Geo 892 – 001: Biophysical Models and Applications in Ecosystem Analysis 10:00 am – 4:30 pm; GEO 120

March 10: Carbon fluxes

Update: manuscript and journal Lecture 1: Modeling Ecosystem Production (Chapter 2) Lecture 2: Modeling Ecosystem Respiration (Chapter 3) Logistics for April 1: Installations at Battle Creek and KBS

Biophysical Models and Applications in Ecosystem Analysis

Modeling Ecosystem Production (Chapter 2)

2.1 Introduction

2.2 Core biophysical Models for Ecosystem Production

- *2.2.1 Michaelis-Menten model*
- *2.2.2 Landsberg model*
- *2.2.3 Farquhar's model*
	- *2.2.4 Photosynthesis based on stomatal conductance (g^s)*
- *2.2.6 Light use efficiency (LUE) model 2.2.7 Nitrogen use efficiency (NUE) model 2.2.8 Water use efficiency (WUE) model*

2.3 The datasets for Modeling Photosynthesis

- *2.4.1 Light response models*
- *2.4.2 Results from Farquhar's model*
- *2.4.3 Results from Ball-Berry Model*
- *2.4.4 Other models*

2.5 Summary Soil respiration (Rs)

Photosynthesis is the first step for assimilating atmospheric CO_2 into organic substances in an ecosystem

- Photosynthesis is a physiological process in which plants, algae and certain bacteria convert solar energy and CO₂ to chemical energy and carbohydrate – such as glucose, sugar, and cellulose.
- "Photosynthesis' is a combination of the Greek words "light" and "putting together".
- The process was discovered by Dutch physician Jan Ingenhousz in the late 1700s
- Chemical conversions take place with Chlorophyll a.
- Two types of chlorophyll pigments absorb light in the blue and red part of the visible spectrum

Plants use sunlight, water, and the gases in the air to make glucose, which is a form of sugar that plants need to survive.

[https://www.youtube.com/watc](https://www.youtube.com/watch?v=FfLLHQDgpjI) [h?v=FfLLHQDgpjI](https://www.youtube.com/watch?v=FfLLHQDgpjI)

Chemical expression has several forms, including the following one:

 $6CO₂ + 12H₂O + Solar Energy \rightarrow C₆H₁₂O₆ + 6O₂ + 6H₂O$

More YouTube videos:

https://www.youtube.com/watch?v=HbLg4lMpUa8 https://www.youtube.com/watch?v=Dq38MpYOb8w Chemical expression has several forms, including the following one:

Measuring photosynthesis: chamber-based at leaf level (snapshots)

LiCor6400 (LI6800) $CO₂$ & H₂O concentration PAR, temperature

Measuring photosynthesis: chamber-based at leaf level (continuous)

Measuring photosynthesis: EC tower
Measuring photosynthesis: EC tower
daytime minus nighttin

daytime minus nighttime $(NEE = GEP - R_{eco})$

Measuring photosynthesis: Biometric approach (tree ring, DBH)

Measuring photosynthesis: remote sensing modeling

Measuring photosynthesis: ecosystem modeling

2.2 Core biophysical Models for Ecosystem Production

2.2.1 Michaelis-Menten model

2.2.2 Landsberg model

2.2.3 Farquhar's model

2.2.4 Photosynthesis based on stomatal conductance (g^s)

2.2.6 Light use efficiency (LUE) model

2.2.7 Nitrogen use efficiency (NUE) model

2.2.8 Water use efficiency (WUE) model

Major variables and Symbols

Pn/An: Photosynthesis rate $(\mu$ mol m⁻² s⁻¹) PAR (PPFD): photosynthetically active radiation (μ mol m⁻² s⁻¹) VPD: vapor pressure deficit (kPa) *I^o or I* **_{comp}** light compensation point (μmol m^{−2} s^{−1}) *Γ * :* CO₂ compensation point (ppm) P_{max/}A_{max}: maximum Pn or A (μmol m^{−2} s^{−1}) V_{max}: maximum Pn under CO2 limited (μmol m^{−2} s^{−1}) J_{max}: maximum Pn under light limited (μmol m^{−2} s^{−1}) g_s : : Stomata conductance (μmol m^{−2} s^{−1}) (stomata conductance (μmol m^{−2} s^{−1})

1. Light response curve **2.** A-C_i curve

https://www.researchgate.net/publication/263642910_Effects_of_Elevated_CO2_Concentration_and_Temperature_on_Physiological_Characters_of_Liriodendron_tulipifera/figures?lo=1

2.2.1 Michaelis-Menten model

$$
P_n = \frac{\alpha \cdot PAR \cdot P_m}{\alpha \cdot PAR + P_m}
$$

Michaelis constant (*Km*) of the enzyme is an inverse measure of affinity. K_m is the value when P_n reaches half of the P_m .

MM model with Respiration (R_d)

$$
P_n = \frac{\alpha \cdot PAR \cdot P_m}{\alpha \cdot PAR + P_m} - R_d
$$

2.2.1 Michaelis-Menten model

$$
P_n = \frac{\alpha \cdot PAR \cdot P_m}{\alpha \cdot PAR + P_m}
$$

Michaelis constant (*Km*) of the enzyme is an inverse measure of affinity. *K^m* is the value when *Pⁿ* reaches half of the *Pm*.

Michaelis Constant (K_m)

2.2.1 Michaelis-Menten model

Landsberg & Sands (2011) introduced an additional shape factor (β) into a non-rectangular hyperbolic model

$$
P_n = p_m \cdot \frac{2 \cdot \alpha \cdot PAR/p_m}{1 + \alpha \cdot \frac{PAR}{Pm} + \sqrt{\left(1 + \alpha \cdot \frac{PAR}{Pm}\right)^2 - 4 \cdot \alpha \cdot \beta \cdot PAR/p_m}}
$$
\nY=a+b*x+c*x²

This model is virtually the same as Eq. 2.1 when β = 0. The value of β should be less than 1 for simulations.

An alternative expression of the non-rectangular hyperbolic model is applied by Peat (1970) as:

$$
P_n = \frac{1}{2 \cdot \beta} \left(\alpha \cdot PAR + P_m - \sqrt{(\alpha \cdot PAR + P_m)^2 - 4 \cdot \alpha \cdot PAR \cdot P_m \cdot \beta} \right)
$$

2.2.2 Landsberg model

$$
P_n = P_m \cdot (1 - e^{\alpha \cdot (PAR - I_{comp})})
$$

In-class exercise

- Create a spreadsheet model for MM and Landsberg model to explore the sensitivity of each parameters.
- PAR values vary from 0 to 2000 (μ mol m⁻² s⁻¹)

Photosynthesis rate for Rubisco-limited, RuBP-limited, and product-limited assimilations (A_c , A_j , and A_p).

Ac as a function of intercellular CO₂ concentration is described by FvCB equation:

$$
A_c = \frac{V_{max} \cdot (c_i - \Gamma^*)}{c_i + K_c \cdot (1 + \frac{O_i}{K_O})}
$$

Vmax is the maximum activity of Rubisco

 c_i is the intercellular CO_2 concentration (µmol mol⁻¹),

 Γ^* is the CO₂ compensation point in the absence of day respiration (R_d),

 K_c is the Michaelis-Menten constant of Rubisco for CO_2 ,

 O_i is the oxygen (O_2) concentration in the atmosphere (209 mol mol⁻¹),

 K_o is the Michaelis-Menten constant of Rubisco for O_2 .

*Γ ** is calculated as:

$$
\Gamma^* = \frac{0.5 \cdot O_i}{2600 \cdot 0.57^{010}}
$$

 K_c for CO_2 is calculated as: $K_c = 30 \cdot 2.1^{Q10}$

 K_o for O_2 is calculated as: $K_c = 30000 \cdot 1.2^{Q10}$

RuBP-limited photosynthesis rate (A_j), also commonly known as lightlimited photosynthesis rate, is calculated as:

$$
A_j = \frac{\mathbf{J} \cdot (c_i - \Gamma^*)}{4 \cdot c_i + 8 \cdot \Gamma^*}
$$

j is the electron transport rate (μ mol m⁻² s⁻¹) and varies with absorbed photosynthetically active radiation (*aPAR*).

Finally, the product-limited photosynthesis rate is calculated as:

$$
A_p = 3 \cdot T_p
$$

Tp (μmol m−2) is the triose phosphate utilization rate. This rarely limits the rate of photosynthesis under physiological conditions

 \bm{A}_n is the least of the three rates: $A_n=minnum(A_c,A_j,A_p)$

The four major parameters that are needed to fit Farquhar's model

$$
V_{max} \text{ (µmol m}^{-2} s^{-1}\text{)},
$$

\n
$$
J_{max} \text{ (µmol m}^{-2} s^{-1}\text{)},
$$

\n
$$
T_p \text{ (µmol m}^{-2} s^{-1}\text{)},
$$

\n
$$
R_d \text{ (µmol m}^{-2} s^{-1}\text{)}
$$

Web Sources for A models

<https://biocycle.atmos.colostate.edu/shiny/photosynthesis/> <https://leafweb.org/>

https://www.researchgate.net/publication/236199968_Modeling_C3_photosynthesis_from_the_chloropl ast_to_the_ecosystem/figures?lo=1

- The diffusion rate is called stomatal conductance (*gs* , μmol m−2 s −1), which is proportional to the photosynthesis rate (*A*_{*n*}, μmol m^{−2} s^{−1}).
- This linear relationship is modulated by leaf surface $CO₂$ and H₂O concentration and varies among leaves and species.

Ball-Berry model:

$$
g_s = K \cdot A_n \cdot \frac{h_s}{c_s}
$$

- *h*^s (ranging 0-1) is the fractional relative humidity at the leaf surface,
- c_s (µmol mol⁻¹) is the CO_2 concentration of leaf surface,
- *K* is the slope constant of the model that represents the composite sensitivity of g_s to CO_2 concentration

By reversing Eq. 2.13, photosynthesis is modeled as:

$$
A_n = \frac{g_s \cdot c_s}{K \cdot h_s}
$$

Stomata do not completely close, there is a minimum conductance value (g_o, mol m⁻² s⁻¹). The Ball-Berry model is also expressed as:

$$
g_s = g_0 + g_1 \cdot A_n \cdot \frac{h_s}{c_s}
$$

Leuning (1990) argued that the use of $[c_{s}-1]$ is more appropriate in the numerator, and he modified the original Ball-Berry model:

$$
g_s = g_0 + \frac{a_1 \cdot A_n}{(c_s - \Gamma)}
$$

Leuning reasoned this new form was applicable because $A_n \rightarrow 0$ when $c_s \rightarrow \Gamma$, rather than when $c_s \rightarrow 0$. With this model, the supply-constraint model of photosynthesis can be expressed as:

$$
A_n = \frac{g_0}{1.6 \cdot (c_s - c_i) - g_1 \cdot h_s \cdot (c_s - r)}
$$

Later, Leuning *et al.* (1995) made an additional modification to the model (Eq. 2.18) for C_3 plants as:

$$
g_s = g_0 + \frac{a_1 \cdot A_n}{(c_s - \Gamma)(1 + \frac{D_s}{D_0})}
$$

where D_0 is the value of *VPD* at which stomatal conductance becomes zero.

Lloyd (1991) proposed that g_s is dependent of \sqrt{D} . Medlyn *et al.* (2011) further emphasized the importance of g_1 in the Ball-Berry model because of its sensitivity to environmental changes (*e.g.*, temperature, soil water and nutrients). They also agreed with Leuning *et al.* (1995) that *VPD*, instead of relative humidity, should be used in modeling [*Aⁿ ~ g^s*] for a new form of:

$$
g_s = g_0 + 1.6 \cdot \left(1 + \frac{g_1}{\sqrt{D}}\right) \cdot \frac{A_n}{c_s}
$$

Figure 2-4. Simulations of stomatal conductance (*g^s*) with different sets of parameters (Eq. 2.13). Other curves can be generated by altering parameters in **S2-2**

Figure 2-6. Changes in photosynthesis rate (A_n) with photosynthetically active radiation (*PAR*) (a) and CO₂ concentration (c*^a*) (b) for two species in Wang *et al.* (2018) (data use permission received from the authors).

Figure 2-7. Fitted light response curves using three Michaelis-Menten (MM) equations (Eqs. 2.2, 2.3. and 2.4) and the Landsberg model (Eq. 2.5) for two species on the Tibetan Plateau (Wang *et al.* 2018). Details are included in the supplement spreadsheet LightR_models.xlsx (S2-4).

Figure 2-8. Changes in photosynthesis rate $\begin{bmatrix} \vdots \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$ (a) (*Aⁿ*) of two species in Wang *et al.* (2018) based on Farquhar's model (Eq. 2.6) with the maximum rate of Rubisco (*Vmax*) (a) and maximum rate of electron transport (*Jmax*) (b). Differences between Rubisco-limited model (Eq. 2.7) and light-limited model (Eq. 2.11) are shown in (c).

Figure 2-9. Changes in stomatal conductance (g_s) with photosynthesis rate (A_n) and leaf surface CO₂ concentration for two species studied in Wang *et al.* (2018). A_n was estimated with Farquhar's model (Eq. 2.6) and g_s was estimated with the Ball-Berry model (Eq. 2.15). The data and regression results are included in the supplement document S-3 (Wang2018.xlsx).

2.2.6 Light use efficiency (LUE) model 2.2.7 Nitrogen use efficiency (NUE) model 2.2.8 Water use efficiency (WUE) model

Scalars

Ecosystem primary production (*GPP*, or *NPP*), or canopy photosynthesis (*Pⁿ*), can be simply molded as a portion of *PAR –* light use efficiency (ε):

 $Pn = \varepsilon \cdot Water$

LUE model for estimating ecosystem primary production is simple, using a*PAR* as the sole independent variable that is more available at ecosystem-regional-global scales. This advantage is the primary reason that the MODIS teams were able to measure global, continuous *GPP* based on Terra satellite data (Running *et al.* 2004). *GPP* is estimated as:

 $GPP = [\varepsilon_{\text{max}} \cdot \text{mod}(\text{Temperature}) \cdot \text{mod}(VPD)] \cdot aPAR$

Figure 2-5. Scalar development for modifying resource use efficiency (ε) from its maximum value (ε_{max}). Both symmetric and asymmetric functions can be used for estimating ϵ from ϵ_{max} . Maximum (T_{min}), maximum (T_{max}) and optimum (T_{out}) temperature are used for deriving temperature scalar of three asymmetric approaches.

PnET model

 P_{max} (µmol CO₂ m⁻² s⁻¹) is calculated with a simple linear model based on a meta-analysis of prior publications:

 $P_{max} = \alpha + \beta \cdot N\%$

Pn is further modified for suboptimal environmental conditions (see Section 2.2.6) as:

$$
P_n = \alpha \cdot P_{max} \cdot \Delta T \cdot \Delta W \cdot \Delta VPD
$$

Water use efficiency (WUE)

Assuming CO₂ uptake and H₂O loss are coupled, *GPP* at ecosystem can be molded as:

 $GPP = WUE \cdot ET$

Multiple resource use model (mRUE)

 GPP = resource supply \times proportion of resource supply \times captured efficiency of resource use

When multiple RUEs are integrated, GPP can be modeled as:

$$
GPP = (R_{avail1} \cdot R_{avail2} \cdot \cdots R_{availn})^{1/n}.
$$

$$
(RUE_1 \cdot RUE_2 \cdot \cdots RUE_n)^{1/n}
$$

Summary

- Models based on light response curve are easy to understand and use. Only a few parameters (2-4) are needed to construct these models. Much more efforts are needed to examine the influences of other potential driving forces on model parameters.
- Physiological models have solid chemical and physical processes and theoretical foundations. Farquhar's model is based on the Kinetic energy concept of the Michaelis-Menten model as well as the chemical processes of photosynthesis, whereas the Ball-Berry family of models are rooted in the gas diffusion process and the corresponding properties of gases and physical conditions.
- A large number of parameters (5-10) are required for both Farquhar's model and the Ball-Berry models. These parameters are often difficult to measure or estimate. When these models are used to model ecosystem production, a tremendous amount of ancillary data on species composition, structure, soil conditions and microclimate are needed.
- Resource use models are also easy to understand and can be based on empirical parameters. They are particularly advantageous for modeling ecosystem production at landscape-region-global scales. These models have specific merits when applied with remote-sensed measures such as vegetation index, phenology, *etc.*
Supplementary Materials

- **S-1:** Light response curves through Michaelis-Menten and Landsburg models (LightResponse.xlsx)
- **S-2:** Simulations of stomatal conductance (g_s) based the Ball-Berry model (Ball Berry Model.xlsx)
- **S-3:** Field measurements and modeled photosynthesis rate $(A_n, \mu \text{mol m}^{-2} s^{-1})$ and parameters for two species in Wang *et al.* (2018) (Wang2018.xlsx)
- S-4: Model performances of Michaelis-Menten and Landsberg models for the two species in Wang et al. (2018) $(Lighth$ models x lsx)
- S-5: Python codes for estimating empirical coefficients through nonlinear regression analysis of Michaelis-Menten models and Landsberg model (Chapter2_PY.RAR). This package has one dataset in Excel for practice and four Python programs for non-linear regression.

Biophysical Models and Applications in Ecosystem Analysis

Modeling Respiration (Chapter 3)

- In-class exercise
- Homework #3

Modeling Respiration (Chapter 3)

3.2.1 Linear and log-linear models 3.2.2. Quadratic and polynomial model 3.2.3. Arrhenius *model 3.2.4 Logistic model 3.2.5 Gamma Model 3.2.6 Biophysically constrained models 3.2.7. Time series models*

Machine learning in modeling carbon fluxes!

Terminology

Autotrophic respiration (R_a): respiration from living plant components (leaves, shoots, roots) for constructions and maintenances

Heterotrophic respiration (R_h): respiration due to decomposition of organic matters (mostly from litter layers and soils)

Soil respiration (R_s): The sum of belowground R_a and R_h

Ecosystem respiration (R_{eco}): The sum of aboveground and belowground respiration

Figure 1: Diagrammatic representation of the main terms describing carbon fluxes in ecosystems.

[http://www.steverox.info/Downloads/Software/C%20Accounting%20Definitions.pdf](http://www.steverox.info/Downloads/Software/C Accounting Definitions.pdf)

Figure 6.1 Illustration of the major carbon fluxes in a forest ecosystem, including gross primary production (GPP), ecosystem respiration (R_e) , aboveground carbon allocation (AGCA), belowground carbon allocation (BGCA), soil respiration (R_s) , aboveground heterotrophic respiration (R_{Ha}) , aboveground autotrophic respiration (R_{Aa}) , surface runoff (S_c) , lateral fluxes of carbon through the wind (W_c) and animals (A_c) , vertical water leaching (G_c) , and upward movement through diffusion after weathering of bedrock (M_c) in the soil

Flux terms and relationships (Chen et al. 2014)

through the wind (T_c) , such as fine litter, leaves) and of organic materials through animals (A_c) may be significant. Finally, surface runoff (S_c) and vertical water leaching (G_c) will carry small amounts of carbon into or out of a forest (Fig. 6.1). These carbon fluxes and their relationships can be summarized as follows:

```
GPP = [NEP + R_{\circ}]NPP = [GPP - R<sub>A</sub>]NPP = [ANPP + BNPP]ANPP = Vegetation Growth - LitterfallBNPP = Root Growth - Root MortalityR_e = [R_A + R_H] - (M_c)R_{\rm A} = R_{\rm A} + R_{\rm Ab}R_{\rm H} = [R_{\rm H_2} + R_{\rm Hb}] - (M_{\rm c})NEP = [AGCA + BGCA] + (S_c + T_c + G_c + A_c - M_c)R_{\rm s} = [R_{\rm Ab} + R_{\rm Hb}] - (M_{\rm c})
```


Soil Food Web

Just like human being, these animals take $O₂$ and breath out CO₂, i.e., respiration

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www.exploringnature.org

Vegetation-Soil Profiles

<https://temperategrasslandsbiomes.weebly.com/soillandform.html>

CARBON DIOXIDE EVOLUTION OF SOIL AND CROP GROWTH HENRIK LUNDEGÅRDH

Ecological Station of Hallands Väderö, Sweden and Central Experiment Station, Stockholm

Received for publication April 5, 1926

INTRODUCTION

Carbon dioxide evolution from the soil, and its relation to microbiological activity and to climatic factors have been studied by a large number of scientists (17, 34, 32, 33, 25, 6, 29), who have found a relation between the carbon dioxide evolution on one hand and the number of bacteria and the intensity of nitrification on the other hand. The influence of mineral salts, humidity, manure, and temperature on the rate of carbon dioxide evolution has been studied by Wollny (36), Petersen (25), König and Hasenbäumer (10), Van Suchtelen (33), Lundegårdh (16, 17), Waksman and Starkey (34), and others.

- (32) STOKLASA, J., AND ERNEST, A. 1905 Ueber den Ursprung, die Menge und die Bedeutung des Kohlendioxyds im Boden. Centbl. Bakt. (II) 14: 723–736.
- (33) SUCHTELEN, H. VAN 1910 Über die Messung der Leppnstätigkeit der äeobiotischen Bakterien im Boden durch die Kohlensäureproduktion. Centbl. Bakt. (II) $28:45-89.$
- (34) WAKSMAN, S. A., AND STARKEY, R. L. 1924 Microbiological analysis of soil as an index of soil fertility: VII. Carbon dioxide evolution. Soil Sci. 17: 141-161.
- (35) WILSON, J. K. 1920 Device for growing large plants in sterile media. Phytopath. $19:425-429.$
- jqchen (36) WOLLNY, E. 1880 Untersuchungen über den Kohlensauregehalt der Bode analysis of CO2 content in soil air Landw. Vers. Sta. 25: 273-391.

6/12/2019 12:17 PM

Type your reply...

SOIL SCIENCE, VOL. XXIII, NO. 6

TABLE 10

Variations in free atmosphere during the summer period

How much is ecosystem respiration?

Three bioenergy crops at the Kellogg Biological Station (KBS): Corn, Mixed parries, and switchgrass

Lessons so far: Aboveground C allocation (NPP:GPP)

- The allocation in 2009 (soybean) was the same
- The allocation at Marshall Farm (CRP) to aboveground is substantially higher

Lessons so far: Aboveground C allocation (NPP:GPP)

• The allocations were the same, except 2013-2014 (drought effects?)

Lessons so far: Aboveground C allocation (NPP:GPP)

• The allocations at Marshall Farm were slightly lower (drought effects)

Globally, Reco can be less than or greater than GPP

How much is ecosystem respiration?

Figure

Caption

Table 3. Summary of simulated trends of global carbon fluxes (Tg C a -2) from different experiments. Simulations are using WFDEI meteorology. Significant trends (p < 0.05) are shown in bold.

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How is respiration measured?

CARBON DIOXIDE EVOLUTION OF SOIL AND CROP GROWTH

HENRIK LUNDEGÅRDH

Ecological Station of Hallands Väderö, Sweden and Central Experiment Station, Stockholm

Received for publication April 5, 1926

FIG. 2. APPARATUS FOR ESTIMATING THE SOIL RESPIRATION ("RESPIRATION BELL")

 h , handles; e, cylindric edge; u, ring up to which e is driven in the soil; sr, tube for drawing the air sample.

FIG 3. SCHEME OF NEW APPARATUS FOR ACCURATE ANALYSIS OF THE CO₂ CONCENTRATION IN THE AIR

How is respiration measured?

STUDIES ON THE VEGETATION OF THE GASPÉ PENINSULA

II. THE SOIL RESPIRATION OF SOME PLANT COMMUNITIES!

HELMUT LIETH² AND ROBERT OUELLETTE³ 1962

Abstract

The present study was undertaken to investigate the soil respiration of different
communities of the boreal forest region in the Gaspé Peninsula. The measure-
ments were done with an absorption method which is described in the lower limit of these values.

The respirometer as shown in the diagram is used to measure the uptake of oxygen by respiring seeds. Any other small living organisms (e.g. insect) could be used for this investigation. This is done simply by measuring the change in the volume of gas surrounding the seeds. It is therefore essential to eliminate volume changes that are caused by anything other than the uptake of oxygen by the respiring seeds.

How is respiration measured?

A SIMPLE RESPIRATION APPARATUS FOR DETERMIN TION OF OXYGEN AND CARBON DIOXIDE IN INDIRECT CALORIMETRY.

BY J. F. MCCLENDON, HILDING C. ANDERSON, F. R. STEGGERL CLAIRE CONKLIN, AND MILDRED WHITAKER.

(From the Laboratory of Physiological Chemistry, University of Minnes Medical School, Minneapolis.)

(Received for publication, March 8, 1928.)

FIG. 1. The prototype of the respiration apparatus of McClendon and ^{*l*an} Slyke.

How is respiration measured? Enclose chambers

How is respiration measured? The Closed chambers

Automated chambers

Open path eddy-covariance system: nighttime flux is considered as R_{eco}

Chapter 7. Carbon in the Low-Temperature Environment

Atmosphere

102

Applications of stable isotopic analysis

775 (-7%) 100 22 60 $0.06 - 0.7$ Surface Ocean 600 (1.5%) Fossil Land biota $36\sqrt{ }$ \mathbf{T} 35 Fuels 1600 5000 Cont. (-23%) silicic (-23%) Dissolved bicarbonate crust Deep Ocean Marine $60\sqrt{ }$ 0.5 7,000,000 36,000 carbonate ↘ (-6%) (0%) **Terrestrial soils** seds. and marine seds. $2500(0\%)$ $1600 (-23\%)$ 0.17 0.3 $|0.2|$ 0.05 Carbonate sedimentary Mantle Organic carbon rocks in sedimentary rocks 324,000,000 60,000,000 $(0-1\%)$ 15,000,000 (-23%) (-6%) 0.2 0.2 0.03 0.05 to atmosphere

McConnaughey, T. A., Burdett, J., Whelan, J. F., & Paull, C. K. (1997). Carbon isotopes in biological carbonates: respiration and photosynthesis. *Geochimica et Cosmochimica Acta*, *61*(3), 611-622.

> Fig. 7.1. Carbon cycle, showing amounts, fluxes and δ^{13} C values of different reservoirs. Abundance shown in bold in 10^{15} g. Flux is shown in italics in 10^{15} g/yr. δ^{13} C values are in parentheses.

https://www.youtube.com/watch?v=1EkkB8JaIzQ

Separating R_a and R_h

Temperature-dependent respiration

Q¹⁰ model (Van't Hoff 1898)

$$
Q_{10} = \left(\frac{R_2}{R_1}\right)^{\left(\frac{10}{T_2 - T_1}\right)}
$$

where respiration rate is measured as R_1 under temperature T_1 and R_2 is measured at temperature T_2 , Q_{10} (a unitless measure) describes the reaction rate increase when the temperature is raised by 10 $\rm{^{\circ}C}$ (or $\rm{^{\circ}K}$).

Figure 3-1. Schematic illustration of change in respiration with temperature by an exponential function (Eq. 3.3) for four *Q¹⁰* values (a). The exponential increase of respiration can be limited by other ecological resources such as moisture (b). The respiration reduction due to low moisture can be linear, polynomial, Gamma, logistic, or take other forms. The threshold point can be empirically determined for a site or a specific time period.

Temperature dependent respiration

Q¹⁰ model (Van't Hoff 1898)

This model (Eq. 3.1) is often used in the literature and has been expressed as well

$$
R = R_0 \cdot Q_{10} \frac{(T2 - T1)}{10}
$$

where R_o is called reference respiration at 0 °C.

Figure 3-1. Schematic illustration of change in respiration with temperature by an exponential function (Eq. 3.3) for four *Q¹⁰* values (a). The exponential increase of respiration can be limited by other ecological resources such as moisture (b). The respiration reduction due to low moisture can be linear, polynomial, Gamma, logistic, or take other forms. The threshold point can be empirically determined for a site or a specific time period.

Temperature dependent respiration

An exponential form is also widely used in respiration studies as:

$$
R = \alpha \cdot e^{\beta \cdot T}
$$

where β is the rate of change with increasing temperature and α is the respiration at near zero temperature (\degree C). Q_{10} is calculated as:

$$
Q10=e^{10\cdot T}
$$

Q¹⁰ values = 2.1 1 to 10 (R_s) (Xu & Qi 2001) 3.4 to 5.6 (R^s), mixed-hardwood forests (Davidson *et al*. (1998) 1.3 to 3.3 (R_s) (Raich & Schlesinger (1992) 1.4±0.1 (Reco) (Mahecha *et al*. 2010),

Figure 3-1. Schematic illustration of change in respiration with temperature by an exponential function (Eq. 3.3) for four *Q¹⁰* values (a). The exponential increase of respiration can be limited by other ecological resources such as moisture (b). The respiration reduction due to low moisture can be linear, polynomial, Gamma, logistic, or take other forms. The threshold point can be empirically determined for a site or a specific time period.

Moisture constraints

- In many ecosystems
- More pronounced in Mediterranean ecosystems and drylands
- The decreasing trend varies by ecosystem type and time (DOY, month, year)
- Moisture as a significant variable needing to be included in the Q10 model
- Time is also needed for the model

3.2.1 Linear and log-linear models

Simple linear models for predicting respiration (R) using temperature $(T, {}^{\circ}C)$:

 $R = \alpha + \beta \cdot T$

Natural logarithm linear model (*i.e.*, Eq. 3.3)

$$
\text{Ln}(R) = \ln(\alpha) + \beta \cdot T
$$

Or

 $R = \exp(\ln(\alpha)) + \exp(\beta)) \cdot T$

Quadratic and polynomial models

$$
R = \alpha + \beta_0 \cdot T + \beta_1 \cdot T^2
$$

$$
R = \alpha + \beta_1 \cdot T + \beta_1 \cdot T^2 + \beta_3 \cdot T^3 + \beta_4 \cdot T^4 + \beta_5 \cdot T^5
$$

The polynomial equation can provide accurate predictions but lacks any theoretical foundation and should not be used beyond the range of *in situ* measurements.

3.2.3. Arrhenius *model*

The Arrhenius form of the model was proposed by Lloyd and Taylor (1994): Lloyd and Taylor model

$$
R = R_{10} \cdot e^{E_0 \left[\frac{1}{56.02} - \frac{1}{T - 227.13}\right]}
$$

 R_{10} : the respiration rate at a reference temperature of 10 °C (a.k.a. reference respiration) E_o : the temperature sensitivity coefficient (°K) *T*: soil temperature at a certain (*e.g.* 5 cm) depth (^oK) Temperature in Kelvin units is used $(K = C + 273.15)$ R_{10} and E_0 are empirically estimated (linear or nonlinear)

3.2.4 Logistic model

Barr et al. (2002)

$$
R = \frac{\alpha}{1 + e^{(\beta_0 - \beta_1 \cdot T)}}
$$

- Nonlinear regression analysis is performed for estimating the parameters
- The logistic model assumes that the rate of change (i.e., density function) in respiration with temperature is not a constant, but peaks at a specific temperature and eventually returns to zero at high temperature.

Demonstration of model application in Excel!

3.2.5 Gamma Model

Gamma model is expressed as Khomik *et al*. (2009) :

 $R = T^{\alpha} \cdot e^{\beta_0 + \beta_1 \cdot T}$

- Coefficients are empirically estimated
- when a is equal to zero, the model becomes an exponential function,
- when b1 is equal to zero, the model becomes a power function
- It allows R to decrease at high temperatures when respiration is constrained
- asymmetric changes by its maximum value

The *T* (°C) value at which *R* peaks (*i.e., T_{max,}* °C) can be determined as:

$$
T_{max} = \left(\frac{\alpha}{-\beta 1} - 40\right)
$$

Demonstration of model application in Excel!

3.2.6 Biophysically constrained models

DeForest *et al*. (2006)

$$
R = [R_{10} \cdot e^{\beta \cdot T}] + [a \cdot \theta + b]
$$

Martin *et al*. (2009)

$$
Ln(R) = \beta_0 + \beta_1 \cdot T + \beta_2 \cdot T^2 + \beta_3 \cdot \theta + \beta_4 \cdot \theta^2 + \beta_5 \cdot (T \cdot \theta)
$$

Concilio *et al*. (2005)

$$
R = R_0 \cdot e^{\beta_0 \cdot T} \cdot e^{\beta_1 \cdot \theta} \cdot \beta_2 \cdot T \cdot \theta
$$
3.2.7. Time series models

Soil and ecosystem respiration change over time due to not only the corresponding changes in significant biophysical variables but also the temporal correlations from memory or legacy effects, especially under extreme climate and disturbances.

Xu et al. (2011)
\n
$$
R = \underline{\alpha \cdot e^{\beta_0 \cdot T} + \beta_1 \cdot (\theta - \beta_2)^2 + (\beta_3 \cdot (DOY - \beta_4)^2)}
$$
\n
$$
R = \kappa_0 + \kappa_1 \cdot \sin(DOY^* + \varphi_1) + \kappa_2 \cdot \sin(2 \cdot DOY^* + \varphi_2)
$$
\n365

3.4 Model performances

Figure 3-4. Modeled soil respiration from three sets of models: (a) linear (log linear) models, (b) nonlinear models, and (c) moisture-included models. Field data were collected at Chamber #1 every 2 hours from March 18 through December 17 in 2015 at a larch plantation in the Mt. Fuji Flux Site, central Japan (Teramoto *et al*. 2019).

3.4 Model performances

Figure 3-5. Comparisons of predicted and measured soil respiration (µmol CO₂ m⁻² s⁻¹) from 9 models (Fig. 3-4). The cyan lines are the 1:1 ratios. Field data were collected with an automated respiration chamber every 2 hours from March 18 through December 17 in 2015 at a larch plantation in the Mt. Fuji Flux Site, Japan (Teramoto *et al*. 2019).

Measured

3.4 Model performances

Figure 3-6. Comparisons of predicted and measured soil respiration (µmol CO₂ m⁻² s⁻¹) between DOY-included model and Lloyd-Taylor model. Field measurements (gray dots) were collected with an automated respiration chamber every 2 hours from March 18 through December 17 in 2015 at a larch plantation in the Mt. Fuji Flux Site, central Japan (Teramoto *et al*. 2019).

Summary

- Simple linear, power, and polynomial forms are not recommended in modeling respiration regardless of their simple-to-use nature.
- Selection of model form is critical for producing reliable predictions. Residual analysis can help development of additional covariates and model forms.
- Incorporating other independent variables is necessary. Soil moisture, soil carbon and nutrient content, biomass or production, canopy cover, litter depth, *etc.* are among the potential factors to be considered.
- Multiple model forms or a unique set of coefficients for the same model need to be used for different times such as seasons (phenophases), climatic conditions, and disturbances. For modeling seasonal changes, day of year should be included in the models.

Supplementary Materials

- S3-1. Spreadsheet models (Schematics.xlsx) for illustrating the roles of two parameters in exponential model (Eq. 3.3) for respiration-temperature relationship, calculations of Q_{10} values, and inclusion of linear constraints by moisture (θ) at high temperature ranges (Fig. 3-1).
- S3-2. Field measurements of soil respiration, soil temperature and moisture in 2015 from Chamber #1 (RespirationData.xlsx) in a mature larch plantation (Larix kaempferi) (35° 26' 36.7" N, 138° 45' 53.0" E; 1105 m a.s.l.) on the northeastern slope of Mt. Fuji in central Japan (Fig. 3-2).
- S3-3. Spreadsheet modeling and model comparisons (Rmodel 1.xlsx) of linear, exponential and quadratic forms (Eqs. $3.5, 3.3, 3.7$).
- S3-4. Spreadsheet modeling and model comparisons (Rmodel 2.xlsx) of Logistic, Lloyd-Taylor and Gamma models $(Eqs. 3.10, 3.9, 3.11).$
- S3-5. Spreadsheet modeling and model comparisons (Rmodel 3.xlsx) of three model forms by including soil moisture (θ) as an additional independent variable (Eqs. 3.14, 3.16, 3.17).
- S3-6. Spreadsheet modeling of soil respiration with day of year (DOY) and soil moisture (θ) as additional covariates of temperature (Rmodel 4.xlsx) (Eq. 3.18) (Fig. 3-6).
- S3-7. Python codes for estimating empirical coefficients through nonlinear regression analysis of Logistic, Lloyd-Taylor, Gamma, DeForest, Xu, Concilio and DOY models (Respitation.PY). This RAR file has two Excel data file and 12 Python programs for linear and non-linear regression.

In class exercise

Find out the Q10 value of soil respiration at Chamber 1 of the Larch forest, Japan (Data file: Q10Model.xlsx)

Machine Learning and Modeling Fluxes

Eddy Covariance (EC) Technology for direct measurement of net exchange of trace gases, momentum, energy, and other materials at **ecosystem level**

- ~2000 EC towers since the first one at the Harvard Forest in 1989
- Lots of experience, tools, maintenance protocols, data process, etc.
- Beyond CO_2 : CH_4 , N₂O, CO, NOx, aerosols, Albedo, etc.
- Goodwill for data sharing => global synthesis and knowledge development
- Communication and coordinated efforts (e.g., FLUXNET, AmeriFlux, USCCC, etc.)
- Many more

- 1) 2000⁺ EC towers are not enough to cover all ecosystems, with their distributions seriously skewed
- 2) Most tower sites are not large enough
- 3) Our understanding of the regulation mechanisms on C fluxes is based on a few biophysical models, often empirical, such as Q10, Michaellis-Menten, Farquar, Penmen-Monteith, etc.
- 4) There lack reliable models for CH₄ and N₂O fluxes

• 2000⁺ EC towers are not enough to cover all ecosystems, with their distributions seriously skewed

• Our understanding of the regulation mechanisms on C fluxes is based on a few biophysical models, often empirically tried, such as Q10, Michaellis-Menten, Farquar, Penmen-Monteith, etc.

Yet, we have dozens of other variables collected at an EC tower, but not used

Inbox - jqchen@msu.edu - Outlool

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• There lack reliable models for CH_4 and N_2 O fluxes

Knox et al. 2019; Delwiche et al. 2021). The growth in available CH_4 data can help improve bottom-up estimates of regional-to-global wetland CH₄ sources (Treat et al. 2018; Peltola et al. 2019; Rosentreter et al. 2021) but this requires data processing standards that ensure eddy covariance CH₄ flux data products are of the same quality and provenance as carbon dioxide $(CO₂)$ and energy fluxes (e.g., FLUXNET2015; Pastorello et al. 2020). Gap-filling is a particularly

Irvin et al. 2021. https://doi.org/10.1016/j.agrformet.2021.108528

Opportunities

1. Rich data

All contribute to the magnitude and dynamics of fluxes Mechanistic and/or empirical explorations

2. Evolving analytical tools

Accurate predictions of fluxes and underline regulations

Machine Learning in flux studies?

Speech Recognition

Human **expertise** does not exist

Personalized Medicine

Models must be **customized**

Genomics

Huge amounts of data

Credit: Dr. Jiliang Tang

The fundamental concept of Machine Learning (ML) in flux studies

All bio-physical variables are responsible, at various degrees, for the magnitude and dynamics of fluxes, with known or unknown mechanisms.

Complex tasks Continuously updated

Credit: Dr. Jiliang Tang

Deep Learning vs Traditional Machine Learning

Predictions based on conventional "biophysical models" and recurrent neural network (RNN) at an agricultural land in KBS

RNN model

Measured Fc

Predicted Fc

Measured Fc

Proposed architecture of GNN & RNN for estimating model parameters with partially known, or unknown mechanisms by assuming missing values of $\varphi_{ij}(t)$ and VI(t) at any giving time (t) and space (i,j) (*i.e.*, nodes)

Fully Connected Layer (FC Layer)

Credit: Dr. Jiliang Tang

Modeling NEE of carbon using RNN at a mixed prairie in MI (Zou et al. in process)

7-3

epoch: 36 validation: rmse: 0.7695824495942905 validation: best rmse: 0.7615167483546836 test rmse: 0.6335910434578435

8-2

epoch: 35 validation: rmse: 0.6659846320595684 validation: best rmse: 0.6572025276120753 test rmse: 0.8090676608599882

Homework #3:

- 1) Q10 model
- 2) One of the biophysically constrained respiration model
- 3) One of the time series model

Briefly describe the model strengths and weakness

Deadline: 2:30 pm, Nov. 18, 2021

Formulas

Data

View

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Q&A from the Class

In class exercise of respiration models by group

Note: Comments and typos for each chapters are welcome!

Field Trip to Battle Creek (Urban Flux Tower) and KBS (chambers and towers)

- 8:30 Leave geography building
- 9:45 Arrive Battle Creek Area Mathematics and Science Center (Kevin Postma arrives) Scott Hanson, Science Instructor
- 10:30 Heading out to KBS, BCSE plots (Kevin Kahmark, kahmark@msu.edu)
- 11:45 LTER installations (Kevin K)
- 12:30 Lunch and KBS Labs (Kellogg Manor House)
- 2:00 Marshal Fam (EC towers)
- 3:00 Heading back to MSU
- 4:300 Arrive Geography Building

Notes

- Bring own lunch and water
- Raingear (?)
- Travel approval (check your email) for acceptance
- ?