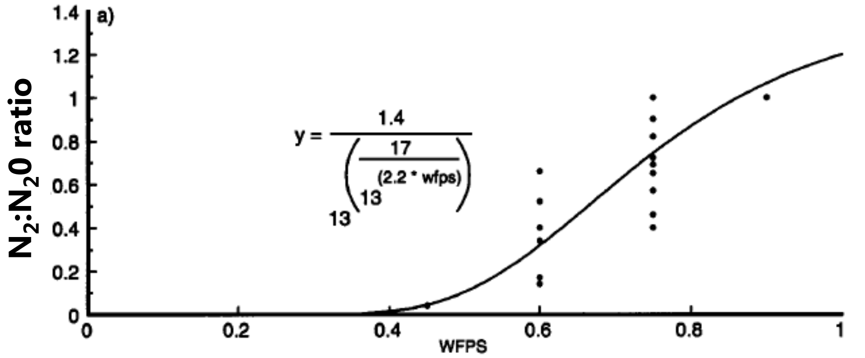
# **NEW (Daisy 7.0.0)** : from actual denitrification to $N_2O$ and $N_2$

**Generalized model for $N_2$ and $N_2O$ production from nitrification and denitrification**

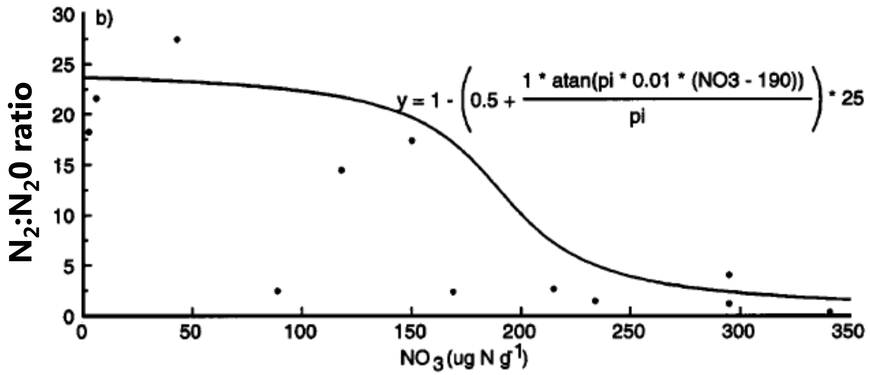
W. J. Parton,[1] A. R. Mosier,[2] D. S. Ojima,[1] D. W. Valentine,[1] D. S. Schimel,[3] K. Weier,[4] and A. E. Kulmala[5]

Actual denitrification is now split between **$N_2$ and $N_2O$** using the "**old" DayCent implementation** by Parton et al. (1996).

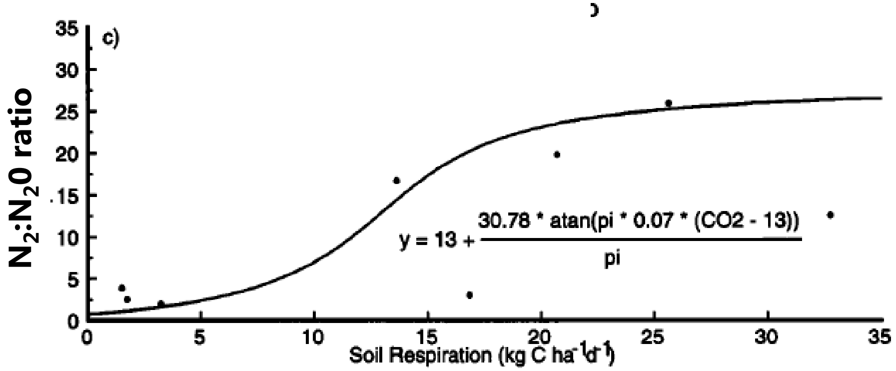
**WFPS :**




**$NO_3^-$ :**




**Respiration :**



# PREDICTING $N_2O$ EMISSIONS WITH DAISY

## A CASE STUDY – CALIBRATING DAISY

# Case study (project: “CatCap”)

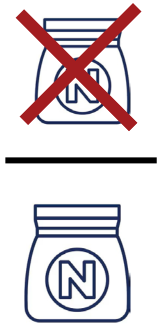
**Soil texture:** loamy sand (eastern Denmark)

**Simulation period:** August 2020 – June 2021 | August 2021 – June 2022

**Crop rotation:**

Calibration | Validation

1. Spring barley →  → fertilization → spring barley




75 kg N/ha

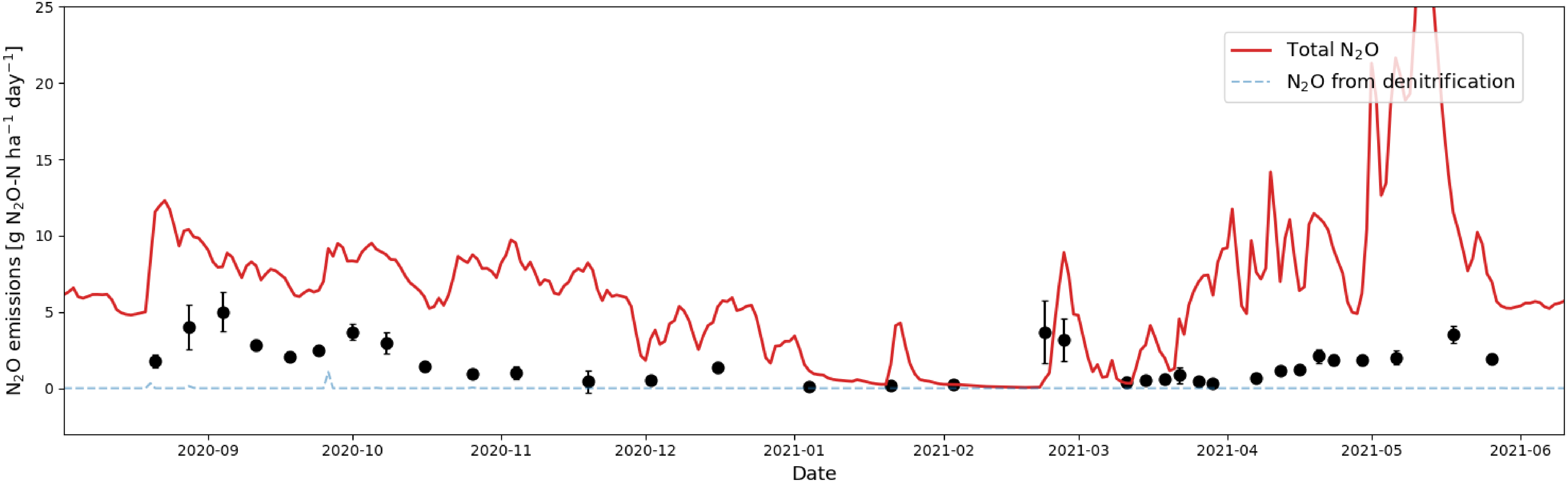
2. Spring barley →  * → fertilization → spring barley
3. Spring barley →  * → fertilization → spring barley

* created using AI

# Calibration – uncalibrated

+

**Bare soil**

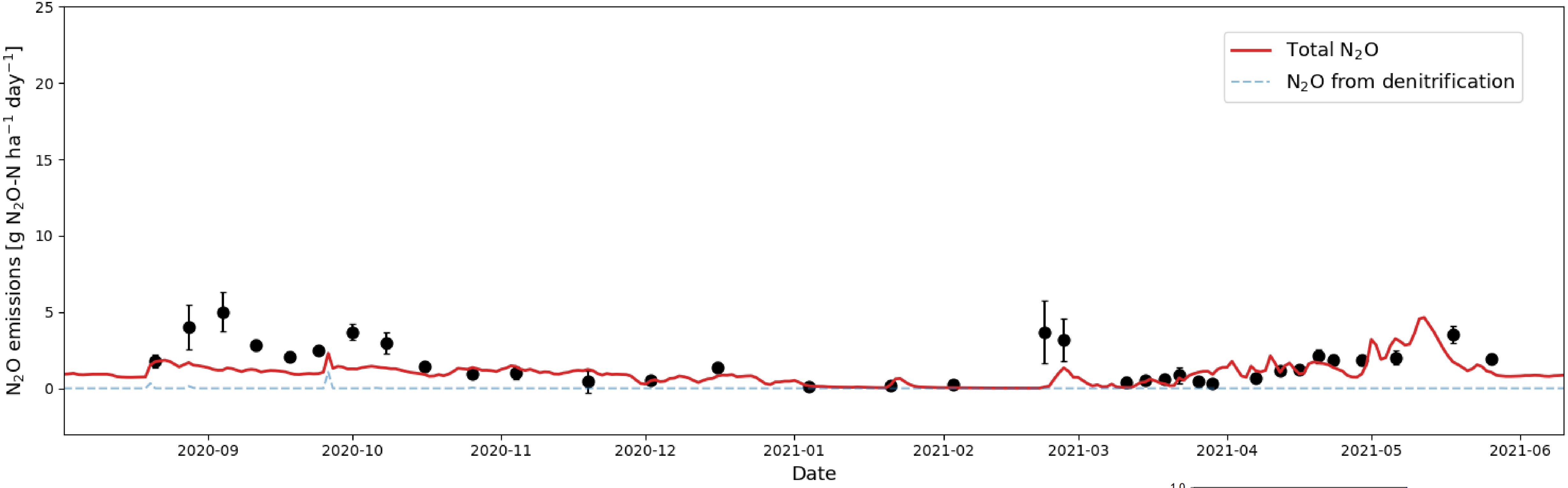



**Nitrification factor ($K_n$) was adjusted from 2% to 0.3%**

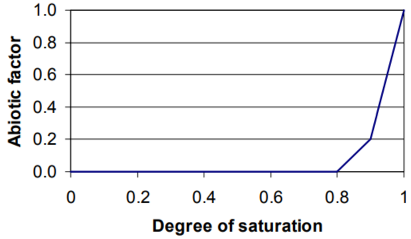
# Calibration – $N_2O$ from nitrification adjusted


+

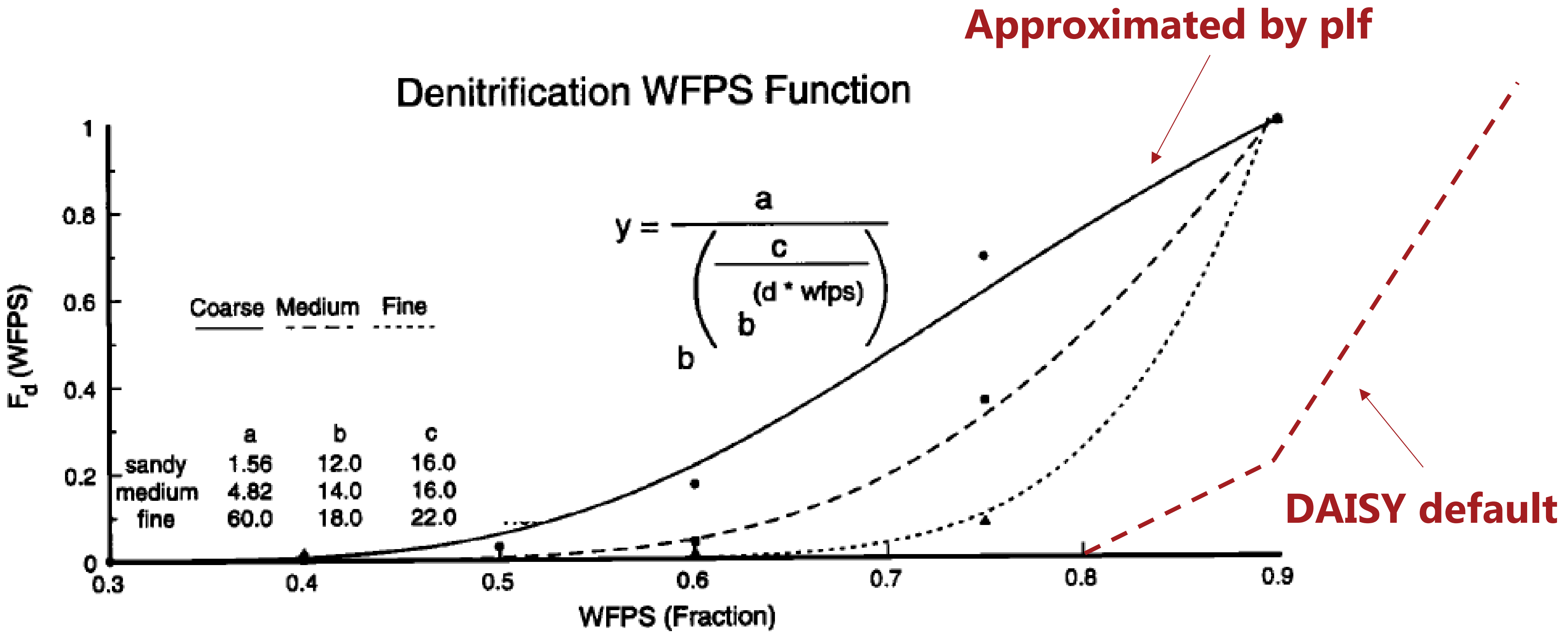

**Bare soil**




**Water-filled pore space function for denitrification was adjusted.**



# Calibration – implement water-filled pore space function by Parton et al. (1996)

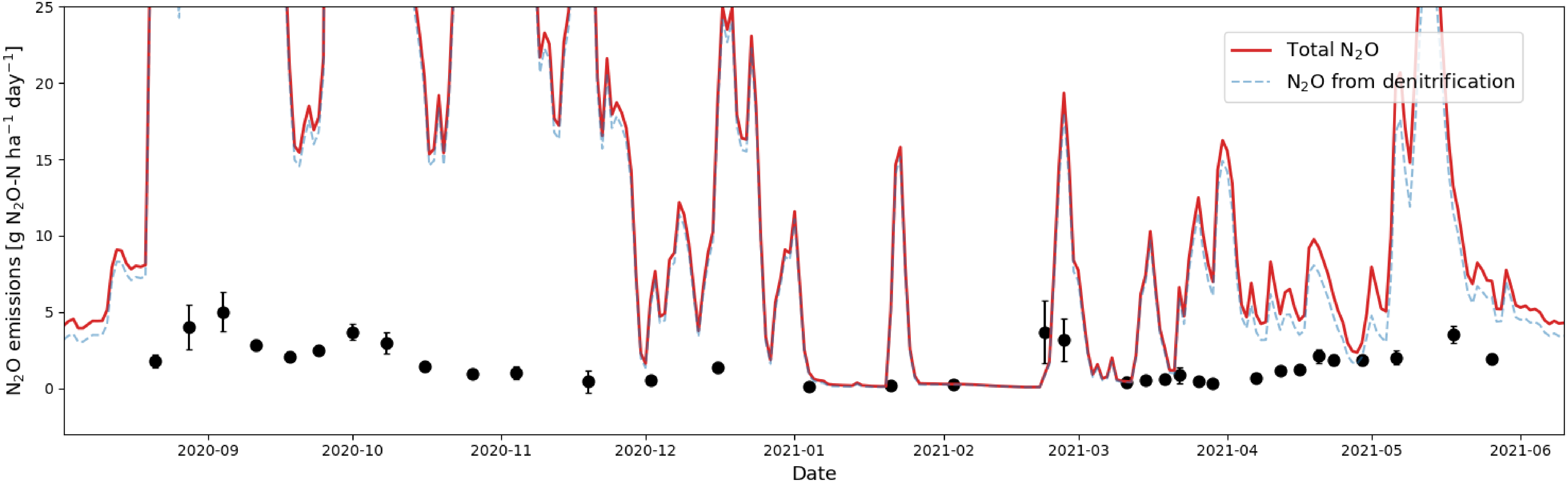



Parton et al. (1996). *Glob. Biogechem. cycles*

# Calibration – WFPS function adjusted


+

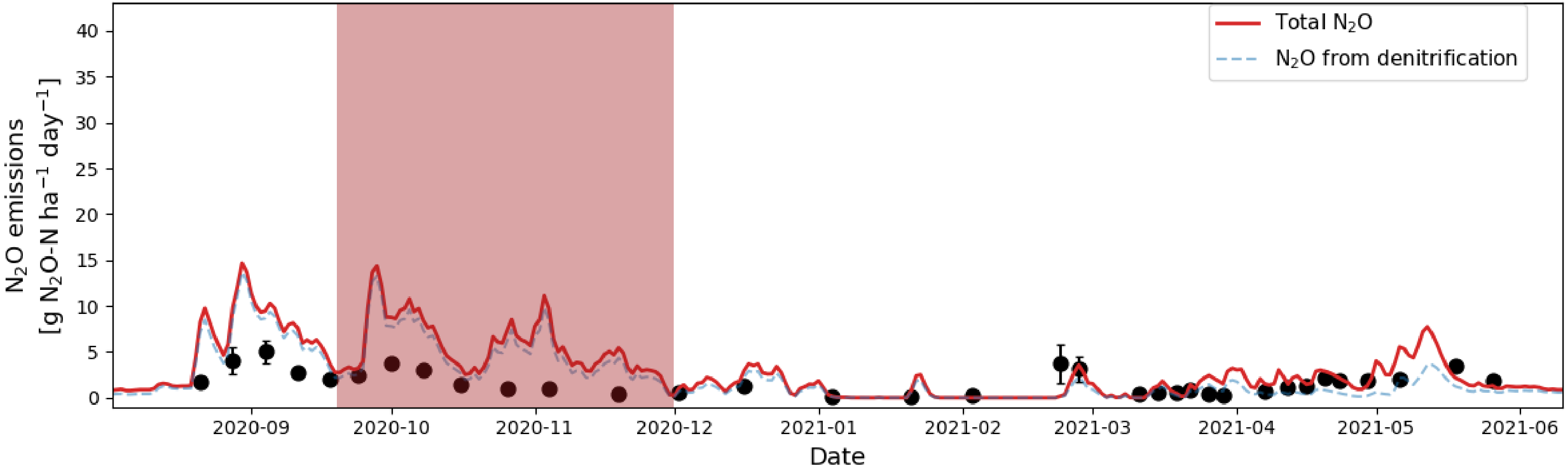

**Bare soil**

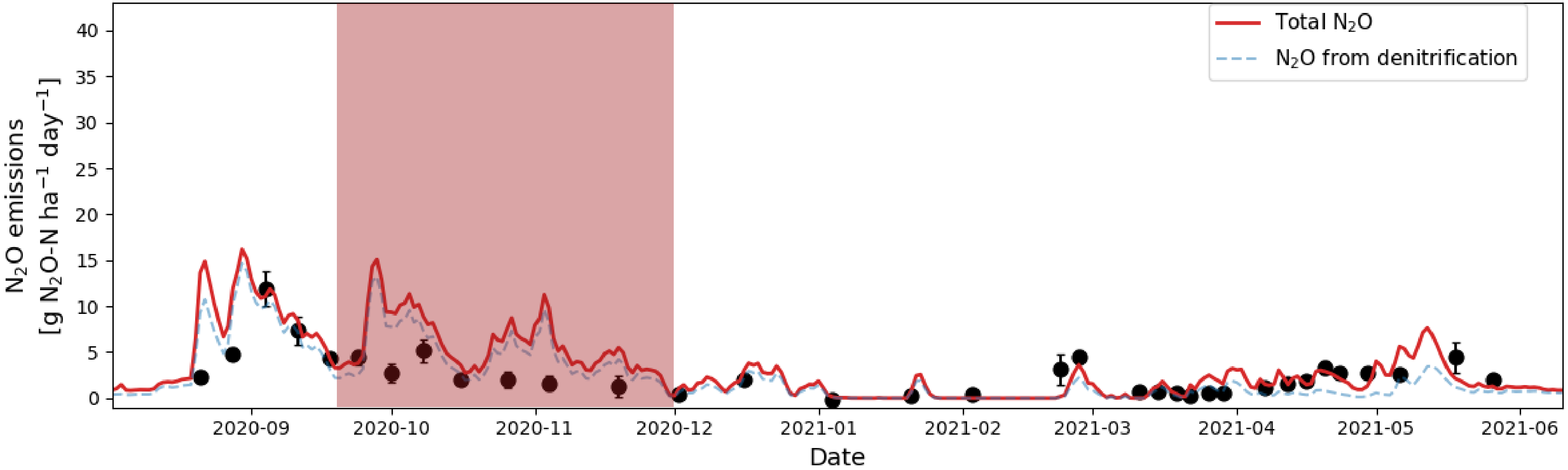



**Alpha value was adjusted from 0.1 to 0.016 (fast SOM pool) and 0.0001 (slow SOM pool).**

# Fully calibrated (bare soil)

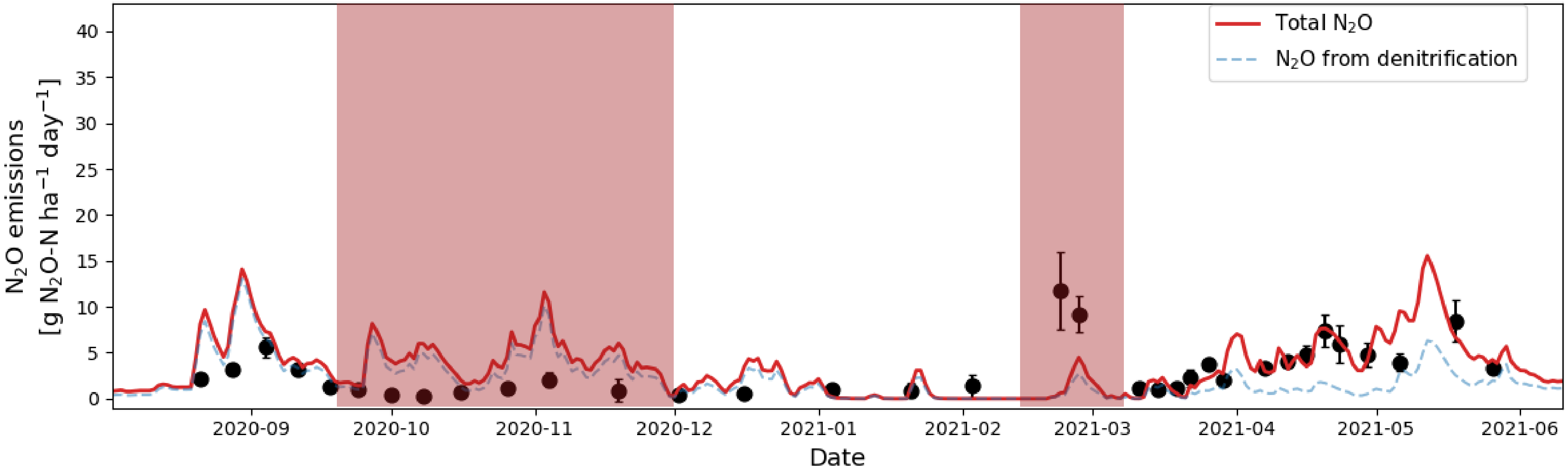
Bare soil

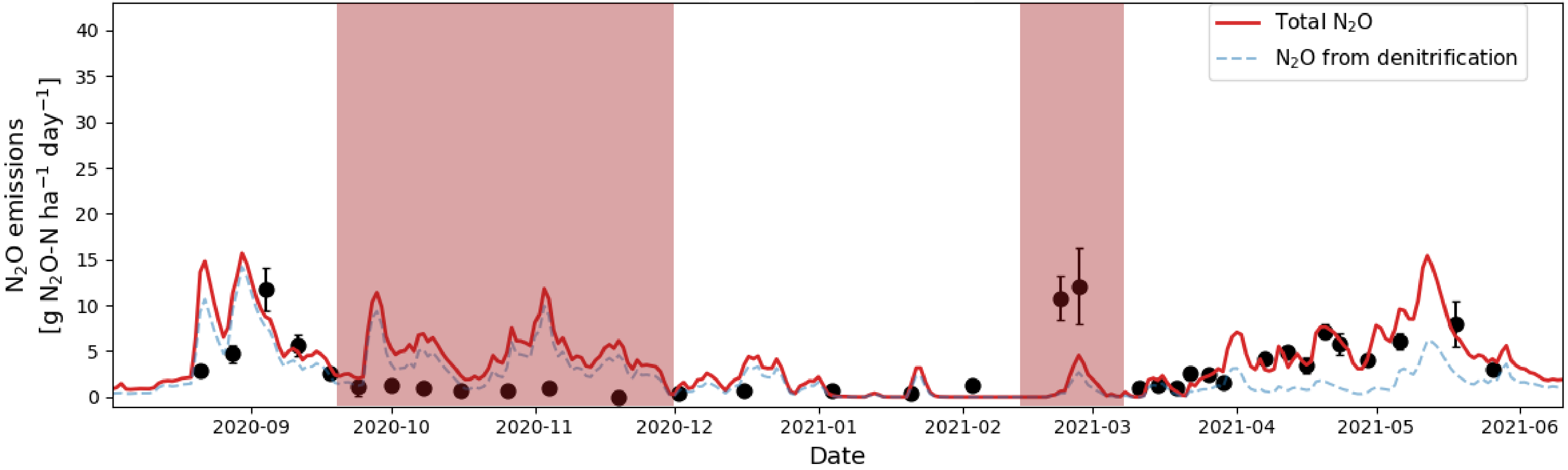


# Fully calibrated (hairy vetch)

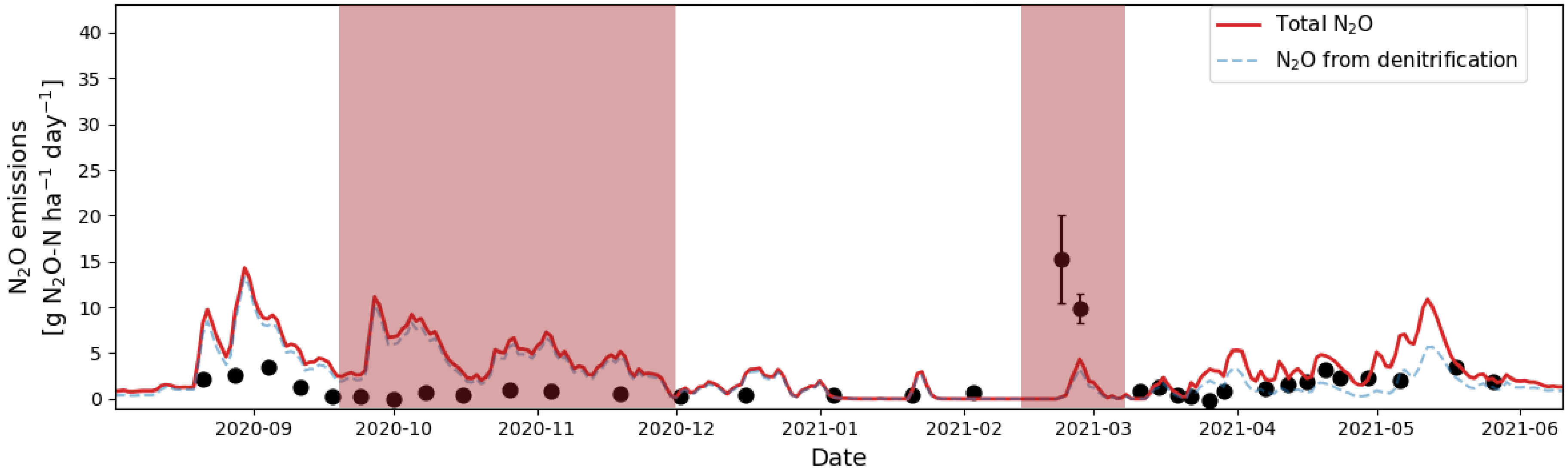
Hairy vetch

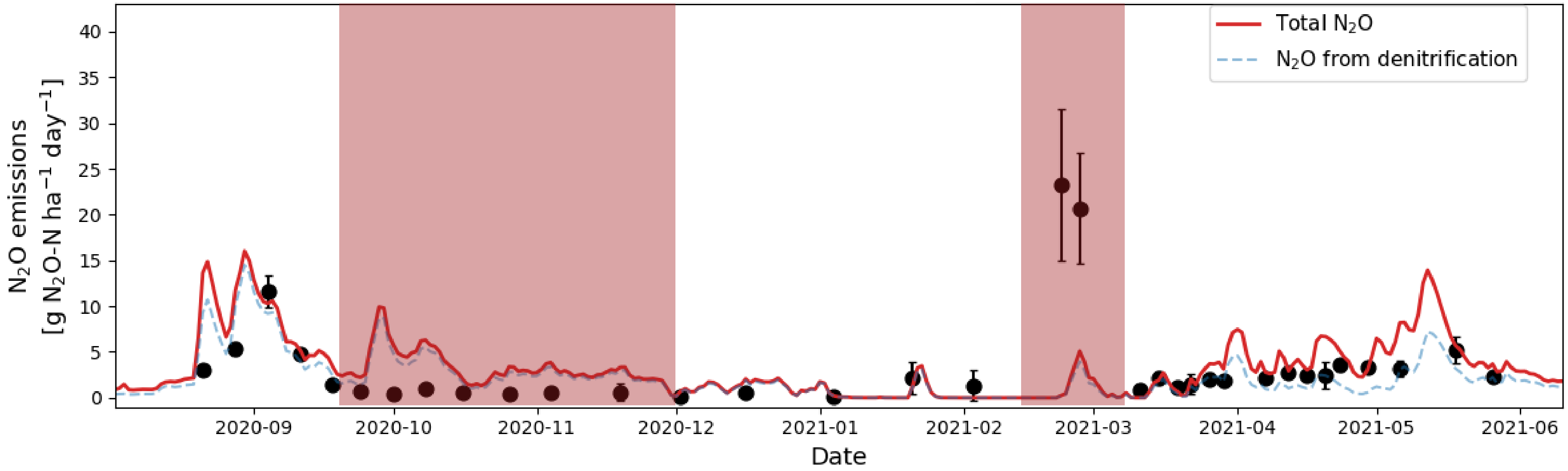


# Fully calibrated (oilseed radish)

**Oilseed radish**



# COMPARING DENITRIFICATION $N_2O$ MODELS

## IMPLEMENTING PARTON ET AL. (1996)

# Setting up the Python interface in Daisy

1. Define *reaction* ($N_2O$ production from denitrification)

```
(defreaction pyDenitN2O Python "Use Python for chemical reaction."
  (module "pyDenitN2O")
  (soil "denitN2O_fullParton1996")
  (in
    (NO3 M_primary "NO3"))
    (texture
        ("clay" 2 [um])
        ("below50" 50 [um]) )
    (extra Theta z rho_b T CO2_C CO2_C_fast)
  (out
    (N2O none "N2O-Denit")
    (NO3 primary "NO3")
    (Act-Denit none "Actual-Denit")
    (Pot-Denit none "Potential-Denit")
    (N2 none "N2-Denit"))
)
```

```python
def denitN2O_fullParton1996(z, Theta, NO3, clay, below50, rho_b, T, CO2_C, CO2_C_fast):
...
return {"N2O-Denit": N2O_deni, "N2-Denit": N2_deni, "NO3": NO3_loss,
        "Actual-Denit": actDenit, "Potential-Denit": potDenit}
```

2. Define *chemistry* that includes the new reaction

```
(defchemistry pyChem N
  (reaction pyDenitN2O nitrification)
)
```

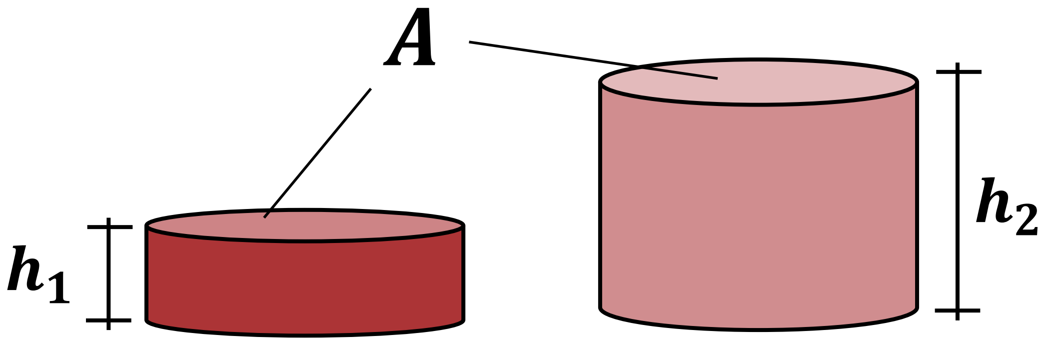
→ The interface set-up was tested by implementing the default Daisy $N_2O$ functions.

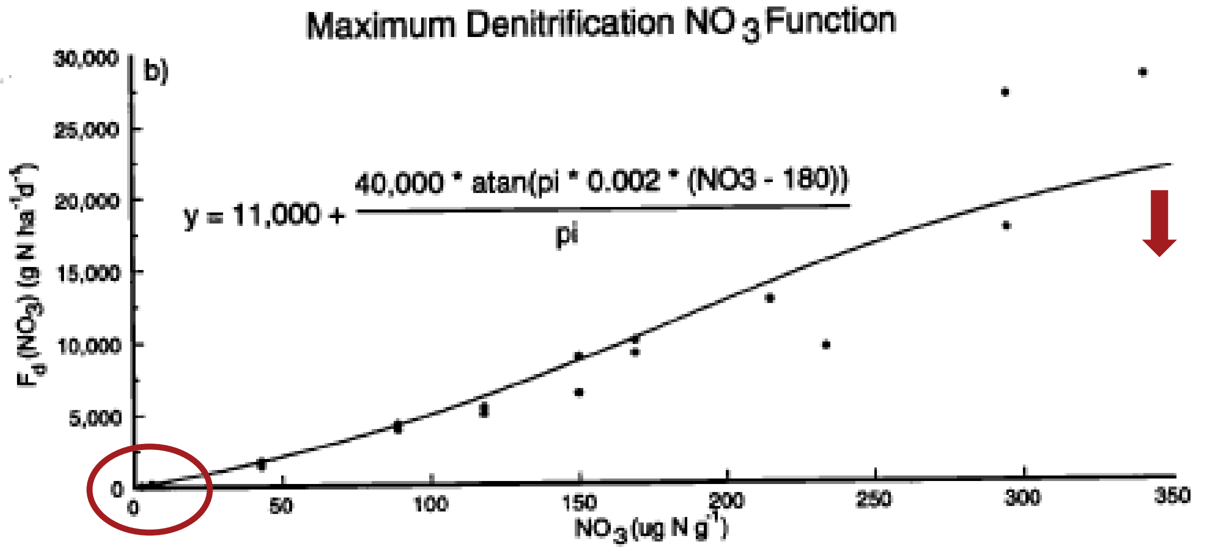
# Parton et al. (1996) – potential denitrification

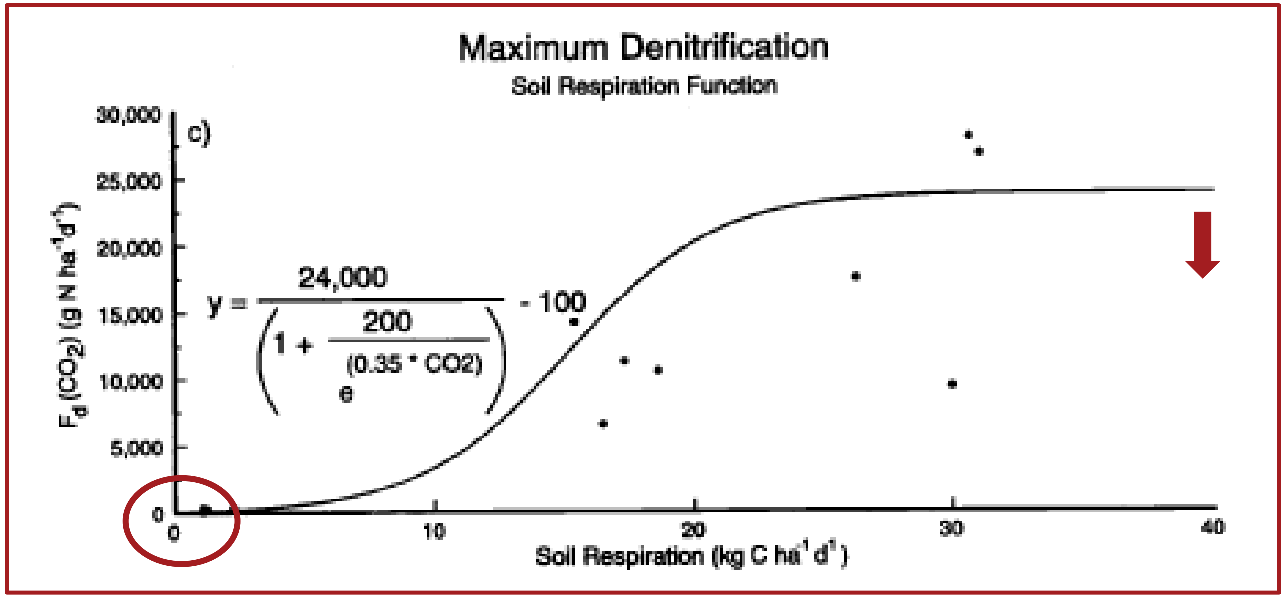
$$\xi_d^* = \min\left(F_d(NO_3^-), F_d(CO_2)\right)$$

Two issues:

1. Denitrification is **not strictly zero** for zero $NO_3^-$ or $CO_2$-C.
2. Volumes must be **converted to areas** for respiration function.



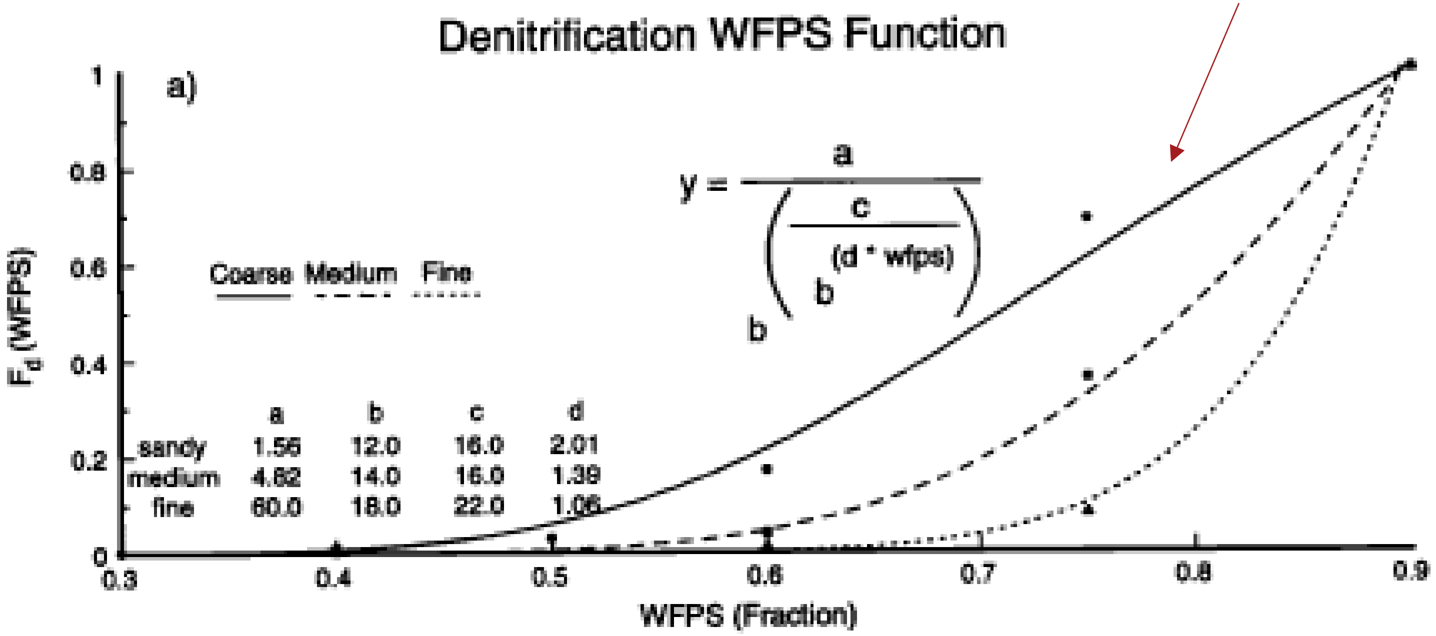



# Parton et al. (1996) – actual denitrification and $N_2O$

$$\xi_d = \xi_d^* F_d(WFPS)$$

**Implemented**



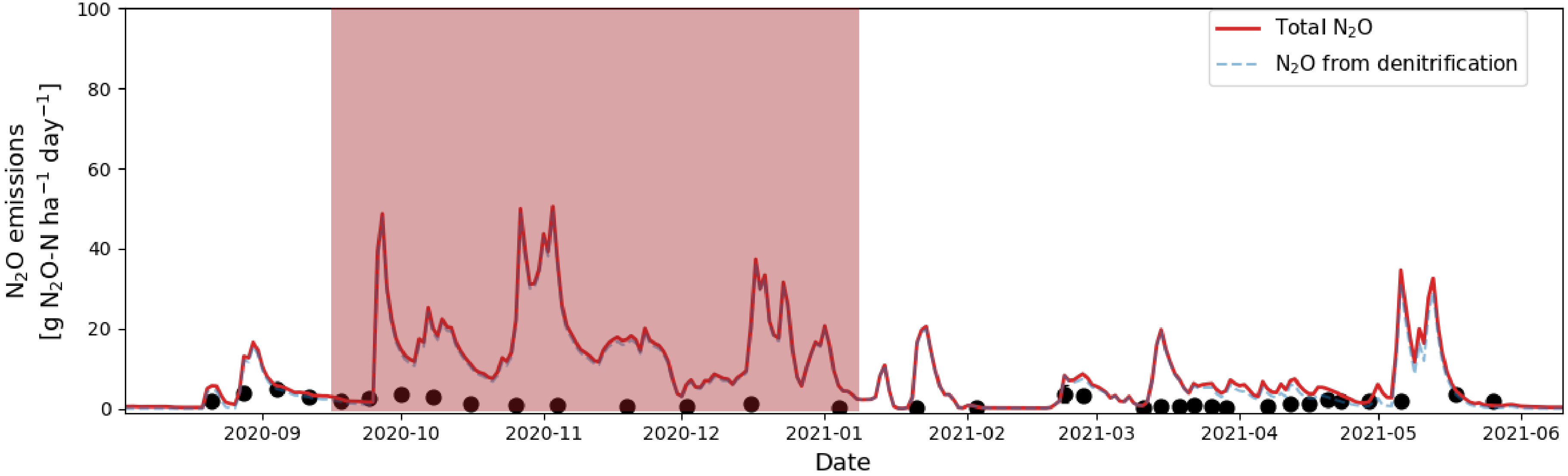

→ The same $N_2$:$N_2O$ partitioning function as in Daisy was implemented.

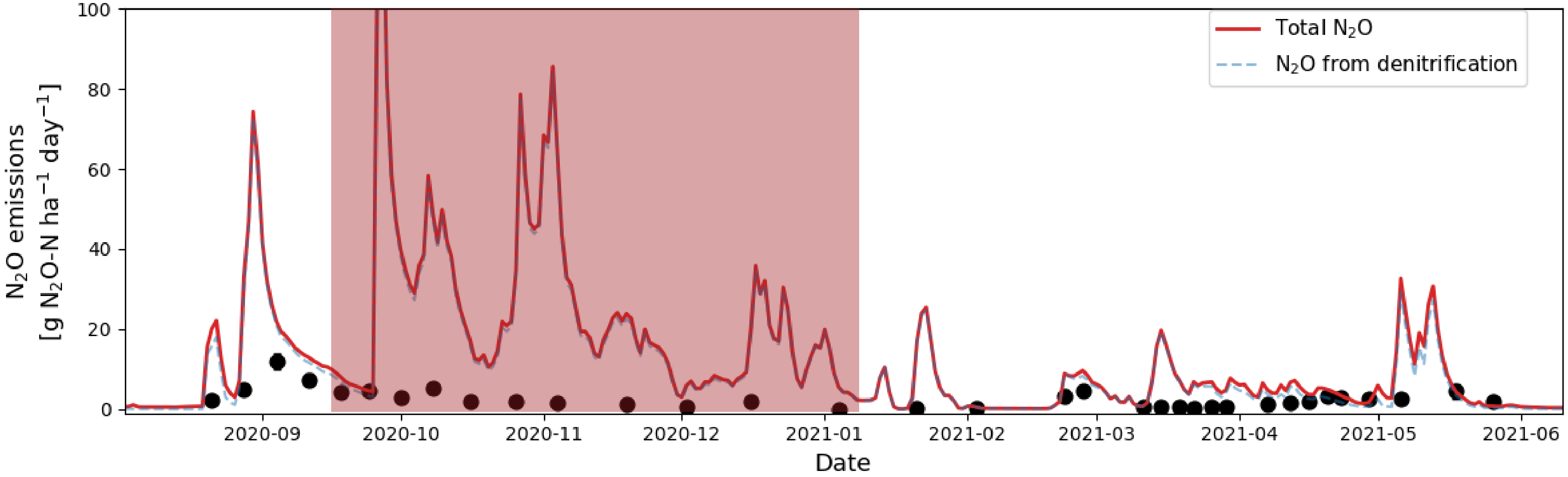
# COMPARING DENITRIFICATION $N_2O$ MODELS

CALIBRATED DAISY VS. (ADJUSTED) PARTON ET AL. (1996)

# Parton et al. (1996) – some example fits (2020-2021)

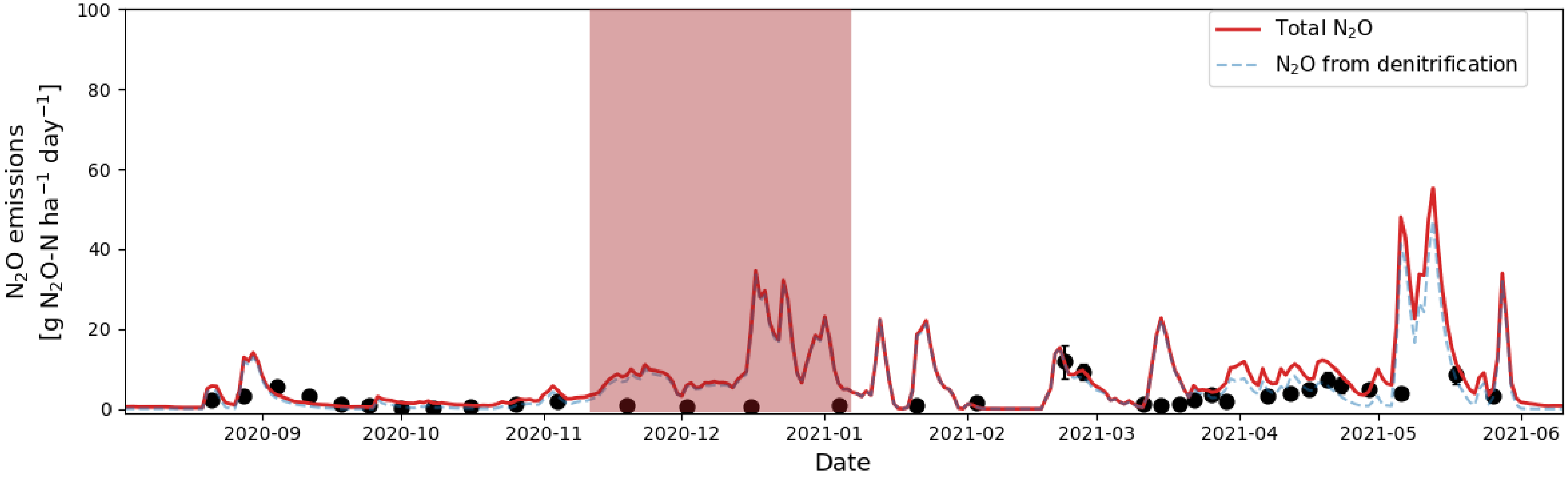
**Bare soil**

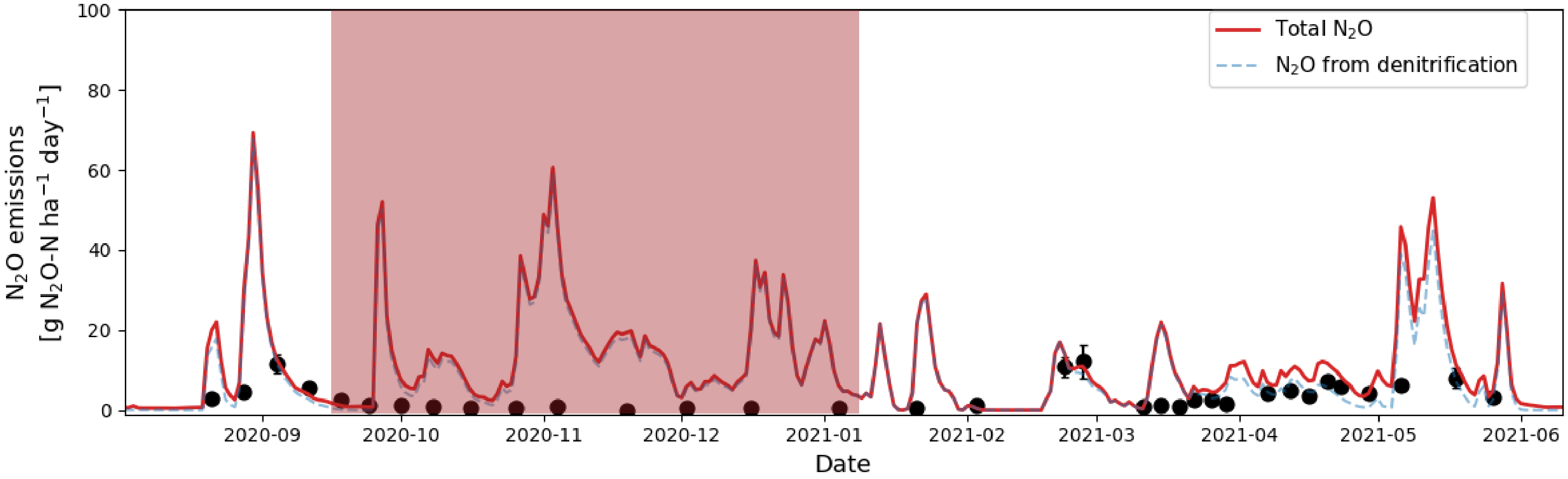


# Parton et al. (1996) – some example fits (2020-2021)

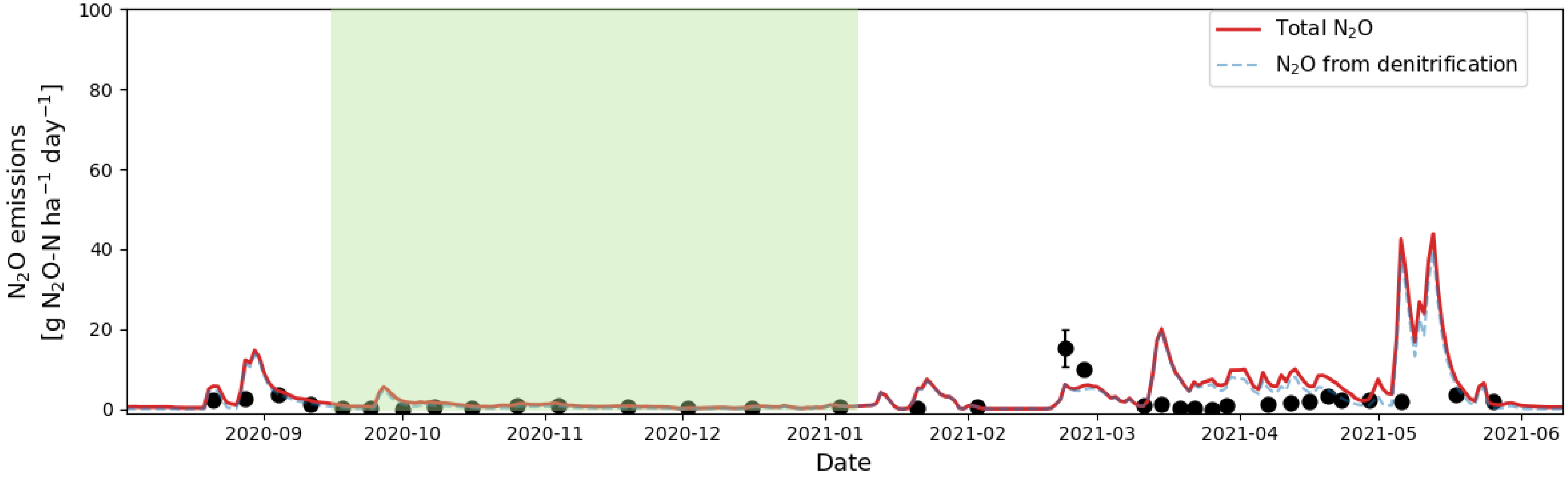
Hairy vetch



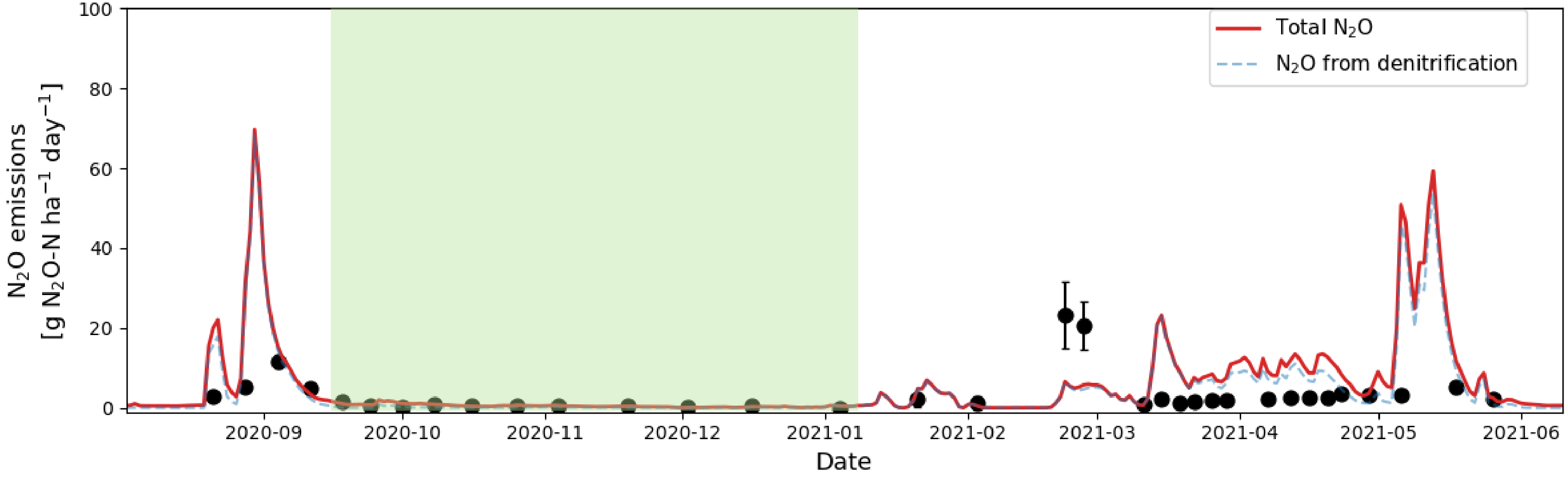



# Parton et al. (1996) – some example fits (2020-2021)

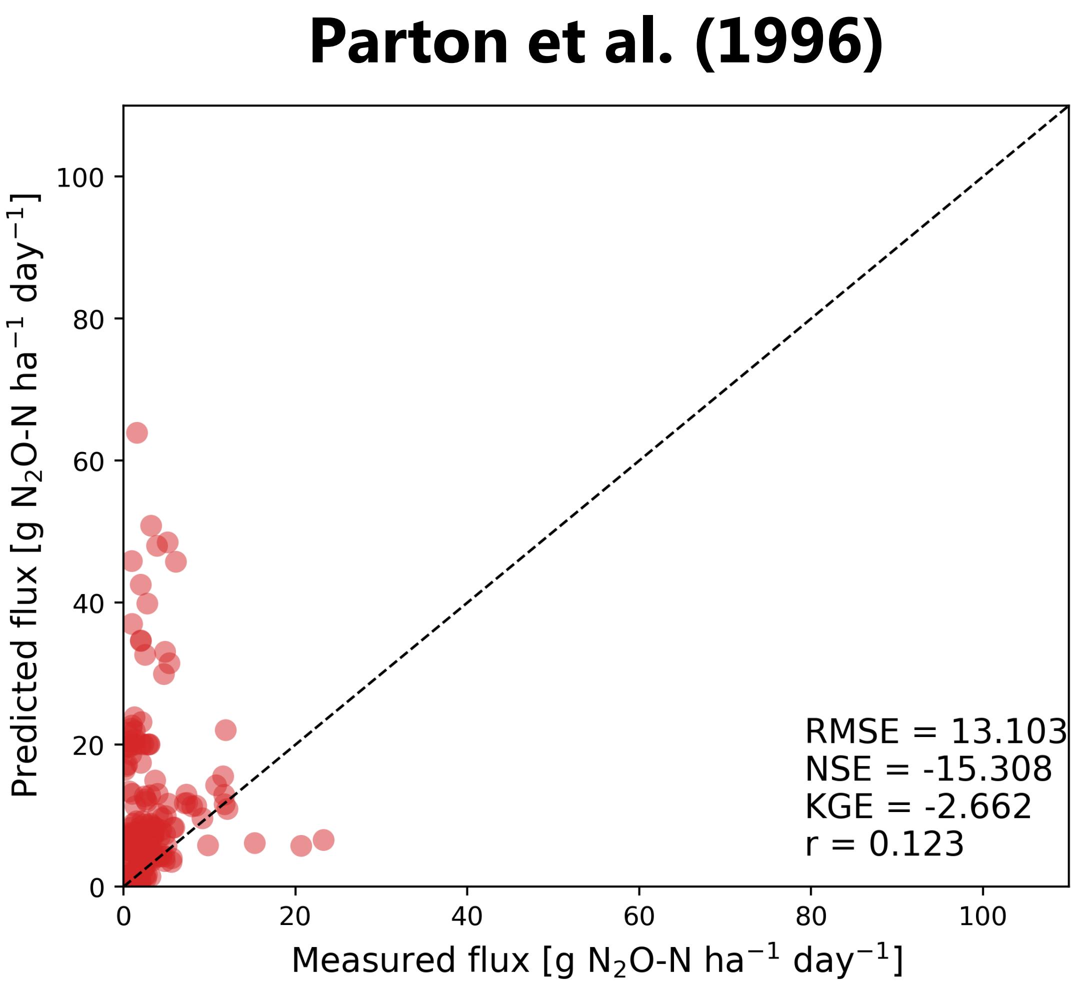
**Oilseed radish**

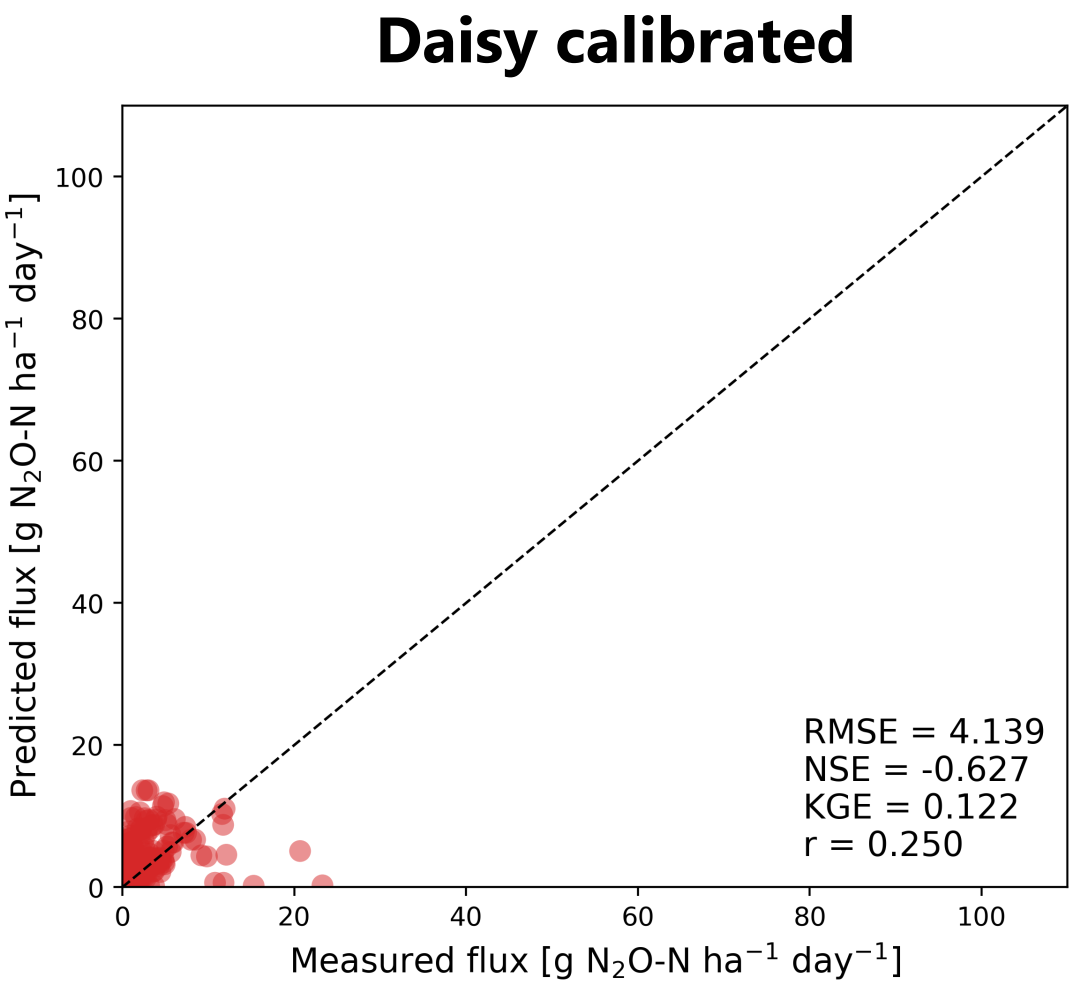





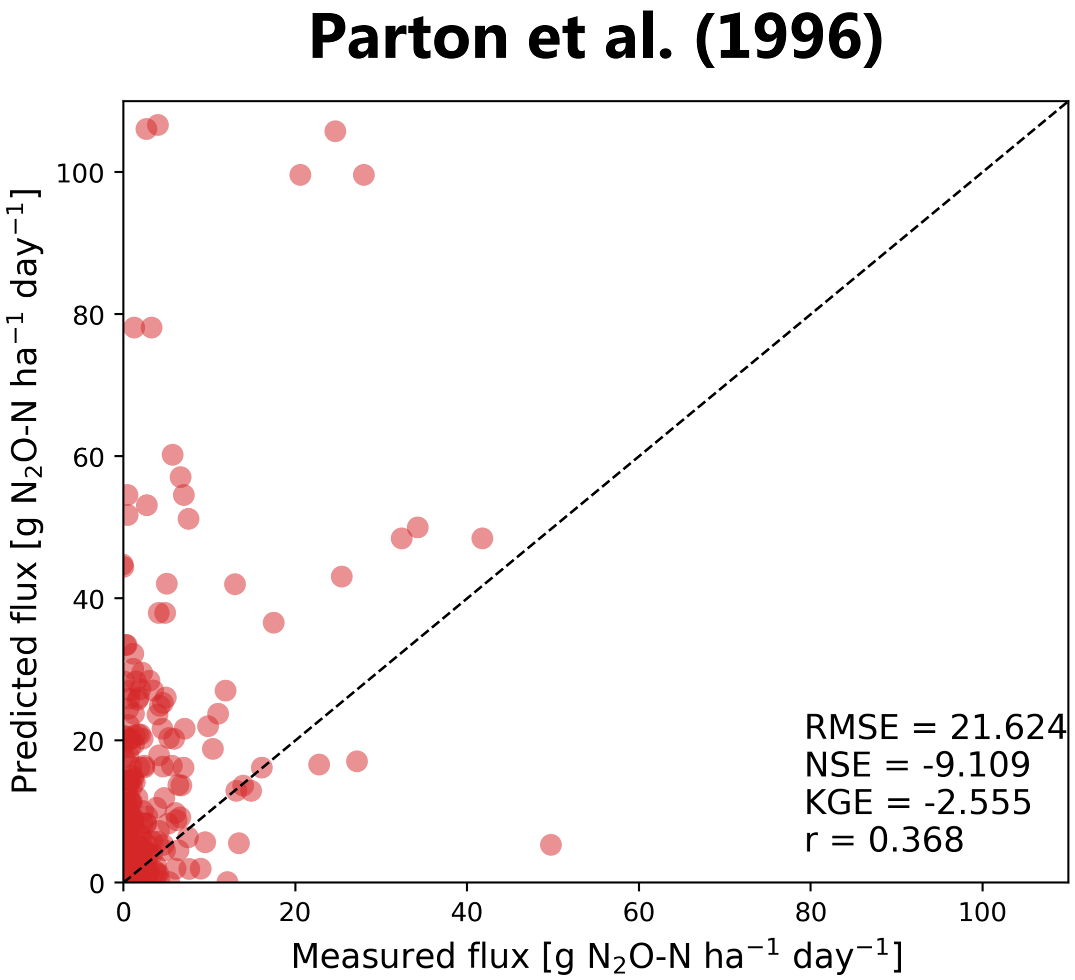


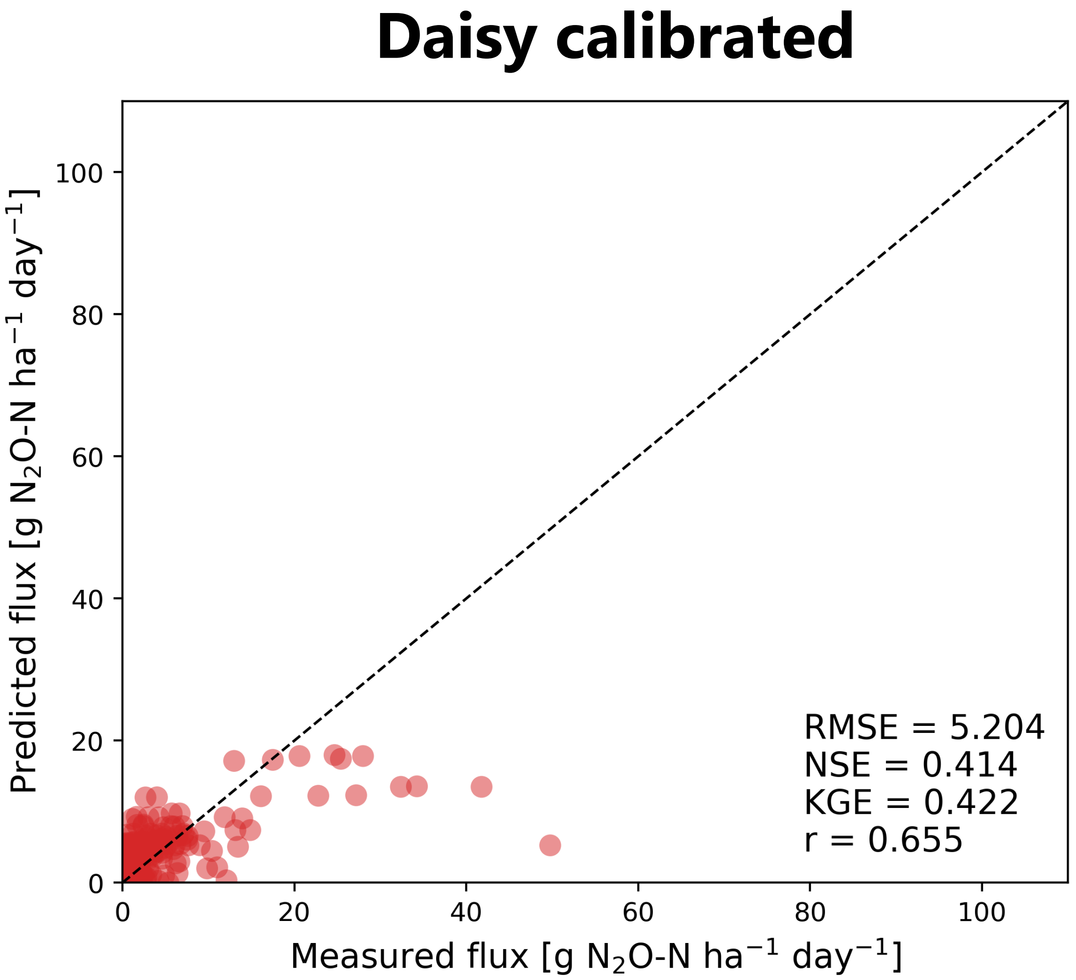
# Model comparison (2020-2021)



# Model comparison (2021-2022)



# CONCLUSIONS AND NEXT STEPS

# Conclusions and next steps

- Daisy's current approach to modelling $N_2O$ emissions looks **promising in the tested conditions (incl. calibration)**.
- Existing $N_2O$ functions seem to **not be easily transferable** to Daisy and may need adjustments.
- $N_2O$ models will be tested on more datasets, incl**. finer-textured soil, organically fertilized soil** and in **hotspot conditions**.
- Other $N_2O$ models will be implemented in Daisy and tested, for example:
    - The **current DayCent** functions (Del Grosso et al., 2000)
    - **NOE** as implemented in STICS (Henault et al., 2005)
    - **Expert-N** (Kaharabata et al., 2003)
    - **FASSET** (Chatskikh et al., 2005)
    - **NITROSIM** as implemented in APSIM (Rolston et al., 1984)

# THANK YOU FOR YOUR ATTENTION

**CONTACT:** tk@plen.ku.dk