Title: A derivation error that affects carbon balance models exists in the current implementation of the modified Arrhenius function

Running Title: Derivation error in modified Arrhenius model

Author: Bridget Murphy^{1,2}, Joseph R. Stinziano^{3,*}

Affiliations: ¹ Department of Biology, University of Western Ontario, London, ON, Canada; ² Current

Affiliation: Department of Cell and Systems Biology, University of Toronto, Toronto, ON, Canada;

³ Department of Biology, University of New Mexico, Albuquerque, NM, USA

* Corresponding author; Email: jstinziano@unm.edu; Tel: +1 (226) 678-1670

Article Type: Modelling/Theory

Word Count: 3,623

Introduction: 559

Description: 1640

Results: 688

Discussion: 710

Acknowledgments: 26

Number of Tables: 3

Number of Figures: 4

Supplementary Files: 1

Summary

- Understanding biological temperature responses is crucial to predicting global carbon fluxes. The current approach to modelling temperature responses of photosynthetic capacity in large scale modelling efforts uses a modified Arrhenius equation.
- We rederived the modified Arrhenius equation from the source publication from 1942 and uncovered a missing term that was dropped by 2002. We compare fitted temperature response parameters between the correct and incorrect derivation of the modified Arrhenius equation.
- We find that most parameters are minimally affected, though activation energy is impacted quite substantially. We then scaled the impact of these small errors to whole plant carbon balance and found that the impact of the rederivation of the modified Arrhenius equation on modelled daily carbon gain causes a meaningful deviation of $\sim 18\% \text{ day}^{-1}$.
- This suggests that the error in the derivation of the modified Arrhenius equation has impacted the accuracy of predictions of carbon fluxes at larger scales since $>40\%$ of Earth System Models contain the erroneous derivation. We recommend that the derivation error be corrected in modelling efforts moving forward.

Keywords: Arrhenius, temperature, photosynthesis, gas exchange, modelling, carbon balance

Introduction

Globally, photosynthesis and autotrophic respiration are the largest biological carbon fluxes, with photosynthesis removing ~120 Gt C year⁻¹ from the atmosphere and autotrophic respiration releasing ~60 Gt C year⁻¹ back to the atmosphere (Amthor, 2000; Ciais *et al.*, 2013). Given the temperature sensitivity of these large carbon fluxes (Lombardozzi *et al.*, 2015), understanding how photosynthesis and respiration respond on acute, acclimatory, and adaptive timescales is crucial for predicting vegetative and carbon cycle responses to future global climates (Rogers *et al.*, 2017; Stinziano *et al.*, 2018). Biological temperature responses including photosynthesis and respiration are typically assumed to be exponential or peaked (Way & Yamori, 2014; Smith & Dukes, 2017; Kumarathunge *et al.*, 2019). Exponential responses are usually modelled based on an Arrhenius-type curve (Arrhenius, 1915):

$$f(T) = k \exp\left(\frac{-E_a}{RT}\right) \quad \text{Equation 1,}$$

or equivalently,

$$f(T) = k_{25} \exp\left[\frac{E_a(T-298.15)}{298.15RT}\right] \quad \text{Equation 2}$$

where $f(T)$ is the rate of the process at temperature T , k is a pre-exponential factor, E_a is the activation energy in J mol⁻¹, R is the universal gas constant of 8.314 J mol⁻¹ K⁻¹, T in K, k_{25} is the rate of the process at 298.15 K, and 298.15 is the reference temperature in degrees Kelvin (K). As for peaked responses, while a few options are available (Kruse *et al.*, 2008; Hobbs *et al.*, 2013; Heskell *et al.*, 2016), the most commonly implemented version is the modified Arrhenius model of Johnson *et al.* (1942) as presented in Medlyn *et al.* (2002):

$$f(T) = k_{25} \exp\left[\frac{E_a(T-298.15)}{298.15RT}\right] \left[\frac{1 + \exp\left(\frac{298.15\Delta S - H_d}{298.15R}\right)}{1 + \exp\left(\frac{T\Delta S - H_d}{RT}\right)} \right] \quad \text{Equation 3}$$

where H_d is the deactivation energy in J mol^{-1} , and ΔS is the entropy of the process in $\text{J mol}^{-1} \text{K}^{-1}$.

Equation 3 (**which will be referred to as M2002 from this point forward as it is conventionally referred to in the literature as the source of the equation**) is used for modelling the temperature responses of photosynthetic capacity (i.e. maximum carboxylation capacity of rubisco, V_{cmax} , maximum electron transport capacity, J_{max} , and triose phosphate utilization capacity (TPU); see Table 1 for a review of which Earth System Models use M2002). These parameters are then used in ecophysiological studies to understand thermal acclimation of photosynthesis (see Kattge & Knorr, 2007; Smith & Dukes, 2017; and Kumarathunge *et al.*, 2019 for examples). Furthermore, this equation is also used in terrestrial biosphere models to predict future carbon cycling (e.g. Rogers *et al.*, 2017).

Due to the ubiquity of M2002 in modelling temperature responses and the thermal acclimation of photosynthetic capacity (e.g. Kattge & Knorr, 2007; Rogers *et al.*, 2017; Smith & Dukes, 2017; Kumarathunge *et al.*, 2019; Table 1), we revisited the original Johnson *et al.* (1942) modified Arrhenius function to rederive M2002. In the process of this rederivation, we uncovered a term that was completely dropped sometime between Johnson *et al.* (1942) and Medlyn *et al.* (2002) which causes a systematic error in the application of the modified Arrhenius for modelling photosynthetic capacity in individual species (e.g. Medlyn *et al.*, 2002) to modelling global scale carbon uptake (e.g. Rogers *et al.*, 2017; Table 1). We then refit a freely available dataset (Kumarathunge *et al.*, 2019), with both versions of the modified Arrhenius model, and fed the temperature response fits through a carbon balance model to estimate the impact of the derivation error on modelled plant carbon balance. We predicted that the derivation error would cause substantial variation in fitted temperature response parameters, and that these differences would propagate through to modelled daily carbon balance.

Description

Rederivation of the modified Arrhenius equation

Johnson *et al.* (1942, equation 24) describe the temperature response of the light intensity of a luciferase reaction whereby the enzyme reversibly denatures or inactivates at high temperatures as:

$$I = \frac{c''T \exp\left(\frac{-\Delta H^\ddagger}{RT}\right)}{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-\Delta H}{RT}\right)} \quad \text{Equation 4}$$

where I is the intensity of the luciferase reaction, c'' is not explicitly defined in Johnson *et al.* (1942), but appears to represent a constant based on the derivation of Equation 4, T is the temperature in K, R is the universal gas constant of $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$, $\Delta H^\ddagger$ is the activation energy in J mol^{-1} , ΔH is the deactivation energy in J mol^{-1} , and ΔS is the entropy in $\text{J mol}^{-1} \text{ K}^{-1}$. First, we harmonize the notation with standard ecophysiological representations such that $\Delta H^\ddagger$ becomes E_a , and ΔH becomes H_d :

$$f(T) = \frac{c''T \exp\left(\frac{-E_a}{RT}\right)}{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-H_d}{RT}\right)} \quad \text{Equation 5}$$

We can relativize the equation to a reference temperature by dividing Equation 5 at a hypothetical temperature by Equation 5 at a standard temperature (i.e. 25°C):

$$\frac{f(T)}{k_{25}} = \frac{\left[\frac{c''T \exp\left(\frac{-E_a}{RT}\right)}{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-H_d}{RT}\right)} \right]}{\left[\frac{c''298.15 \exp\left(\frac{-E_a}{298.15R}\right)}{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-H_d}{298.15R}\right)} \right]} \quad \text{Equation 6}$$

Next, rearrange fractions so that there is one numerator and one denominator on each line for clarity:

$$\frac{f(T)}{k_{25}} = \left[\frac{c''T \exp\left(\frac{-E_a}{RT}\right)}{c''298.15 \exp\left(\frac{-E_a}{298.15R}\right)} \right] \left[\frac{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-H_d}{298.15R}\right)}{1 + \exp\left(\frac{\Delta S}{R}\right) \exp\left(\frac{-H_d}{RT}\right)} \right] \quad \text{Equation 7}$$

Cancel out the constant c'' , use exponent rules to simplify so that E_a is contained within a single exponential function, and the ΔS and H_d terms are grouped together:

$$\frac{f(T)}{k_{25}} = \frac{T}{298.15} \exp\left(\frac{-E_a}{RT}\right) \left[\frac{1 + \exp\left(\frac{\Delta S}{R} + \frac{-H_d}{298.15R}\right)}{1 + \exp\left(\frac{\Delta S}{R} + \frac{-H_d}{RT}\right)} \right] \quad \text{Equation 8}$$

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120 Simplify further by setting a common denominator within exponential terms:

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$$f(T) = k_{25} \frac{T}{298.15} \exp\left(\frac{-298.15E_a + E_aT}{298.15RT}\right) \left[\frac{1 + \exp\left(\frac{298.15\Delta S - H_d}{298.15R}\right)}{1 + \exp\left(\frac{T\Delta S - H_d}{RT}\right)} \right] \quad \text{Equation 9}$$

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124 Simplify exponential terms further to reduce the number of instances that E_a appears in the equation:

125

$$f(T) = k_{25} \frac{T}{298.15} \exp\left(\frac{E_a(T - 298.15)}{298.15RT}\right) \left[\frac{1 + \exp\left(\frac{298.15\Delta S - H_d}{298.15R}\right)}{1 + \exp\left(\frac{T\Delta S - H_d}{RT}\right)} \right] \quad \text{Equation 10}$$

127

128 Note the difference between M2002 and the rederived equation 10 (**which will be referred to as**

129 **J1942**): the term $T / 298.15$ is missing from M2002. There are several alternative expressions of

130 Equation 4 (e.g. Farquhar *et al.*, 1980; Harley *et al.*, 1986; Harley *et al.*, 1992; Harley & Baldocchi,

131 1995; Lloyd, 1995), however when relativized to a common temperature, the equations presented in

132 Farquhar *et al.* (1980), Harley *et al.* (1992), Harley & Baldocchi (1995), and Lloyd (1995) are all

133 identical to M2002 when relativized by temperature, while the Harley *et al.* (1986) equation is

134 identical to our derivation (J1942) when relativized to a common temperature (see Appendix A for the

135 relativizations of Farquhar *et al.* (1980), Harley *et al.* (1986), and Harley *et al.* (1992); Harley &

136 Baldocchi (1995) uses an identical equation to Eq. 18 from Medlyn *et al.* (2002), while Lloyd (1995)

137 uses an identical equation to Eq. 17 from Medlyn *et al.* (2002)).

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139 We traced the origin of the dropped term to two papers: Hall (1979) and Farquhar *et al.* (1980). Both

140 papers cite the M2002 equation as belonging to Sharpe and DeMichele (1977) when in fact it belongs

141 to Johnson *et al.* (1942). In Hall (1979), the reasoning behind the dropped term is given as: "In

142 addition their linear T term was omitted because it has little influence on the function and would have

143 prevented Eq. 22 [the M2002 equation] from approaching Eq. 21 [Equation 1 in the present study] in

the limiting conditions of low temperatures” (Hall, 1979, page 305). Considering J1942, at 5 °C the error due to the dropped term would be $\sim 278 \text{ K} / 298 \text{ K} = \sim 0.93$, and at 45 °C would be $318 \text{ K} / 298 \text{ K} = \sim 1.07$, so $\sim 7\%$ error at those temperatures. In context of measurement precision, such an assumption of “little influence” may have been reasonable at the time. However, the reason regarding the convergence of the two equations is simply tuning the model equations to fit their expectations. Meanwhile, Farquhar et al. (1980) report that: “Eq. (36) is a simplified version of an equation developed by Sharpe and DeMichelle [sic] (1977) to describe the effect of temperature on enzyme inactivation” (Farquhar et al., 1980, page 84). In both cases, it appears that the intention was to simplify the equation, which in the process of simplifying, generated an error that was propagated for over 40 years.

The derivation error introduces multiple systematic errors. First, errors are introduced into the fitted parameters E_a , H_d , and ΔS . Second, k_{25} is scaled using the wrong equation, introducing an error in $f(T)$. And third, acclimation equations describing E_a , H_d , and ΔS will then be in error due to errors in the fitted parameters at each temperature. Here we focus on the impact of the dropped term on fitted temperature response parameters and modelling whole-plant carbon balance.

Data analysis

Using A-C_i curve data compiled in Kumarathunge *et al.* (2019), available from the Kumarathunge *et al.* (2018) repository, we used the {fitacis} function from the R package {plantecophys} (Duursma, 2015), setting fitmethod = “bilinear”, Tcorrect = FALSE, and fitTPU = TRUE, to obtain V_{cmax} and J_{max} . We then fit Equations 3 and 10 to the data, allowing H_d to be fit. To ensure that the curves could be fit (i.e. that there were enough data to fit 4 parameters), we only used data where A-C_i curves were measured at 5 or more temperatures. This reduced the number of candidate temperature responses from 729 to 403. We used the R package {minpack.lm} (Elzhov *et al.*, 2016), using Equation 2 to obtain starting values for E_a and k_{25} , while the other initial parameters were $\Delta S = 0.650 \text{ kJ mol}^{-1} \text{ K}^{-1}$, and H_d varying from 1 to 1000 kJ mol^{-1} , followed by the {BIC} function to select the best model based on Bayesian Information Criteria. We obtained 341 and 337 successful V_{cmax} temperature response curve fits for M2002 and J1942, respectively, and 241 and 242 successful J_{max} temperature response curve fits for M2002 and J1942, respectively. This resulted in a total of 547 fitted temperature response curves

which we filtered further, requiring that E_a , ΔS , and H_d were all positive values and that the V_{cmax} and J_{max} data were paired, resulting in 196 complete pairs of V_{cmax} and J_{max} temperature responses for analysis. The data covered a temperature range from 1 °C to 50 °C across all curves, with a median range of 14 °C to 42.6 °C.

Modelling

We modelled the impact of the M2002 and J1942 equations on daily net plant carbon balance. Data for leaf area, root and shoot masses, as well as leaf dark respiration at 25 °C were taken for white spruce (*Picea glauca*) from Stinziano & Way (2017), while stomatal conductance model parameters were calculated with the gas exchange data reported in Stinziano & Way (2017). Briefly, Stinziano and Way (2017) grew white spruce in growth chambers under a simulated autumn treatment based on temperatures and photoperiods from Trenton, ON, with weekly harvesting of biomass and gas exchange measurements across 17 weeks as a control treatment, along with a warming treatment where temperatures were +5 °C of the control, a constant summer day/night temperature with declining photoperiod, and a constant summer photoperiod with ambient changes in temperature. Here we only used data from Stinziano & Way (2017) that were from the control treatment. Mean data were taken from the control treatment at weeks 0 and 12 to provide contrasting biomass allocation patterns such that week 0 is a low respiration scenario and week 12 is a high respiration scenario. These different respiration scenarios were used to reduce bias in any conclusions regarding the impact of the M2002 and J1942 equations on carbon balance, as the ratio of photosynthesis to respiration may alter the sensitivity of net carbon balance to the Arrhenius equation used. Root respiration for white spruce was taken from Weger & Guy (1991) and we assumed that stem respiration was equal to root respiration (Table 2).

For the full model structure and equations, please see the accompanying R package {arrhenius.comparison} ("arrhenius.comparison_1.0.2.tar.gz"; Stinziano & Murphy, 2020) (see Table 3 for equations). Briefly, we linked the Medlyn *et al.* (2011) stomatal conductance model with the Farquhar *et al.* (1980) C_3 photosynthesis model, assuming infinite mesophyll conductance to CO_2 as these same assumptions were used in fitting the data from Kumarathunge *et al.* (2018). Photosynthetic capacity, both maximum rubisco carboxylation capacity, V_{cmax} , and maximum electron

transport rate, $J_{\max}$, were scaled to temperature using either M2002 or J1942, while respiration was scaled according to (Atkin & Tjoelker, 2003). Photosynthesis and respiration were summed across each modelled day to calculate daily plant carbon assimilation.

Modelling was performed on 18 total days of environmental data, with three days of data from three months (17th – 19th of May, August, and October, 2019) obtained from external irradiance sensors at the Biotron Experimental Climate Change Research Centre at the University of Western Ontario and the remaining environmental data from Environment Canada historical climate data for South London (43.01°N, 81.27°W, altitude: 251 m; temperature range: -0.1 – 27.9 °C) and the rooftop greenhouse at the University of New Mexico (35.08°N, 106.62°W, altitude: 1587 m; temperature range: 7.2 – 42.2 °C) to capture different levels of environmental variability (see *Impacts on modelled net carbon balance* for environmental data).

Overall, the modelling approach allows us to assess the relative differences between Equations 3 and 10 under a low- and high- respiration scenario across different ranges of seasonal variability.

Statistical analysis

Data were analyzed using the {lm} function in R v.3.6.2 (R Core Team, 2019), regressing the data obtained from M2002 against the data obtained from J1942 for each of $V_{\max,25}$, $J_{\max,25}$, $E_a,V_{\max}$, $E_a,J_{\max}$, $\Delta S_{V_{\max}}$, $\Delta S_{J_{\max}}$, $H_{d,V_{\max}}$, $H_{d,J_{\max}}$, BIC values for the fits of Equations 3 and 10, daily photosynthesis, daily net carbon balance, and daily photosynthesis : daily respiration ratios. Intercepts in the regression, when significant, were interpreted as a bias in the parameter, while deviations in slope from a 1:1 relationship were interpreted as percentage over- or under- estimation of the parameter (i.e. $[\text{parameter slope} - 1] \cdot 100 = \% \text{ estimation error}$). All p-values were corrected for multiple testing using the p.adjust() function in R with Holm's method. All code and data will be made freely available on GitHub upon publication in the {arrhenius.comparison} R package (Stinziano & Murphy, 2020).

Results

Equations M2002 and J1942 exhibited similar performance

The performance between M2002 and J1942 for fitting $V_{\text{cmax},25}$ temperature responses were essentially identical when assessed based on BIC, with a slope of 1.001 ± 0.001 ($F_{1,195} = 5.52 \cdot 10^5$, $R^2 = 0.9996$, $P < 2.2 \cdot 10^{-16}$; Fig. **1a**), as was the case for $J_{\text{max},25}$ with a slope of 1.001 ± 0.001 ($F_{1,195} = 2.43 \cdot 10^6$, $R^2 = 0.9999$, $P < 2.2 \cdot 10^{-16}$; Fig. **1b**). However, while fitted temperature responses based on BIC appeared identical, the largest discrepancy between fitted responses was observed when comparing $J_{\text{max},25}$ of both plant species scaled across 10 °C and 50 °C (Figs. **1c-f**; note the differences between the blue and red hatched lines).

Estimates of $V_{\text{cmax},25}$ were essentially identical between the M2002 fitting (y-axis) and the J1942 fitting (x-axis) with a slope of 1.002 ± 0.004 ($F_{1,195} = 5.84 \cdot 10^4$, $R^2 = 0.9967$, $P < 2.2 \cdot 10^{-16}$; Fig. **2e**), as was the case for $J_{\text{max},25}$ with a slope of 1.001 ± 0.001 ($F_{1,195} = 6.56 \cdot 10^5$, $R^2 = 0.9997$, $P < 2.2 \cdot 10^{-16}$; Fig. **2f**). $E_{a,V_{\text{cmax}}}$ was generally underestimated with a slope of 0.847 ± 0.024 and a positive bias of 9.73 ± 2.59 kJ mol⁻¹ when using M2002 ($F_{1,194} = 1202$, $R^2 = 0.8610$, $P < 2.2 \cdot 10^{-16}$; Fig. **2a**), while $E_{a,J_{\text{max}}}$ was underestimated with a slope of 0.832 ± 0.013 and a positive bias of 5.98 ± 1.06 kJ mol⁻¹ ($F_{1,194} = 3834$, $R^2 = 0.9518$, $P < 2.2 \cdot 10^{-16}$; Fig. **2b**). $\Delta S_{V_{\text{cmax}}}$ was essentially identical between M2002 and J1942 with a slope of 1.000 ± 0.0233 ($F_{1,195} = 1849$, $R^2 = 0.9046$, $P < 2.2 \cdot 10^{-16}$; Fig. **2c**), as was the case with $\Delta S_{J_{\text{max}}}$ with a slope of 0.988 ± 0.033 ($F_{1,195} = 904$, $R^2 = 0.8226$, $P < 2.2 \cdot 10^{-16}$; Fig. **2d**), and $H_{d,V_{\text{cmax}}}$ with a slope of 1.002 ± 0.005 ($F_{1,195} = 4.12 \cdot 10^4$, $R^2 = 0.9953$, $P < 2.2 \cdot 10^{-16}$; Fig. **2g**). However, $H_{d,J_{\text{max}}}$ was underestimated with a slope of 0.952 ± 0.024 and a positive bias of 31.48 ± 8.93 kJ mol⁻¹ ($F_{1,194} = 1592$, $R^2 = 0.8914$, $P < 2.2 \cdot 10^{-16}$; Fig. **2h**).

Impacts on modelled net carbon balance

In general, the differences in thermal response parameters were amplified when integrated at the whole-plant level across a range of environmental conditions (Fig. **3**). For modelled daily photosynthesis (A), the slope for the low respiration model was 0.819 ± 0.013 and the intercept was 0.018 ± 0.002 g plant⁻¹ day⁻¹ (M2002 versus J1942; approximately 18% of modelled A) ($F_{1,3523} = 4.168 \cdot 10^3$, $R^2 = 0.5418$; $P < 2.2 \cdot 10^{-16}$) (Fig. **4a**). For the high respiration model of daily A, the slope was 0.819 ± 0.013 and the intercept was 0.031 ± 0.003 g plant⁻¹ day⁻¹ (approximately 18% of modelled A) ($F_{1,3523} = 4.168 \cdot 10^3$, $R^2 = 0.5418$; $P < 2.2 \cdot 10^{-16}$) (Fig. **4b**). The low respiration model of total daily carbon (C) gain had a slope of 0.836 ± 0.012 and an intercept of 0.012 ± 0.001 g plant⁻¹ day⁻¹ (approximately 16%

of modelled C gain) (M2002 versus J1942; $F_{1,3523} = 4.539 \cdot 10^3$, $R^2 = 0.5629$; $P < 2.2 \cdot 10^{-16}$) (Fig. 4c). The high respiration of total C gain similarly had a slope of 0.859 ± 0.012 and an intercept of 0.011 ± 0.002 g plant⁻¹ day⁻¹ (approximately 14% of modelled C gain) (M2002 versus J1942; $F_{1,3523} = 5.364 \cdot 10^3$, $R^2 = 0.6035$; $P < 2.2 \cdot 10^{-16}$) (Fig. 4d). The ratio of the total daily photosynthesis: respiration (A/R) was also considered when comparing models. The low respiration model of A/R had a slope of 0.982 ± 0.007 and the intercept was 0.146 ± 0.031 (approximately 2% of modelled A/R) (M2002 versus J1942; $F_{1,3523} = 2.096 \cdot 10^4$, $R^2 = 0.8561$; $P < 2.2 \cdot 10^{-16}$) (Fig. 4e). The high respiration model had a similar slope of 0.982 ± 0.007 and the intercept was 0.082 ± 0.017 (approximately 2% of modelled A/R) (M2002 versus J1942; $F_{1,3523} = 2.097 \cdot 10^4$, $R^2 = 0.8562$; $P < 2.2 \cdot 10^{-16}$) (Fig. 4f).

Discussion

We sought to determine whether the missing term in M2002 had a meaningful impact on fitted temperature response parameters due to its prevalence in photosynthetic temperature response data and vegetation modelling (Kattge & Knorr, 2007; Duursma & Medlyn, 2012; Rogers *et al.*, 2017; Smith & Dukes, 2017; Stinziano *et al.*, 2018; Stinziano *et al.*, 2019; Kumarathunge *et al.*, 2019). Our present analysis suggests that there is a large impact on E_a for both V_{cmax} and J_{max} , however there were minimal impacts on k_{25} , H_d , and ΔS (though note that $H_{d,Jmax}$ was underestimated) (Fig. 2). In general, fitting M2002 instead of J1942 results in E_a reductions of around 15% with positive bias, even though fitted responses are *visually* similar (Fig. 1). These findings are promising in that one of the parameters to which modelled carbon gain is particularly sensitive, H_d (Stinziano *et al.*, 2018), is minimally affected by the missing term. However, since temperature responses are non-linear, small changes in the shape of an accelerating curve can have a strong impact on the integral of the response (Jensen, 1906; e.g. changes in the shape of the temperature response of carbon assimilation can have strong impacts on total carbon fixation). Despite fit performance being nearly identical and visually similar (Fig. 1), the differences due to E_a values between the equations led to an 18% reduction in modelled daily photosynthesis for M2002 compared to J1942, leading to a ~14-16% reduction in modelled net daily carbon gain. Overall, comparisons of low-respiration to high-respiration scenarios resulted in similar percent changes in daily C balance with similar variation.

Not only did we compare the impact of the missing term in M2002 on different respiration scenarios, but we also modelled data across a range of environmental conditions to understand the impact on C balances of plants under different temperature regimes and how these impacts could scale up in global models. A ~15% reduction in net daily carbon gain is substantial by itself, but this difference would also be amplified over time for a single plant. Plant growth follows the compound interest law (Blackman, 1919). As leaf area increases with growth so too does the rate of photosynthesis and thus the amount of carbon available to further increase growth and metabolism, hence why relative growth rates are commonly utilized in the literature (e.g. Shipley, 1989; Causton, 1991; Tjoelker *et al.*, 1999; Loveys *et al.*, 2003; Poorter *et al.*, 2012; Pommereng & Anders, 2015). A reduction of 18% in modelled daily photosynthesis caused by using the modified equation with the missing term (M2002) would become compounded long-term with plant growth and may result in underestimations of future carbon uptake. It is thus likely that the differences we observed would accumulate to even larger carbon flux errors across large spatial and temporal scales with fluctuating temperatures.

Based on the above analysis, the impact of the missing term in the modified Arrhenius equation substantially alters E_a and net daily carbon balance at a whole-plant level. While our models of plant carbon uptake were indicative of problems caused by using M2002, it would be worth comparing how the use of this derivation has affected the interpretation of temperature response data and whole plant carbon balances collected from previous studies. Future work comparing the impact of using M2002 opposed to J1942 on interpreting whole tree carbon balance and net primary production data could lead to better estimations of the temperature sensitivity of carbon uptake. Given that carbon balance is the time integral of net CO_2 assimilation, this may also lead to substantial impacts over a long time period. On a larger scale, a correction of this derivation error will also be necessary when considering Earth system models, as 17 out of 40 models in the CMIP6 simulations are affected by the derivation error (Table 1). We therefore recommend the switch from M2002 to J1942 because: 1) M2002 is the result of a derivation error circa 1979, and 2) M2002 and J1942 lead to different net daily carbon estimates due to the derivation error, which may currently be compensated by other factors in large-scale models, most notably in the Community Land Model which currently relies on the M2002 equation (Bonan, 1996; Lawrence *et al.*, 2018) and underlies 30% of Earth System Models (Table 1).

322

323 **Acknowledgments**

324 We would like to thank Wesley J. Noe at the University of New Mexico for providing climate data. This
325 research was supported by personal funds.

326

327 **Author Contributions**

328 Both authors contributed to all aspects of the study.

329

330 **Additional Information**

331 A version of this manuscript was posted on bioRxiv (manuscript ID: BIORXIV/2020/921973).

332 **Tables**

333 **Table 1. List of land surface models affected by the derivation error in M2002 and the affected Earth Systems Models (ESMs) being used**
 334 **in the CMIP6 simulations. Note that 17 of the 40 (42.5%) CMIP6 ESMs are affected by the derivation error. Affected models are in bold.**

Land Surface Model Family		# of ESMs	Contains M2002?	Affected ESMs	References
Atmosphere-Vegetation Interaction Model	AVIM	2	No	BCC-CSM2-MR, BCC-ESM1	Ji, 1995
Community Atmosphere-Biosphere Land Exchange Model	CABLE	2	Yes	ACCESS-CM2, ACCESS-ESM1-5	Haverd et al., 2018
Canadian Land Surface Scheme	CLASS	1	Yes	CanESM5	Swart et al., 2019
Community Land Model	CLM	12	Yes	CAMS-CSM1-0, CESM2, CESM2-FV2, CESM2-WACCM, CESM2-WACCM-FV2, NorESM2-LM, NorESM2-MM, E3SM-1-0, FGOALS-f3-L, FGOALS-g3, TaiESM1, SAM0-UNICON	Bonan, 1996; Lawrence et al., 2018
Goddard Institute for Space Studies Global Circulation Model	GISS-GCM	3	No	GISS-E2-1-G, GISS-E2-1-H, GISS-E2-2-G	Friend & Kiang, 2005
Interaction Soil Biosphere	ISBAcc	3	No	CNRM-CM6-1, CNRM-CM6-1-HR, CNRM-ESM2-1	Calvet et al., 1998; Joetzjer et al., 2015
Atmosphere Carbon Cycle	JSBACH	4	No	AWI-CM-1-1-MR, MPI-ESM1-2-HR, MPI-ESM1-2-LR, NESM3	Rogers et al., 2017; Cao et al., 2018
Joint Scheme for Biosphere	JULES	3	No	HadGEM3-GC31-LL, HadGEM3-GC31-MM, UKESM	Clark et al., 2011
Atmosphere Coupling in Hamburg					
Joint UK Land Environment Simulator					
Land Model 4	LM4	2	No	GFDL-CM4, GFDL-ESM4	Milly et al., 2014
Lund-Potsdam-Jena Model	LPJ	3	No	EC-Earth3, EC-Earth3-Veg, IPSL-CM6A-LR	Sitch et al., 2003; Arora et al., 2020
Simple Biosphere Model	SiB	3	No*	INM-CM4-8, INM-CM5-0, MRI-ESM2-0	Sato et al., 1989; Volodin & Lykosov, 1998; Hosaka, 2011
Vegetation Integrative Simulator for Trace Gases	VISIT	2	Yes	MIROC6, MIROC-ESL2	Ito, 2010; Arora et al., 2020

335 *The SiB model does not include photosynthesis.

Table 2. Parameters used in modelling daily carbon gain.

Parameter	Group	Value	Reference
Respiration	R _{dark}	2.78 $\mu\text{mol m}^{-2} \text{s}^{-1}$	Stinziano & Way, 2017
	R _{day}	0.7 * R _{dark}	Ayub <i>et al.</i> , 2011
	R _{root}	0.0095 $\mu\text{mol g}^{-1} \text{s}^{-1}$	Weger & Guy, 1991
	R _{stem}	0.0095 $\mu\text{mol g}^{-1} \text{s}^{-1}$	Assumed
	Q ₁₀	2.015	Atkin & Tjoelker, 2003
Γ^*	25 °C	42.75 $\mu\text{mol mol}^{-1}$	Bernacchi <i>et al.</i> , 2001
	E _a	37.83 kJ mol^{-1}	Bernacchi <i>et al.</i> , 2001
K _m	25 °C	718.4 $\mu\text{mol mol}^{-1}$	Bernacchi <i>et al.</i> , 2001
	E _a	65.51 kJ mol^{-1}	Bernacchi <i>et al.</i> , 2001
α		0.8	Norman & Campbell, 1998
ϕ		0.08	Norman & Campbell, 1998
Leaf Area	Low R	0.015 m^2	Stinziano & Way, 2017
	High R	0.025 m^2	Stinziano & Way, 2017
Stem Mass	Low R	0.496 g	Stinziano & Way, 2017
	High R	2.523 g	Stinziano & Way, 2017
Root Mass	Low R	0.498 g	Stinziano & Way, 2017
	High R	5.072 g	Stinziano & Way, 2017

Q₁₀: thermal sensitivity coefficient; Γ^* : photorespiratory CO₂ compensation point; K_m: apparent Michaelis-Menten constant for rubisco carboxylation in 21% O₂/air (i.e. K_{c,air}); α : absorbance of photosynthetically activation radiation; ϕ : maximum quantum efficiency of photosynthetic electron transport; E_a: activation energy; R_{dark}: leaf respiration in the dark; R_{day}: leaf respiration in the light; R_{root}: root respiration; R_{stem}: stem respiration; Low R: low respiration scenario; High R: high respiration scenario.

345 **Table 3. Equations used in modelling daily carbon uptake.**

Equation	Reference
$f(T) = k_{25} Q_{10}^{\frac{T-298.15}{10}}$	Atkin & Tjoelker, 2003
$f(T) = k_{25} e^{\left[\frac{E_a(T-298.15)}{298.15RT}\right]}$	Arrhenius, 1915
$f(T) = k_{25} e^{\left[\frac{E_a(T-298.15)}{298.15RT}\right]} \left[\frac{1 + e^{\frac{298.15\Delta S - H_d}{298.15R}}}{1 + e^{\frac{T\Delta S - H_d}{RT}}} \right]$	Medlyn <i>et al.</i> , 2002
$f(T) = k_{25} \frac{T}{298.15} e^{\left[\frac{E_a(T-298.15)}{298.15RT}\right]} \left[\frac{1 + e^{\frac{298.15\Delta S - H_d}{298.15R}}}{1 + e^{\frac{T\Delta S - H_d}{RT}}} \right]$	Johnson <i>et al.</i> , 1942; this study
$W_c = V_{cmax} \frac{C_i - \Gamma^*}{C_i + K_m}$	Farquhar <i>et al.</i> , 1980
$W_j = J \left(\frac{C_i - \Gamma^*}{C_i + 2\Gamma^*} \right)$	Farquhar <i>et al.</i> , 1980; Way <i>et al.</i> , 2011
Where J is calculated as the minimum root of: $\theta J^2 - (0.5\alpha\phi Q_{in} + J_{max})J + 0.5\alpha\phi Q_{in}J_{max} = 0$	
$A_{gross} = \min(W_c, W_j)$	
$A_{net} = A_{gross} - R_{day}$	
$g_s = g_0 + 1.6 \left(1 + \frac{g_1}{\sqrt{VPD}} \right) \left(\frac{A_{net}}{C_a} \right)$	Medlyn <i>et al.</i> , 2011
$C_i = C_a - 1.6 \frac{A_{net}}{g_s}$	
$A_{plant} = A_{net} \times LA - R_{dark} \times LA - R_{stem} \times SM - R_{root} \times RM$	
$C_{balance} = \sum A_{plant} \times 3600 \times \frac{12.01}{1,000,000}$	
<p>346 f(T): rate of a process at a given temperature; T: temperature in K; k₂₅: rate of a process at 25 °C;</p> <p>347 Q₁₀: thermal sensitivity coefficient; E_a: activation energy in kJ mol⁻¹; ΔS: entropy parameter in kJ</p> <p>348 mol⁻¹; H_d: deactivation energy in kJ mol⁻¹; R: universal gas constant in 0.008314 kJ mol⁻¹ K⁻¹; W_c: rate</p> <p>349 of CO₂-limited carboxylation in μmol m⁻² s⁻¹; W_j: rate of RuBP regeneration-limited carboxylation in</p>	

$\mu\text{mol m}^{-2} \text{s}^{-1}$; V_{cmax} : maximum rate of rubisco carboxylation capacity in $\mu\text{mol m}^{-2} \text{s}^{-1}$; J_{max} : maximum rate of electron transport in $\mu\text{mol m}^{-2} \text{s}^{-1}$; C_i : intercellular CO_2 concentration in $\mu\text{mol mol}^{-1}$; Γ^* : photorespiratory CO_2 compensation point in $\mu\text{mol mol}^{-1}$; K_m : Michaelis-Menten constant for rubisco in $\mu\text{mol mol}^{-1}$; α : absorbance of photosynthetically active radiation; ϕ : maximum quantum efficiency of electron transport; Q_{in} : incident photosynthetically active radiation; A_{gross} : gross CO_2 assimilation in $\mu\text{mol m}^{-2} \text{s}^{-1}$; A_{net} : net CO_2 assimilation in $\mu\text{mol m}^{-2} \text{s}^{-1}$; R_{day} : leaf day respiration in $\mu\text{mol m}^{-2} \text{s}^{-1}$; g_s : stomatal conductance to water in $\text{mol m}^{-2} \text{s}^{-1}$; g_o : intercept for the Medlyn et al. 2011 model; g_1 : slope for the Medlyn et al. 2011 model; VPD: vapor pressure deficit in kPa; C_a : CO_2 concentration at the leaf surface in $\mu\text{mol mol}^{-1}$; A_{plant} : whole plant net CO_2 assimilation; LA: leaf area in m^2 ; R_{dark} : leaf dark respiration in $\mu\text{mol m}^{-2} \text{s}^{-1}$; R_{stem} : stem respiration in $\mu\text{mol m}^{-2} \text{s}^{-1}$; R_{root} : root respiration in $\mu\text{mol m}^{-2} \text{s}^{-1}$; SM: stem mass in g; RM: root mass in g; C_{balance} : whole plant daily carbon balance in $\text{g plant}^{-1} \text{day}^{-1}$.

Figure Captions

Figure 1. Relative performance and fit for Equations 3 (M2002) and 10 (J1942) for temperature responses of $V_{\text{cmax } 25}$ and $J_{\text{max } 25}$ based on a,b) Bayesian Information Criterion (BIC), and c-f) visual inspection of curve fits across 10-50 °C for c,d) *Elymus canadensis* and 20-50 °C of e,f) *Betula alleghaniensis*. Red dashed lines indicate curves fitted with the M2002 equation and blue dotted lines indicate curves fitted with the J1942 equation. Parameters for c-f) are as follows: c) M2002: k_{25} : 46.4 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 29.0 kJ mol^{-1} , ΔS : 0.692 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 221.4 kJ mol^{-1} ; J1942: k_{25} : 46.4 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 29.0 kJ mol^{-1} , ΔS : 0.655 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 209.0 kJ mol^{-1} ; d) M2002: k_{25} : 68.9 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 0.0 kJ mol^{-1} , ΔS : 0.746 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 240.5 kJ mol^{-1} ; J1942: k_{25} : 69.5 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 0.0 kJ mol^{-1} , ΔS : 0.625 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 201.0 kJ mol^{-1} ; e) M2002: k_{25} : 37.6 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 57.7 kJ mol^{-1} , ΔS : 0.579 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 185.4 kJ mol^{-1} ; J1942: k_{25} : 37.0 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 57.7 kJ mol^{-1} , ΔS : 0.557 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 178.1 kJ mol^{-1} ; f) M2002: k_{25} : 66.7 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 23.0 kJ mol^{-1} , ΔS : 0.761 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 246.6 kJ mol^{-1} ; J1942: k_{25} : 65.5 $\mu\text{mol m}^{-2} \text{s}^{-1}$, E_a : 23.0 kJ mol^{-1} , ΔS : 0.668 $\text{kJ mol}^{-1} \text{K}^{-1}$, H_d : 216.1 kJ mol^{-1} .

Figure 2. The modified Arrhenius equation missing the term (M2002) compared to J1942 fits different values for E_a (a,b), but mostly similar values for ΔS (c,d), k_{25} (e,f) and H_d (f, g) for both V_{cmax}

(a, c, e, g) and $J_{\max}$ (c, d, f, h). E_a : activation energy, ΔS : entropy parameter, k_{25} : rate of the process at 25 °C, H_d : deactivation energy, $V_{\max}$: maximum capacity of rubisco carboxylation, $J_{\max}$: maximum rate of electron transport. Black line indicates 1:1 line and grey dashed line indicates respective modelled slopes and intercepts.

Figure 3. Hourly environmental data used to drive the model in Table 3 covering 3 days (17th, 18th, and 19th) of 3 months. (a,c,e) Albuquerque, NM, USA (ABQ); (b,d,e) London, ON, Canada (LDN). Environmental parameters include: a,b) temperature; c,d) vapour pressure deficit; and e,f) irradiance (Q_{in}).

Figure 4. The modified Arrhenius equation without the missing term (M2002) gives differences in modelled daily carbon fluxes compared to J1942 for low R (a,c,e) and high R (b,d,f) under scenarios where H_d is allowed to vary. Modelled carbon fluxes include: a,b) Total daily photosynthesis; c,d) total daily C gain; and e,f) total daily A/R. A: photosynthesis, R respiration, Low R: low respiration, High R: high respiration. Black line indicates 1:1 line and grey dashed line indicates respective modelled slopes and intercepts.

Figures

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Supplementary information

Appendix A – Alternate derivations of the modified Arrhenius equation

Below are the temperature relativizations of Farquhar et al. (1980), Harley et al. (1986), and Harley et al. (1992) showing that Farquhar et al. (1980) and Harley et al. (1992) can be transformed to be identical to Equation 3 in the manuscript, while Harley et al. (1986) can be transformed to be identical to Equation 10 in the manuscript.

Farquhar et al. (1980)

From Eq. 36 in Farquhar et al. (1980):

$$k = \frac{c \times \exp [-E/(RT_k)]}{1 + \exp [(ST_k - H)/(RT_k)]} \quad \text{Equation A1}$$

Relativizing to 25 °C:

$$k/k_{25} = \left[\frac{c \times \exp [-E/(RT_k)]}{1 + \exp [(ST_k - H)/(298.15R)]} \right] \left[\frac{1 + \exp [(ST_k - H)/(298.15R)]}{c \times \exp [-E/(RT_k)]} \right] \quad \text{Equation A2}$$

Simplifying:

$$k/k_{25} = \exp [E/(298.15R) - E/(RT_k)] \left[\frac{1 + \exp [(S298.15 - H)/(298.15R)]}{1 + \exp [(ST_k - H)/(RT_k)]} \right] \quad \text{Equation A3}$$

$$k = k_{25} \exp \left[E \frac{(T_k - 298.15)}{(298.15RT_k)} \right] \left[\frac{1 + \exp [(298.15S - H)/(298.15R)]}{1 + \exp [(ST_k - H)/(RT_k)]} \right] \quad \text{Equation A4}$$

where E is activation energy (E_a), S is deactivation entropy (ΔS), and H is deactivation energy (H_d).

Harley et al. (1986)

From Eq. 7 in Harley et al. (1986):

$$k = \frac{T_k \exp [c - \Delta H_d/(RT_k)]}{1 + \exp [(\Delta ST_k - \Delta H_d)/(RT_k)]} \quad \text{Equation A5}$$

Relativizing to 25 °C:

$$k/k_{25} = \left[\frac{T_k \exp [c - \Delta H_d/(RT_k)]}{1 + \exp [(\Delta ST_k - \Delta H_d)/(RT_k)]} \right] \left[\frac{1 + \exp [(\Delta S298.15 - \Delta H_d)/(R298.15)]}{298.15 \exp [c - \Delta H_d/(R298.15)]} \right] \quad \text{Equation A6}$$

625 Simplifying:

$$626 \quad k/k_{25} = \frac{T_k}{298.15} \exp [\Delta H_a / (R298.15) - \Delta H_a / (RT_k)] \left[\frac{1 + \exp [(\Delta S298.15 - \Delta H_d) / (R298.15)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \right] \quad \text{Equation A7}$$

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$$628 \quad k = k_{25} \frac{T_k}{298.15} \exp \left[\Delta H_a \frac{(T_k - 298.15)}{(298.15 R T_k)} \right] \left[\frac{1 + \exp [(298.15 \Delta S - \Delta H_d) / (298.15 R)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \right] \quad \text{Equation A8}$$

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630 where ΔH_a is activation energy (E_a), and ΔH_d is deactivation energy (H_d).

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632 *Harley et al. (1992)*

633 From Eq. 9 in Harley et al. (1992):

$$634 \quad k = \frac{\exp [c - \Delta H_a / (RT_k)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \quad \text{Equation A9}$$

635

636 Relativizing to 25 °C:

$$637 \quad k/k_{25} = \left[\frac{\exp [c - \Delta H_a / (RT_k)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \right] \left[\frac{1 + \exp [(\Delta S298.15 - \Delta H_d) / (R298.15)]}{\exp [c - \Delta H_a / (R298.15)]} \right] \quad \text{Equation A10}$$

638

639 Simplifying:

$$640 \quad k/k_{25} = \exp [\Delta H_a / (R298.15) - \Delta H_a / (RT_k)] \left[\frac{1 + \exp [(\Delta S298.15 - \Delta H_d) / (R298.15)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \right] \quad \text{Equation A11}$$

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$$642 \quad k = k_{25} \exp \left[\Delta H_a \frac{(T_k - 298.15)}{(298.15 R T_k)} \right] \left[\frac{1 + \exp [(298.15 \Delta S - \Delta H_d) / (298.15 R)]}{1 + \exp [(\Delta S T_k - \Delta H_d) / (RT_k)]} \right] \quad \text{Equation A12}$$

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644 where ΔH_a is activation energy (E_a), and ΔH_d is deactivation energy (H_d).

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