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## 2 **A dynamic hydro-mechanical and biochemical model of stomatal** 3 **conductance for C<sub>4</sub> photosynthesis**

4 Chandra Bellasio, Joe Quirk, Thomas N. Buckley, and David J. Beerling

5

### 6 **Supporting notes**

7 **Note S1.** Equations to derive a set of key photosynthetic quantities consistent with Eqn 16 in the  
8 main paper.

9 A smoothed value for CO<sub>2</sub> concentration in the BS is given by:

$$C_{BS\ MOD} = \frac{C_{BS(C)} + C_{BS(J)} - \sqrt{(C_{BS(C)} + C_{BS(J)})^2 - 4\theta_A C_{BS(C)} C_{BS(J)}}}{2\theta_A}. \quad S1$$

10 Consistently,

$$V_{C\ MOD} = \frac{A_{MOD} + R_{LIGHT}}{1 - \gamma^* \frac{O_{BS}}{C_{BS\ MOD}}}, \quad S2$$

11 where O<sub>BS</sub> is calculated with Eqn 4.

12 V<sub>OMOD</sub> is given by:

$$V_{O\ MOD} = V_{C\ MOD} 2 \gamma^* \frac{O_{BS}}{C_{BS\ MOD}}. \quad S3$$

13 Leakiness is:

$$L_{MOD} = g_{BS}(C_{BS\ MOD} - C_M), \quad S4$$

14 where C<sub>M</sub> is calculated through Eqn 17.

15 Finally,

$$V_{P\ MOD} = L_{MOD} + A_{MOD} + R_M. \quad S5$$

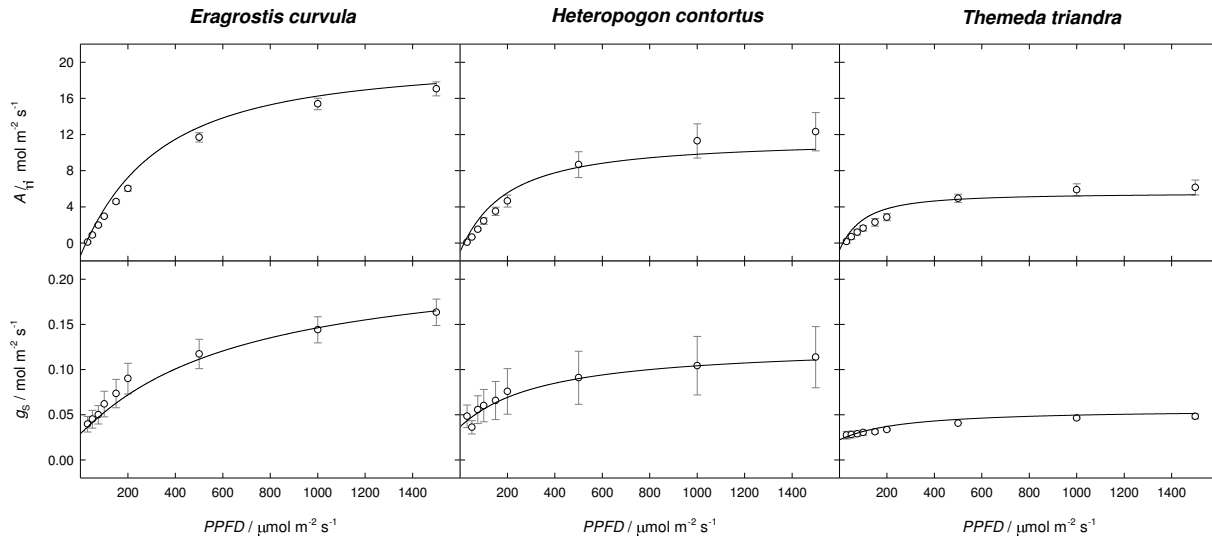
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18 **Supporting Figures**

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20 **Figure S1.** Responses to incident irradiance (PPFD) of assimilation rate, A<sub>H</sub> (top), and stomatal  
 21 conductance, g<sub>s</sub> (bottom), for three C<sub>4</sub> grasses: *Eragrostis curvula* (left), *Heteropogon contortus*  
 22 (middle) and *Themeda triandra* (right). Symbols show observed means ± S.E. (n = 8, 5 and 3,  
 23 respectively) and lines show model simulations.

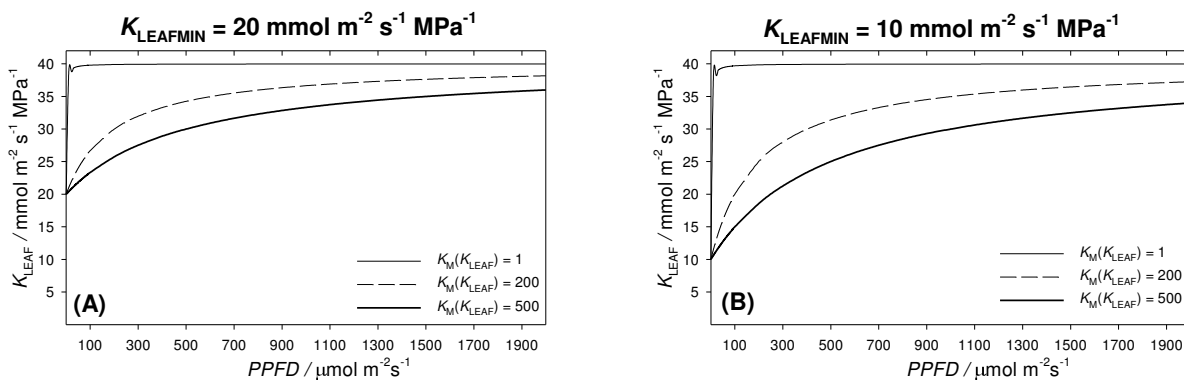


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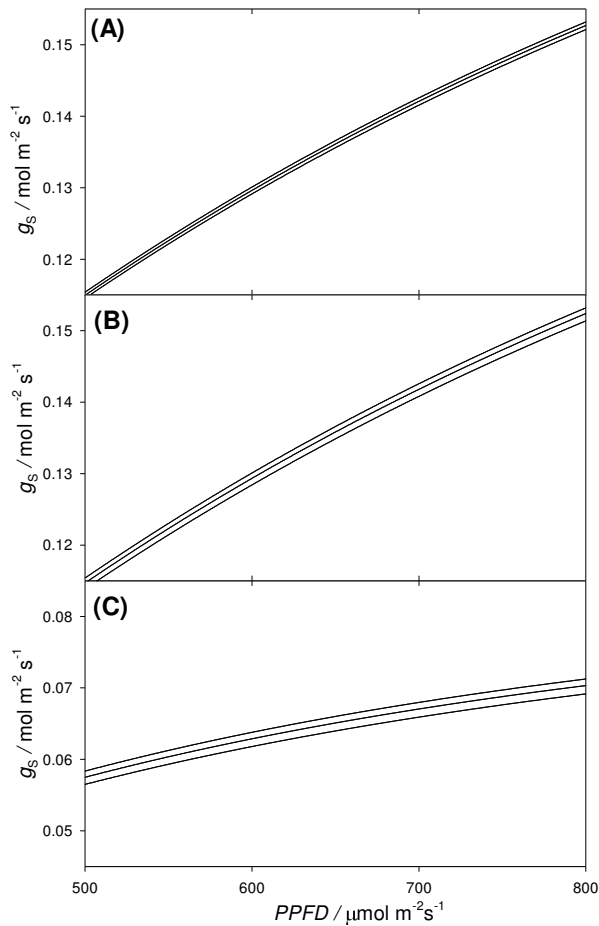
27 **Figure S2.** Simulated dynamics of K<sub>LEAF</sub> in response to PPFD. K<sub>LEAF</sub> increases from a value of  
 28 K<sub>LEAFMIN</sub>=20 mmol m<sup>-2</sup> s<sup>-1</sup> MPa<sup>-1</sup> (panel A) or K<sub>LEAFMIN</sub>=10 mmol m<sup>-2</sup> s<sup>-1</sup> MPa<sup>-1</sup> (panel B), with  
 29 three different induction patterns: an induction in the dark (K<sub>M</sub>(K<sub>LEAF</sub>)=1 μmol m<sup>-2</sup> s<sup>-1</sup>), an  
 30 induction in moderate light (K<sub>M</sub>(K<sub>LEAF</sub>)=200 μmol m<sup>-2</sup> s<sup>-1</sup>), or an induction in high light  
 31 (K<sub>M</sub>(K<sub>LEAF</sub>)=500 μmol m<sup>-2</sup> s<sup>-1</sup>).



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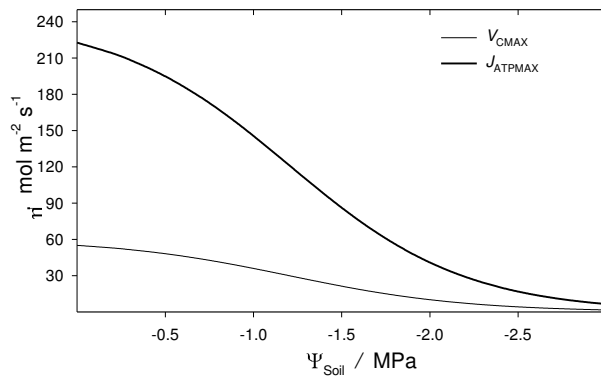
34 **Figure S3.** Simulated dynamics of  $g_s$  in response to PPFD, when  $K_{LEAF}$  is allowed to vary.  
 35 Three increasingly pronounced patterns were simulated. Panel **A** shows outputs generated for  
 36  $K_{LEAFMIN}=20 \text{ mmol m}^{-2} \text{ s}^{-1}$ ,  $D_S=10 \text{ mmol H}_2\text{O mol air}^{-1}$ ,  $\Psi_{Soil}=0 \text{ MPa}$ , with three different  
 37 induction patterns (see Figure S2):  $K_M(K_{LEAF})=1 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$ ,  $K_M(K_{LEAF})=200 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$ , or  
 38  $K_M(K_{LEAF})=500 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$  (curves from top to bottom). Panel **B** shows outputs generated for  
 39  $K_{LEAFMIN}=10 \text{ mmol m}^{-2} \text{ s}^{-1}$   $D_S=10 \text{ mmol H}_2\text{O mol air}^{-1}$ ,  $\Psi_{Soil}=0 \text{ MPa}$  and the same three  
 40  $K_M(K_{LEAF})$  described above. Panel **C** shows outputs generated for  $K_{LEAFMIN}=10 \text{ mmol m}^{-2} \text{ s}^{-1}$   
 41  $D_S=50 \text{ mmol H}_2\text{O mol air}^{-1}$ ,  $\Psi_{Soil}=-1 \text{ MPa}$  and the same three  $K_M(K_{LEAF})$  described above.



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44 **Figure S4.** Empirical correction of model inputs  $V_{\text{CMAX}}$  and  $J_{\text{ATPMAX}}$  for non-stomatal limitations  
45 under decreasing  $\Psi_{\text{Soil}}$  (Eqn 15).

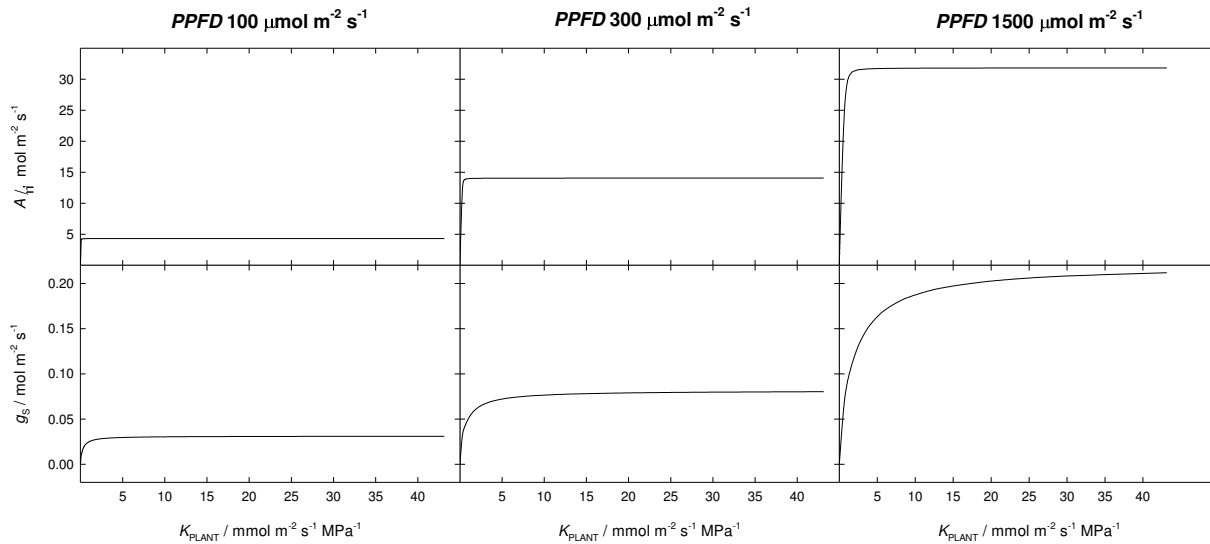


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49 **Figure S5.** Simulated responses of  $A$  and  $g_s$  to variable  $K_{\text{PLANT}}$  at three levels of PPFD. External  
50  $\text{CO}_2$  concentration  $C_a$  was set at  $400 \mu\text{mol mol}^{-1}$  and  $D_s$  at  $10 \text{ mmol mol}^{-1}$ , for other inputs see  
51 Table 1 of the main paper.



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54 **Supporting Tables**

55 **Table S1.** Additional definitions and units used in Table S2.

Symbol	Definition	Values / Units / source
$A_{SAT}$	CO <sub>2</sub> -saturated A, under the PPFD of A/C <sub>i</sub> -curves	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$b$	$\gamma$ -intercept of the $Y(II)$ - $Y(\text{CO}_2)$ linear fit i.e. the fraction of $Y(II)$ used by alternative ATP sinks	dimensionless (Valentini et al., 1995)
$F$	Photorespiration rate, or rate of photorespiratory CO <sub>2</sub> evolution $F = 0.5 \cdot V_O$	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$GA$	Gross assimilation, $GA=A+R_{LIGHT}$ . Represents the net biochemical CO <sub>2</sub> uptake $GA=V_C-F$	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$GA_{SAT}$	Light-saturated GA, under the CO <sub>2</sub> concentration of light-curves	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$g_{BS}$	BS conductance to CO <sub>2</sub> diffusion	$\text{mol m}^{-2} \text{s}^{-1}$
$J_{ATPSAT}$	Light-saturated ATP production rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$k'$	Slope of the linear fit of $Y(II)$ against $Y(\text{CO}_2)$	dimensionless (Valentini et al., 1995)
$LCP$	Light compensation point, i.e. PPFD when A=0. At the LCP ( $V_C=R_{LIGHT}+F$ ).	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$PPFD_{50}$	PPFD which half saturates either GA or J	$\mu\text{mol m}^{-2} \text{s}^{-1}$
$R_{LIGHT}$	Respiration in the light	$\mu\text{mol m}^{-2} \text{s}^{-1}$ $R_M = \frac{1}{2} R_{LIGHT}$
$s'$	A calibration factor to calculate $J_{ATP}$	dimensionless (Yin et al., 2004)
$V_{CMAX}$	CO <sub>2</sub> -saturated Rubisco carboxylation rate	$65 \mu\text{mol m}^{-2} \text{s}^{-1}$
$Y(\text{CO}_2)_{LL}$	Initial (or max.) quantum yield for CO <sub>2</sub> fixation, i.e. quanta required per CO <sub>2</sub> assimilated	CO <sub>2</sub> /Quanta, dimensionless
$Y(II)_{LL}$	Initial Yield of photosystem II $Y(II)$ extrapolated to PPFD=0	dimensionless
$Y(J_{ATP})_{LL}$	Initial (or max.) quantum yield for ATP production, i.e. conversion efficiency of PPFD into $J_{ATP}$	dimensionless
$\Gamma$	C <sub>i</sub> -A compensation point, i.e. C <sub>i</sub> at which A=0 and $V_C=R_{LIGHT}+F$	$\mu\text{mol mol}^{-1}$
$\gamma^*$	Half the reciprocal Rubisco specificity $\gamma^*=0.5/S_{C/O}$	0.000233 (Ubierna et al., 2016)
$\theta$	Curvature of the non-rectangular hyperbola describing the PPFD dependence of $J_{ATP}$	dimensionless
$\omega$	Curvature of the non-rectangular hyperbola describing the C <sub>i</sub> dependence of A	dimensionless
$m$	Curvature of the non-rectangular hyperbola describing the PPFD dependence of GA	dimensionless

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58 **Table S2.** Output obtained by analysing the primary gas exchange responses of maize plants,  
59 n=9. Quantities in bold were used in the simulations. The full dataset is in File S2.

Quantity	Unit	Method	Ambient O <sub>2</sub>		Low O <sub>2</sub>		Source
			Mean	S.E.	Mean	S.E.	
$R_{LIGHT}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Fluorescence-Light (Yin)	1.65	0.15	1.46	0.14	Gas Exchange
$Y(II)_{LL}$	dimensionless	Quadratic	0.693	0.012	0.660	0.012	Gas Exchange
LCP	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	25.3	2.8	22.0	2.6	Gas Exchange
$GA_{SAT}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	40.7	0.74	40.2	1.1	Gas Exchange
$Y(\text{CO}_2)_{LL}$	CO <sub>2</sub> /quanta	Hyperbola	0.0669	0.0018	0.0679	0.0014	Gas Exchange
$PPFD_{50}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	395	14	384	18	Gas Exchange
$m$	dimensionless	Hyperbola	0.714	0.029	0.708	0.040	Gas Exchange
$CE$	$\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	2.13	0.54	4.08	2.0	Gas Exchange
$A_{SAT}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	32.9	0.97	33.5	0.93	Gas Exchange
$\omega$	dimensionless	Hyperbola	0.601	0.10	0.633	0.13	Gas Exchange
$\Gamma$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Hyperbola	1.96	1.24	1.01	0.67	Gas Exchange
$s'$	CO <sub>2</sub> /quanta	Yin	–	–	0.312	0.0036	Gas Exchange
$k'$	quanta/CO <sub>2</sub>	Valentini	–	–	8.21	0.30	Gas Exchange
$b$	dimensionless	Valentini	–	–	0.0984	0.015	Gas Exchange
$Y(J_{ATP})_{LL}$	ATP/quanta	Valentini	0.363	0.0062	0.343	0.0051	Gas Exchange
$J_{ATPSAT}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Valentini	243	12	–	–	Gas Exchange
$\theta$	dimensionless	Valentini	0.583	0.061	–	–	Gas Exchange
$PPFD_{50}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Valentini	483	39	–	–	Gas Exchange
$g_{BS}$	$\text{mol m}^{-2} \text{s}^{-1}$	$J_{ATP}$ from Valentini	0.00147	$1.8 \times 10^{-4}$	–	–	Gas Exchange
$V_{P_{MAX}}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Mechanistic	94.9	8.9	–	–	Gas Exchange

60 **Table S3.** Input quantities for grasses simulations.  $J_{ATP_{MAX}}$ ,  $R_{LIGHT}$ ,  $V_{P_{MAX}}$  were obtained by  
 61 analysis of gas exchange data (the full dataset is in File S2) within the  $C_3$  and  $C_4$  photosynthesis  
 62 modelling framework of Bellasio et al. (2016) for three  $C_4$  grass species.  $\chi\beta$  was obtained by  
 63 fitting the output of Eqn 10 to the data in figure S1. Mean values ( $\pm 1$  S.D. in parenthesis).  $\theta$  was  
 64  $10^{-4}$ . All other inputs are the same as for maize and listed in Table 1 of the main paper.

Symbol	Units	<i>Eragrostis curvula</i>	<i>Heteropogon contortus</i>	<i>Themeda triandra</i>
$J_{MAX/SAT}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	153 (68.6)	35.9 (24.3)	43.5 (8.64)
$R_{LIGHT}$	$>0 \mu\text{mol m}^{-2} \text{s}^{-1}$	1.37 (0.22)	0.938 (0.066)	0.700 (0.171)
$V_{C_{MAX}}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	38.2 (17.2)	8.98 (6.06)	10.9 (2.16)
$V_{P_{MAX}}$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	36.0 (8.97)	15.3 (0.808)	11.24 (1.85)
$g_{S0}$	$\text{mol m}^{-2} \text{s}^{-1}$	0.0292 (0.012)	0.0367 (0.023)	0.0223 (0.004)
$\chi\beta$	$\text{mol air mmol}^{-1} \text{ATP s}^{-1} \text{MPa}^{-1}$	0.115	0.07	0.016

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