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# An analytical approach for estimating CO<sub>2</sub> and heat fluxes over the Amazonian region

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#### 10 Abstract

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Accurate assessments of the  $CO_2$  fluxes between the terrestrial ecosystems and the atmosphere are pressingly needed for the 11 climate change and carbon cycle studies. The Collatz et al. parameterization of leaf photosynthesis-stomatal conductance has 12 been widely applied in land surface parameterization schemes for simulating the land surface CO<sub>2</sub> fluxes. The study in this paper 13 developed an analytical solution approach for the Collatz et al.'s parameterization for stable solution and computational efficiency. 14 This analytical approach is then applied to the simplified biosphere model (SSiB), enhancing its capability of simulating land 15 surface CO<sub>2</sub> fluxes. The enhanced SSiB model is tested with field observation data sets from two Amazonian field experiments 16 (ABRACOS missions and Manaus Eddy Covariance Study). Simulations of the land surface fluxes of latent heat, sensible heat 17 and soil heat by the enhanced SSiB agree very well with observations with correlation coefficients being larger than 0.80. 18 However, the correlation coefficient for the daily means of  $CO_2$  fluxes is only 0.42 for the Manaus data set. A day-time "square 19 wave" in the simulated CO<sub>2</sub> flux diurnal curves is found. The discrepancies between simulation and observation were found to 20 be the results of incorrect parameter setup or improper leaf to canopy scaling strategy. A modification to the scaling strategy 21 22 improves significantly the accuracy of the photosynthesis-stomatal conductance model. 23 © 2002 Published by Elsevier Science B.V.

*Keywords*: Photosynthesis; Stomatal conductance; CO<sub>2</sub>; Energy balance; Simplified biosphere model (SSiB); Analytical solution; ABRACOS;
 LBA

#### 26 1. Introduction

Since the late 1970s, numerical modeling experiments using the coupled atmospheric and land surface models have been carried out to explore the relationship between land surface characteristics and the global as well as regional climate. These studies have shown that the changes in land surface characteristics,

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such as albedo, surface roughness length, vegetation 33 properties, and soil properties, could substantially al-34 ter terrestrial hydrologic system at global and regional 35 scales (see reviews by Sellers et al., 1997; Kabat and 36 Claaussen, 2002). In these studies, biophysical models 37 with different complexity have been developed. The 38 project for intercomparison of land-surface parameter-39 ization scheme (PILPS, Henderson-Seller et al., 1993, 40 1995) has also been carried out to evaluate and im-41 prove the land surface parameterizations, and, there-42 fore, to enhance the models' ability predicting the wa-43 ter cycle. In these models, however, empirical work 44

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had correlated stomatal conductance to the environmental conditions independent from any consideration
of photosynthesis. By the late 1980s, scientific interest on global change, particularly on the "greenhouse
effect" had promoted the development of more complete models, which directly couple water and carbon
cycle processes (Sellers et al., 1997).

Increase in greenhouse gases, in particular CO<sub>2</sub>, 52 has great impacts on global climate change. The po-53 tential importance of land carbon cycle to the global 54 climate was suggested in Cox et al. (2000) who per-55 formed future climate simulations with interactive 56 vegetation and ocean carbon cycles. Their simula-57 tions produced significant climate warming caused by 58 climate-induced loss of Amazonian rainforests. Re-59 cent studies have shown that terrestrial ecosystems, 60 especially tropical rain forest, may be an important 61 sink of atmospheric CO<sub>2</sub> (Tian et al., 2000; Schimel 62 et al., 2001). Regional studies based on in situ mea-63 surements are consistent with carbon sinks associated 64 with tropical forests (Phillips et al., 1998). The Ama-65 zon region contains the largest area of tropical forest 66 on Earth. Over the past 25 years, rapid development 67 has led to the destruction of over  $500,000 \,\mathrm{km^2}$  of 68 forest in Brazil (Houghton et al., 2000), producing a 69 large source for atmospheric CO<sub>2</sub>. Study has found 70 that the Amazonian region acted as a net source for 71 carbon in a range of  $0.2-1.2 \text{ Pg year}^{-1}$  from 1992 72 to 1993 mainly because of the deforestation (Keller 73 et al., 2001). Since emissions from land clearing in 74 the tropics are thought to be large, there must be off-75 setting sinks to balance these emissions. All of these 76 indicate a pressing need for accurate assessments of 77 the CO<sub>2</sub> fluxes between the terrestrial ecosystems and 78 79 the atmosphere.

Two efforts are required to address this need: one 80 is the observation of CO<sub>2</sub> fluxes between a terrestrial 81 ecosystem and the atmosphere in field for ground 82 truth; and the other is the development and validation 83 of models to understand the observed evidence and to 84 85 extrapolate the modeling results to the other regions. The first effort has been made in many large-scale 86 field experiments, one of which is the Large-Scale 87 Biosphere-Atmosphere Experiment in Amazonia 88 (LBA, Keller et al., 1997). A number of other field 89 data sets have been collected in this region for analy-90 ses and model validation. In the study of this paper, 91 the data from Anglo-Brazilian Amazonian Climate 92

Observation Study (ABRACOS, Gash et al., 1996)93and another measurement in central Amazonian rain94forest (Malhi et al., 1998) are used.95

In addition to field measurement, great deal of 96 effort has been carried out to develop plant photo-97 synthesis models since 1970s (Thornley and Johnson, 98 1990) and has gained more attention from the ecolog-90 ical science (Jorgensen, 1997) and climate modeling 100 communities (Sellers et al., 1992). This model de-101 velopment effort is still going on (Boonen et al., 102 2002). Collatz et al. (1991, 1992) combined the bio-103 chemical photosynthesis model in Farquhar et al. 104 (1980) with the semi-empirical stomatal conductance 105 model of Ball (1988) to estimate stomatal conduc-106 tance and photosynthesis rate of leaves simultane-107 ously. We will refer Collatz et al. parameterization of 108 leaf photosynthesis-stomatal conductance as Collatz 109 et al. model in this paper. Taking advantages of its 110 strong physical and biochemical bases, Sellers et al. 111 (1996a) adapted this coupled photosynthesis-stomatal 112 conductance model in the revised Simple Biosphere 113 model (SSiB\_2) for simulating land surface energy 114 and CO<sub>2</sub> fluxes by scaling up leaf responses to the 115 canopy level. The SSiB\_2 model has been applied 116 in global climate and carbon cycle studies (Sellers 117 et al., 1996a,b; Sellers et al., 1997; Denning et al., 118 1996a,b). However, the iterative solution used in the 119 photosynthesis-stomatal conductance model is com-120 putationally expensive and also may become numeri-121 cally unstable under certain environmental conditions 122 (Baldocchi, 1994). Proper procedure must be taken to 123 avoid such circumstances. In contrast, an analytical 124 solution for the coupled leaf photosynthesis-stomatal 125 conductance model can avoid these problems. 126

Baldocchi (1994) made an early attempt to derive an 127 analytical solution of the leaf photosynthesis equations 128 in Farquhar et al. (1980) and stomatal conductance in 129 Ball (1988). The equations used in Baldocchi (1994) 130 are similar to those in Collatz et al. (1991), but they dif-131 fer from those in Sellers et al. (1996a), which includes 132 scaling from leaf to vegetation canopies. In addition, 133 the version of the Collatz et al.' model in Sellers et al. 134 (1996a) considers broader environmental conditions. 135 For example, the photosynthesis equations of Collatz' 136 coupled model in Sellers et al. (1996a) takes accounts 137 of three photosynthetic limitations rather than the two 138 photosynthetic limitations considered by Baldocchi 139 (1994). Thus, an analytical approach for the Collatz' 140

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coupled model in Sellers et al. (1996a) should be dif-141 ferent from those in Baldocchi (1994). Because of the 142 wide applications of the Collatz et al. model (Bonan, 143 1995; Sellers et al., 1996a,b; Denning et al., 1996a,b; 144 145 Chen et al., 1999), deriving its analytical solutions of the more complex form should provide a useful ap-146 proach for the global climate and carbon cycling stud-147 ies. 148

The simplified biosphere model (SSiB) of Xue et al. 149 (1991) has been evaluated by observational data from 150 different vegetation types and different geographical 151 location, and has been broadly used in global and re-152 gional climate studies, including the LBA (for exam-153 ple, Xue et al., 1996a; Chou et al., 2002). However, 154 the current version of SSiB uses Jarvis' empirical ap-155 proach (Jarvis, 1976) for the formulation of stomatal 156 conductance. It does not consider the photosynthetic 157 activities of land surface vegetation and is thus unable 158 to estimate land surface CO<sub>2</sub> fluxes for carbon cycling 159 studies. In this paper, we attempt to enhance the SSiB 160 model by deriving an analytical solution from Col-161 latz et al. model and to apply it to SSiB. Replacing 162 the empirical stomatal resistance submodel in SSiB 163 with Collatz et al. model, the SSiB model is then re-164 vised to have the CO<sub>2</sub> flux simulation capability. To 165 test this extended capability of the SSiB model as a 166 part of our effort within the LBA frame, we ran the 167 model with the observational data from two large-scale 168 field experiments held in Amazonian tropical forests. 169 The output from the model is analyzed against their 170 corresponding field observations. Discrepancies be-171 tween simulation and observation were found as a re-172 sult of incorrect parameter setup or improper leaf to 173 canopy scaling strategy. A modification to the scal-174 175 ing strategy improves significantly the accuracy of the photosynthesis-stomatal conductance model. Finally, 176 further improvement of the revised SSiB model is dis-177 cussed. It is important to note that the net  $CO_2$  flux 178 from the land surface is a function of both photosyn-179 thetic uptake and respiratory release by plants and de-180 181 composition. The latter is not addressed here and will be the focus of future updates to the model. 182

#### 183 2. Collatz et al. model

The equations and parameterizations of plant photosynthesis  $A_n$  and stomatal conductance  $g_s$  developed



Fig. 1. Schematic diagram of Collatz' coupled photosynthesis-stomatal conductance model (canopy version in Sellers et al., 1996a). See Appendix A for symbol definition.

by Collatz et al. (1991) for C<sub>3</sub> plants and by Collatz 186 et al. (1992) for C<sub>4</sub> plants are scaled up from leaf to 187 canopy level in Sellers et al. (1996a). These equations 188 have sound physiological bases and thorough descrip-189 tions to the interactive effects of environmental fac-190 tors and stomatal control of plant photosynthesis and 191 transpiration. In the leaf to canopy scaling-up strat-192 egy used in Sellers et al. (1996a), a plant canopy is 193 simplified as a "big leaf". Fig. 1 is the schematic di-194 agram showing the exchanges of sensible heat, latent 195 heat and CO<sub>2</sub> between atmosphere and the canopy in 196 Collatz et al. model (1991, 1992). The formations of 197 Sellers et al. (1996a) can be summarized in the fol-198 lowing five equations: 199

$$A_n = \frac{g_{\rm b}}{1.4} \frac{C_{\rm a} - C_{\rm s}}{p}$$
(1) 200

$$A_n = \frac{g_s}{1.6} \frac{C_s - C_i}{p}$$
(2) 201

$$g_{\rm s} = m \frac{pA_n e_{\rm s}}{C_{\rm s} e^*(T_{\rm c})} + bF \tag{3}$$

$$A_n = \min(W_c, W_e, W_s) - R_d$$
 (4) 203

$$g_{\rm s}(e^*(T_{\rm c}) - e_{\rm s}) = g_{\rm b}(e_{\rm s} - e_{\rm a})$$
 (5) 204

The symbols in these equations are listed in Appendix 205 A. Eq. (1) describes CO<sub>2</sub> transfer rate from canopy 206

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airspace to leaf surface. Eq. (2) estimates CO<sub>2</sub> trans-207 fer rate from leaf surface to inside the stomata. Eq. (3) 208 shows the relationship between stomatal conductance 209 and photosynthesis at canopy scale based on Ball's 210 211 (1988) stomatal conductance model. Eq. (4) is the leaf biochemical model that includes the leaf to canopy 212 scaling approach of Sellers et al. (1992). Eq. (5) is 213 the conservation equation for water transfer from in-214 side stomata through stomata to the canopy airspace. 215 The three limitations ( $W_c$ ,  $W_e$  and  $W_s$ ) of photosyn-216 thetic rate in Eq. (4) are computed as follows for  $C_3$ 217 218 plants:

219 
$$W_{\rm c} = V_{\rm max} \frac{C_{\rm i} - \Gamma_*}{C_{\rm i} + K_{\rm c}(1 + O_{\rm i}/K_{\rm o})} \Pi$$
 (6)

$$W_{\rm e} = {\rm PAR}(1 - \omega_{\Pi})\varepsilon_3 \frac{C_{\rm i} - \Gamma_*}{C_{\rm i} + 2\Gamma_*} \Pi\left(\frac{\overline{G(\mu)}}{\mu}\right)$$
(7)

$$W_{\rm s} = 0.5 V_{\rm max} \Pi \tag{8}$$

For  $C_4$  plants, they are calculated with the following equations:

$$W_{\rm c} = V_{\rm max} \Pi \tag{9}$$

$$W_{\rm e} = {\rm PAR}(1 - \omega_{\Pi})\varepsilon_4 \Pi \left(\frac{\overline{G(\mu)}}{\mu}\right) \tag{10}$$

$$W_{\rm s} = V_{\rm max} 2 \times 10^4 \frac{C_{\rm i}}{p} \Pi \tag{11}$$

227 In these equations, the leaf to canopy scaling factor:

228 
$$\Pi = \frac{VN(1 - e^{-kF/VN})}{\bar{k}}$$
(12)

The inputs needed by these equations include PAR,  $T_a$ ,

230  $T_c$ ,  $e_a$ ,  $C_a$  and  $g_b$ . The unknown variables are  $A_n$ ,  $g_s$ , 231  $C_i$ ,  $C_s$  and  $e_s$  (see Appendix A for symbol definitions).

#### 232 3. Semi-analytical solution approach

Since Eqs. (1)–(5) are high-order non-linear functions, full analytical solutions cannot be obtained. Collatz et al. (1991, 1992) and Sellers et al. (1996a) use iterations to obtain numerical solutions. In this study, a semi-analytical solution procedure is developed. To simplify the solution, we first set the value of  $e_s$  to be the average of  $e_a$  and  $e^*(T_c)$ . Therefore, only Eqs. (1)–(4) are used to derive analytical solutions. We further rewrite Eq. (4) in a general form as follows: 242

$$A_n = A_1 \frac{C_i - A_2}{A_3 C_i + A_4} + A_5 \tag{13}$$

The expression for each  $A_i$  (i = 1, 2, 3, 4, 5) for C<sub>3</sub> 244 and C<sub>4</sub> plants is listed in Table 1. 245

If  $A_1 \neq 0$  and  $A_3 \neq 0$  in Eq. (13), a cubic equation 246 of  $C_i$  can be derived from Eqs. (1)–(3) and (13): 247

$$AC_i^3 + BC_i^2 + CC_i + D = 0 (14) 248$$

If  $A_1 \neq 0$  and  $A_3 = 0$  in Eq. (13), a quadratic equation 249 would be obtained: 250

$$a_{\rm c}C_{\rm i}^2 + b_{\rm c}C_{\rm i} + c_{\rm c} = 0 \tag{15}$$

A detailed derivation and the definitions of the coefficients in Eqs. (14) and (15) are presented in 253 Appendix B. 254

With the valid solution of  $C_i$  obtained from the 255 above procedure, we use Eq. (13) to computer  $A_n$  if 256  $A_3 \neq 0$ . Otherwise, 257

$$A_n = A_1 C_1 + A_5 \tag{16} 258$$

From the value of  $A_n$ , we can inverse Eq. (1) to obtain 259 the value of  $C_s$  and finally the value of  $g_s$  can be 260 obtained from Eq. (3). 261

Fig. 2 is a flow chart of the above semi-analytical 262 solution procedure. It starts from estimating the "leaf" 263 surface water vapor pressure with the average of the 264 canopy space water vapor pressure and the water va-265 por pressure insides the stomata. For any set of envi-266 ronmental conditions, the coefficients of Eq. (14) can 267 be computed with the equations in Appendix B. Then 268 an analytical solution of  $C_i$  can be obtained by ana-269 lytically solving the cubic equation. Once the value of 270  $C_{\rm i}$  corresponding to the set of the environmental con-271 ditions is obtained, the values of  $A_n$ ,  $g_s$ ,  $C_s$  and a new 272  $e_s$  can be obtained. The new  $e_s$  value is normally very 273 close to its previous value. If not, the coefficients of 274 Eq. (14) can be re-computed with the new  $e_s$  value 275 and the steps to solve the cubic equation and to com-276 pute the values of  $A_n$ ,  $g_s$ ,  $C_s$  and  $e_s$  will be repeated. 277 This procedure has two important aspects: (1) with the 278 analytic approach, the physically and biologically un-279 realistic solutions are avoided. Under any specific en-280 vironmental conditions, whether reasonable solutions 281 of the model can be obtained depends on whether the 282

225

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Plant type	Photosynthetic limitation	$A_1$	$\overline{A_2}$	A <sub>3</sub>	$A_4$	$A_5$
C <sub>3</sub>	W <sub>c</sub>	$V_{\max}\Pi$	$\Gamma_*$	1	$K_{\rm c}(1+O_{\rm i}/K_{\rm o})$	$-R_{\rm d}$
	We	$PAR(1 - \omega_{\Pi})\varepsilon_{3}\Pi(\overline{G(\mu)}/\mu)$	$\Gamma_*$	1	$2\Gamma_*$	$-R_{\rm d}$
	Ws	$0.5V_{\max}\Pi$	0	1	0	$-R_{\rm d}$
$C_4$	W <sub>c</sub>	$V_{\max}\Pi$	0	1	0	$-R_{\rm d}$
	We	$PAR(1 - \omega_{\Pi})\varepsilon_4\Pi(\overline{G(\mu)}/\mu)$	0	1	0	$-R_{\rm d}$
	Ws	$2 \times 10^4 (V_{\rm max}/p)\Pi$	0	0	1	$-R_{\rm d}$

lable 1	
Expressions of the variables $A_i$ $(i = 1, 2, 3, 4, 5)$ in Eq. (13)	

283 cubic equation of  $C_i$  has a realistic solution. We have tested the above method under a range of environmen-284 tal conditions, and have not found any case with no 285 valid solution. (2) The initial value of  $e_s$  is very close 286 to its solution when wind speed is not very large which 287 is true for most leaves within a canopy, so that ex-288 cluding  $e_s$  in the analytical solution procedure makes 289 the derivation simple. Although we list iteration for  $e_s$ 290 in Fig. 2, in most cases, no iteration is needed when 291 the initial conditions of  $e_s$  are selected as described 292 293 above.

Fig. 3 demonstrates the results from the above semi-294 analytical solution method compared with the re-295 sults from the iterative numerical solution method 296 for a set of typical environmental conditions listed 207 in Table 2. Sensitive parameters are also listed in 298 Table 2. Other parameter values are adopted from 299 Sellers et al. (1996a). The results are almost identi-300 cal in most cases except that the numerical solution 301

Table 2

The typical environmental conditions and model parameters for the plots in Fig. 3

Canopy leaf area index LAI	3.0
Above canopy $CO_2$ concentration $C_a$	34 Pa
Above canopy air temperature $T_a$	25 °C
Above canopy vapor pressure $e_a$	2000 Pa
"Leaf" boundary layer resistance rb	$50  { m s}  { m m}^{-1}$
Rubisco maximum catalytic capacity V <sub>max</sub>	$60 \mu mol m^{-2} s^{-1}$
PAR extinction coefficient $\kappa$	0.45
Time-mean projection of leaves $[G(\mu)/\mu]$	1.0
Photosynthesis optimal temperature top	30 °C
Photosynthesis minimum temperature $T_{low}$	15 °C
Photosynthesis maximum temperature $T_{high}$	45 °C

method may become unstable when the value of PAR  $_{302}$  becomes higher than 400 (W m<sup>-2</sup>). This confirms the  $_{303}$  potential instability problem in iterations as claimed  $_{304}$  in Baldocchi (1994).  $_{305}$ 



Fig. 2. The semi-analytical solution procedure for the Collatz et al.  $A_n$ - $r_s$  coupled model.

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Fig. 3. Comparison between the analytical and numerical solution methods for the Collatz et al.  $A_n - r_s$  coupled model. The symbols  $aA_n$ ,  $aW_c$ ,  $aW_e$ ,  $aW_s$  represent results from the analytical solution approach. The symbols  $nA_n$ ,  $nW_c$ ,  $nW_e$ ,  $nW_s$  are the results from the numerical iteration method.

# 306 4. Implementing Collatz et al. model in the307 simplified biosphere model (SSiB)

Stomatas on plant leaves control both water vapor 308 transfer from inside to outside and CO<sub>2</sub> transfer from 309 outside to inside as indicated in Fig. 1. The original 310 SSiB model (Xue et al., 1996a,b) simulates only the 311 water vapor transfer by using the Jarvis' empirical ap-312 proach (Jarvis, 1976) to compute the stomatal resis-313 tance  $r_{\rm c}$  to water vapor transfer. With the reasons stated 314 previously, we enhance the SSiB model with the CO<sub>2</sub> 315 simulation capability by replacing the submodel of 316 stomatal resistance in the original SSiB with the Col-317 latz et al. model introduced in the previous sections. 318

To compute the canopy resistance (the inverse of 319 320 canopy stomatal conductance) with the photosynthesis-stomatal conductance model (Eqs. (1)–(5)), one 321 322 needs to know the canopy airspace CO<sub>2</sub> concentration  $C_{\rm a}$ . The value of  $C_{\rm a}$  needs to be specified first, which 323 is the product of the balance of CO<sub>2</sub> fluxes into and 324 out of the canopy airspace. For a typical day-time, 325 the influxes include the CO<sub>2</sub> transfer from the at-326 mosphere and from the soil surface into the canopy 327

airspace, namely  $F_{ca}$  and  $F_{cs}$ . The sink of the canopy 328 airspace CO<sub>2</sub> is the canopy photosynthesis  $A_n$ . If  $F_{cs}$  329 and the CO<sub>2</sub> concentration of the atmosphere above 330 the canopy,  $C_m$ , are known, then we have 331

$$C_{\rm a} = C_{\rm m} - pr_{\rm a}(A_n - F_{\rm cs})$$
 (17) 332

because

$$F_{\rm ca} = \frac{C_{\rm m} - C_{\rm a}}{pr_{\rm a}} = A_n - F_{\rm cs}.$$
 (18) 334

333

Eq. (18) can be used to simulate the CO<sub>2</sub> flux above 335 a plant canopy. The soil respiration term  $F_{cs}$  in the 336 above equations will be the focus of future updates of 337 the model. In this paper, it is setup to be a constant 338 (e.g.  $F_{cs} = 4.0 \,\mu\text{mol m}^{-2} \,\text{s}^{-1}$  for the Manaus data set 339 described in Section 6.2). 340

Soil moisture is an important factor influencing the 341 carbon flux. In SSiB, the equation of the adjustment 342 factor  $f(\psi)$  of the stomatal conductance  $g_s$  for soil 343 moisture limitation is 344

$$f(\psi) = 1 - \exp\{-C_2[C_1 - \ln(-\psi)]\}$$
(19) 345

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where  $\psi$  is the soil water potential.  $C_2$  depends on the 346 vegetation type, and  $C_1$  is a constant obtained using 347 the wilting point. The stomates completely close at the 348 wilting point in the model.  $C_2$  is a slope factor. A large 349 350  $C_2$  means that the  $f(\psi)$  changes from 0 to 1 very fast when soil water content varies from wilting point to 351 the point stomates start to close. This approach differs 352 from that of Sellers et al. (1996a,b) who apply water 353 stress scaling to the maximum photosynthetic capacity 354  $(V_{\text{max}})$  rather than the stomatal conductance directly. 355 Note that in Table 1 of Xue et al. (1991) the values of 356  $C_1$  and  $C_2$  should be interchanged. 357

# **5.** Scaling up the Collatz et al. model from leaf to canopy

360 Fig. 3 indicates that canopy net photosynthesis rate gets saturated when photosynthetically active radia-361 tion PAR is greater than about 50 (W m<sup>-2</sup>). Accord-362 ing to field measurements introduced in Section 6 and 363 documentations in the literature (e.g. Thornley and 364 Johnson, 1990), this saturation PAR level for most 365 leaves is greater than 200 (W m<sup>-2</sup>). One of the causes 366 may be that implementation of the Collatz et al. model 367 in the SSiB\_2 model (Sellers et al., 1996a,b) assumes 368 equal acceptance of PAR by all leaves within a canopy 369 when the equations are integrated for all leaves in the 370 canopy. In reality, only sunlit leaves in plant canopy 371 receive direct PAR while shaded leaves receive diffu-372 373 sive PAR only. To consider this fact, we implement the Collatz et al. model for sunlit leaves and shaded leaves 374 separately while the equation set (Eqs. (1)–(12)) and 375 the analytical solution approach introduced previously 376 are kept the same. 377

Instead of using the total PAR for the Collatz et al. model, we separate PAR to direct radiation  $PAR_{dr}$ and diffusive radiation  $PAR_{df}$ . According to Norman (1982), if the PAR measurement above the canopy is PAR<sub>0</sub> and the fraction of diffusive PAR is  $f_d$ , then

384 
$$PAR_{df} = f_d PAR_0 \exp(-0.5F^{0.7})$$
  
385  $+ 0.07(1 - f_d) PAR_0(1.1 - 0.1F) e^{-\sin\theta_s}$   
386 (20)

PAR<sub>dr</sub> = 
$$\frac{(1 - f_d) PAR_0 \cos \theta_{ls}}{\sin \theta_s}$$
 (21)

З

where  $\theta_s$  is elevation angle of the sun and calculated 388 from the time of day, the day of year and the latitude of 389 observational site with the equation used in Campbell 390 (1977, p. 55). The  $\theta_{1s}$  is the mean angle between the 391 leaf normal and the sunlight. We select  $\theta_{ls} = 60^{\circ}$  for a 392 canopy with spherical leaf angle distribution (Norman, 393 1982). Accordingly, the PAR received by the sunlit 394 leaves  $PAR_{slt} = PAR_{dr} = PAR_{df}$  while the PAR re-395 ceived by the shaded leaves  $PAR_{shd} = PAR_{df}$ . 396

Assuming random leaf positioning and spherical 397leaf angle distribution, the sunlit leaf area index  $F_{slt}$  398as 399

$$F_{\rm slt} = 2[1 - \exp(-0.5F/\sin\theta_{\rm s})]\sin\theta_{\rm s}$$
(22) 400

the shaded leaf area index  $F_{\text{shd}} = F - F_{\text{slt}}$ .

Using PAR<sub>slt</sub> to run the analytical solution proce-402 dure for the Collatz et al. model introduced previously 403 for a unit sunlit leaf (leaf area index = 1.0), one ob-404 tains the net photosynthesis rate  $A_{nslt}$  and stomatal 405 conductance  $g_{slt}$ . Similarly using PAR<sub>shd</sub> for a unit 406 shaded leaf, one obtains  $A_{n \text{ shd}}$  and  $g_{\text{shd}}$ . The canopy 407 total net photosynthetic rate  $A_n$  and stomatal conduc-408 tance are then computed as 409

$$A_n = A_{nslt}F_{slt} + A_{nshd}F_{shd}$$
(23) 410

$$g_{\rm c} = \frac{1}{(F_{\rm slt}/g_{\rm slt}) + (F_{\rm shd}/g_{\rm shd})} \tag{24}$$

By this point, we have introduced three different ver-412 sions of implementing the Collatz et al. model of 413 plant photosynthesis and stomatal conductance: (1) 414 the original implementation in SSiB\_2 using iteration 415 solution method; (2) a modified version using analyt-416 ical solution method; and (3) another modified ver-417 sion using both the analytical solution method and the 418 sunlit-shaded leaf separation scaling method. For this 419 study of enhancing the SSiB for carbon simulation, 420 we use field measurements to evaluate the following 421 three versions of SSiB: (1) the original SSiB model 422 using Jarvis' stomatal model (for convenience we will 423 refer this version as SSiB\_0); (2) the SSiB model us-424 ing the Collatz et al. model in Sellers et al. (1996a) 425 modified with the analytical solution method (referred 426 to as SSiB\_1); and (3) the SSiB model using the Col-427 latz et al. model modified with the analytical solution 428 method and the sunlit-shaded leaf separation scaling 429 method (referred to as SSiB\_2). 430

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# 431 6. Field measurement data sets for model432 evaluation

Three data sets from two field experiments are used
to evaluate the enhanced SSiB model. The two field
experiments are the ABRACOS field experiment and
the Manaus Eddy Covariance Study.

#### 437 6.1. ABRACOS field experiment (1990 and 1991)

The ABRACOS is a comprehensive observational 438 study of land surface-atmosphere interactions in 439 large-scale clearings caused by tropical deforestation 440 (Shuttleworth et al., 1991). The main objective of 441 ABRACOS was to provide comparative data from ad-442 jacent forested and cleared areas, and to provide rep-443 resentative parameters and data from clearings for 444 GCM studies. The data used in this study were collec-445 ted during the first two experimental seasons of 446 ABRACOS at the Fazenda Dimona ranch site 447  $(02^{\circ}19'S, 60^{\circ}19'W)$ , 100 km north of Manaus in 448 central Amazonia. Mission 1 was conducted from 449 4 October to 2 November 1990 and Mission 2 was 450 451 conducted from 29 June to 10 September 1991. Vegetation at the experiment site is mainly C<sub>4</sub> grass. 452 Further details of the ranch and the experimental site 453 are described by Wright et al. (1992), McWilliams 454 et al. (1993), and Bastable et al. (1993). 455

The ABRACOS Mission 1 (M1) and Mission 2 456 (M2) data sets include incoming and reflected radia-457 tion of wavelength  $0.3-3.0 \,\mu\text{m}$ , global radiation, soil 458 heat flux, ambient air and wet-bulb temperatures, soil 459 temperature, precipitation, and wind speed and di-460 rection. Manufacturer supplied calibrations were used 461 462 for all the radiation instruments. The thermometers were calibrated against a standard and are accurate 463 464 to within  $\pm 0.1$  K. The data were recorded using solid state recorder, which sampled every 10 s. 465

Three measurement systems, including a Campbell 466 Scientific Ltd. (UK) Bowen-ratio system, the Mk 2 467 'Hydra' Eddy correlation device, and a logarithmic 468 wind and scalar profile measurement rig were used to 469 estimate fluxes of water vapor and sensible heat. There 470 was excellent agreement between the three measure-471 ment systems, the data from which were combined to 472 form a complete hourly time series record for each 473 experimental period. No CO<sub>2</sub> fluxes were measured 474 during ABRACOS. Therefore, this data set is used to 475



#### 6.2. Manaus Eddy Covariance Study (1996) 481

Another data set used for this paper was obtained 482 from an Eddy Covariance Study which was conducted 483 from 6 July 1995 to 24 August 1996 in the Reserva 484 Biologica do Cuieiras (2°35′22″S, 60°6′55″W), some 485 60 km north of Manaus (Malhi et al., 1998). This is 486 part of a very extensive, continuous area of dense low-487 land terra firm tropical rain forest. Vegetation of the 488 site is very similar to the site studied by Fan et al. 489 (1995). One of the primary focuses in the measure-490 ment is to examine and describe the nature and mag-491 nitude of the diurnal CO<sub>2</sub> flux and its relationship to 492 meteorological conditions (Williams et al., 1998). The 493 fluxes were measured in an Edisol Eddy covariance 494 system (Malhi et al., 1998). Meteorological data were 495 collected with an automatic weather station. The gas 496 analyzers were calibrated at least weekly using zero 497 and fixed concentration CO2 and water vapor sam-498 ples. Very little drift in analyzer concentration was 499 noted over a diurnal cycle or on a week-to-week ba-500 sis. Real time data were collected as 10 min average. 501 Corrections were applied for the dampening of fluc-502 tuations at high frequencies using the approach out-503 lined by Moore (1986) and Moncrieff et al. (1997). 504 For the study in this paper, the data collected only 505 from late December 1995 to mid-January, 1996 were 506 used because of the better continuity and certainty of 507 biophysical parameters. For convenience, this data set 508 is called "Manaus data". 509

#### 7. Results and discussion

510

The SSiB model will be used to study the impact 511 of land cover change in Amazonia region on the regional climate and carbon balance using the Collatz 513 et al. photosynthesis and stomatal conductance model. 514 Thus, proper simulations in both carbon flux and heat 515 fluxes are necessary. The original SSiB model using 516 the empirical Jarvis stomatal model (SSiB\_0) has produced reasonable simulations of heat fluxes in the 518



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off-line tests for Amazon sites (e.g. Xue et al., 1991,
1996a). As the first step, we must check whether the
more realistic but more complex approach for simulation of stomatal control is still able to yield reasonable
simulations in heat fluxes. Then we will evaluate how
the two modified SSiB versions (SSiB\_1 and SSiB\_2)
perform for the CO<sub>2</sub> flux simulations.

#### 526 7.1. Simulation of heat fluxes (SSiB\_0, SSiB\_1 and 527 SSiB\_2 versus observations)

In the off-line numerical experiments, we used ob-528 served temperature, humidity, and wind speed at the 529 reference height, precipitation and net radiation at the 530 surface as forcing to test SSiB. SSiB calculates en-531 ergy components, including the latent heat, sensible 532 heat, and ground heat fluxes, momentum flux, canopy 533 534 photosynthesis, and upward short wave and long wave radiation. All of these components, except long wave 535 radiation, were measured during ABRACOS field ex-536 periments. The values of vegetation parameters used 537 for this off-line validation were from measurements 538 in the ABRACOS field campaign and are listed in 539 Table 3. 540

ABRACOS intensive flux observations were made
for a continuous 30-day period during Mission 1 (M1)
and for 74 days during Mission 2 (M2). Figs. 4 and 5

Table 3

Vegetation	parameters	of	the	ABRACOS	data	set
recountion	parameters	<b>U</b> 1	unc	110101000	autu	

Vegetation parameters	Values
Surface albedo	0.18
Leaf area index (LAI)	1 (M1), 2 (M2)
Greenness	0.7 (M1), 0.9 (M2)
Vegetation cover fraction	0.85
Soil layer thicknesses (m)	0.02, 0.98, 1
Soil hydraulic conductivity at saturation $(ms^{-1})$	$2.2e^{-5}$
Sorption parameter, B	6.9
Soil water potential at saturation (m)	-0.035
Porosity	0.59
Minimum stomatal resistance (sm <sup>-1</sup> )	140
Adjustment factor for water vapor deficit	0.020
Adjustment factor for temperature	295, 276, 323
Adjustment factor for soil moisture	1.73, 5.8
Rooting depth (m)	1.0
Surface roughness length (m)	0.026
Displacement height (m)	0.18
Vegetation height (m)	0.28

Table	4		

Correlation coefficients between the hourly output of heat fluxes from the three model versions and the field observations

Flux	Model	ABRACOS Mission 1 (M1)	ABRACOS Mission 2 (M2)	Manaus
H	SSiB_0	0.87	0.91	0.86
	SSiB_1	0.88	0.90	0.91
	SSiB_2	0.88	0.89	0.91
LE	SSiB_0	0.94	0.96	0.96
	SSiB_1	0.94	0.97	0.97
	SSiB_2	0.94	0.95	0.98
G	SSiB_0	0.83	0.91	0.91
	SSiB_1	0.82	0.90	0.73
	SSiB_2	0.82	0.83	0.84

are the comparisons between the observed and sim-544 ulated daily means of latent heat, sensible heat and 545 soil heat fluxes for three versions of the SSiB model 546 (SSiB\_0, SSiB\_1 and SSiB\_2). The correlation coeffi-547 cients of the daily mean fluxes for the entire periods of 548 both M1 and M2 are listed in Table 4. The three ver-549 sions of SSiB produce very similar simulations for the 550 three fluxes. Fig. 5a shows that in M2 the simulated 551 latent heat flux closely follows observations. The ob-552 served latent heat fluxes dropped sharply several times 553 during M2 (3, 4, and 25 August and 2 September). 554 The model simulated these dramatic changes and re-555 covered very well. In M1, although the three versions 556 of the model generally followed the trend, the sim-557 ulations of the three heat fluxes fluctuated about the 558 observations (Fig. 4). In the early October, the mod-559 els underestimated latent heat flux and overestimated 560 sensible heat flux by about 30%. But in the middle 561 October, the model overestimated latent heat flux 562 and underestimated sensible heat flux by about 20%. 563 These fluctuations might result from the biases of soil 564 heat flux simulations from their observations (Fig. 4c). 565 In general, the simulations of the heat fluxes from 566 the two modified SSiB versions (SSiB\_1 and SSiB\_2) 567 are very similar to those from the original SSiB 568 (SSiB\_0). 569

For the Manus data set, detailed soil and vegetation 570 information was not available except that the vegetation cover of the study site is a continuous area of 572 dense lowland terra firm tropical rainforest and that 573 the leaf area index was 5–6 and canopy height 30 m 574 according to Malhi et al. (1998). In an off-line test, 575 it is important to have a proper set of vegetation and 576

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Fig. 4. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Mission 1 of the ABRACOS field experiment (line marked with open circles), the simulations of SSiB\_0 (solid squares), the simulations of SSiB\_1 (solid circles) and the simulations of SSiB\_2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

soil parameters and it may cause systematic errors if
these parameters are not setup correctly (Xue et al.,
1996b; Xue et al., 1997). Because we have no measured surface vegetation and soil information, we use
the vegetation and soil parameters from a vegetation
and soil parameter table, which is used in the cou-

pled atmospheric/SSiB model (e.g. Xue et al., 2001). 583 In this study, we base on the above-mentioned vegetation type information to specify the land parameter values. Fig. 6 shows the result from three versions of SSiB. It is evident that all three versions are able to simulate the variability in latent heat, sensible heat



Fig. 5. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Mission 2 of the ABRACOS field experiment (line marked with open circles), the simulations of SSiB\_0 (solid squares), the simulations of SSiB\_1 (solid circles) and the simulations of SSiB\_2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

and soil heat fluxes well. The correlations between the
model outputs and the field observations are similar to
the results for the ABROCOS data sets (Table 4). This
result further indicates that the two modified versions
of SSiB do not compromise the capability of the original SSiB in simulating the latent heat, sensible heat
and soil heat fluxes.

7.2. Simulations of CO<sub>2</sub> flux (SSiB\_1 and SSiB\_2 596 versus observations) 597

The primary goal of this work is to enhance the 598 SSiB model with  $CO_2$  flux simulation capability. How 599 the two modified versions of the SSiB model perform in  $CO_2$  flux simulation is of the most concern. 601

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Fig. 6. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Eddy Covariance Study (line marked with open circles), the simulations of SSiB\_0 (solid squares), the simulations of SSiB\_1 (solid circles) and the simulations of SSiB\_2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

Using the only CO<sub>2</sub> flux measurements in the Manaus data set, we can find the answer to this question from the results demonstrated in the following figures.

Fig. 7 is a comparison between the simulations (marked with solid) circles) by (a) SSiB\_1 or (b) SSiB\_2 and their corresponding observations (open circles) of the above canopy hourly  $CO_2$  flux for 609 the 26 days in the Manaus data set. The correlation 610 coefficient between the hourly simulation and field 611 observation is 0.73 for SSiB\_1 and 0.84 for SSiB\_2. 612 Although both SSiB\_1 and SSiB\_2 simulated the 613 diurnal cycles of the  $CO_2$  flux, the simulations by 614 SSiB\_1, which uses the same leaf to canopy scaling 615

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Fig. 7. The hourly above canopy  $CO_2$  flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB\_1; (b) for SSiB\_2. Negative value means that  $CO_2$  is transported from the above canopy atmosphere downward to the canopy.

strategy as in SSiB\_2 (Sellers et al., 1996a), have very 616 similar maximums during midday for all 26 days. 617 The simulations by SSiB\_2, which computes net pho-618 tosynthetic rate and stomatal conductance for sunlit 619 and shaded leaves, respectively, have diurnal cycles 620 varying mainly with incoming photosynthetically ac-621 tive radiation. The observed diurnal cycles of  $CO_2$ 622 flux follow the PAR diurnal pattern. Thus, the SSiB\_2 623

simulations have a higher correlation coefficient 624 (0.84).

**Fig. 8** is the diurnal cycles of the model simulations 626 plotted against the field observations averaged over 627 the 26 days. Despite general consistency of the simulations of both SSiB\_1 and SSiB\_2 with observations, 629 a noontime square wave in the simulations of SSiB\_1 630 is evident. To more clearly examine the difference in 631

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Fig. 8. The averaged diurnal curve of the above canopy  $CO_2$  flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB\_1; (b) SSiB\_2. Negative value means that  $CO_2$  is transported from the above canopy atmosphere downward to the canopy.

the CO<sub>2</sub> flux diurnal cycle simulations by SSiB\_1 and SSiB\_2, the simulated plant photosynthetic rate  $A_n$ and their three limitations (namely, the RuBP saturation limited rate  $W_c$ , the electron transportation limited rate  $W_e$ , and the sink limited rate  $W_s$ ) averaged over the 26 days are plotted in Fig. 9 for SSiB\_1 and Fig. 10 for SSiB\_2. As in Eq. (4), the photosynthetic rate  $A_n$  is the minimum of these three limitations adjusted with a quadratic equation (Collatz et al., 1991). 640 Thus, the curve of net photosynthetic rate  $A_n$  in Fig. 9 641 goes beneath the lowest of  $W_c$ ,  $W_e$  and  $W_s$ . For most 642 of the day-time,  $W_c$  simulated by SSiB\_1 is the lowest 643 and does not change much for more than 6 h around 644 noontime. Thus, the net photosynthetic rate  $A_n$  follows 645

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Fig. 9. The averaged diurnal curve of the canopy  $CO_2$  photosynthetic rate and its three components simulated by Phost\_1. Canopy net photosynthesis rate  $A_n$  is marked with solid squares. The Rubisco limitation  $W_c$  is open circles. The PAR limitation  $W_e$  is solid circles. The sink limitation  $W_s$  is open squares.

 $W_{\rm c}$  and shows a day-time square wave. This day-time 646 square wave is not consistent with observations well 647 documented in the literature (Thornley and Johnson, 648 1990). One of the reasons for this incorrect simula-649 tion by SSiB\_1 in Fig. 9 may be that the parameters 650 of the Collatz et al. model were setup incorrectly so 651 that the simulations of  $W_{\rm e}$  are too large or the com-652 puted values of  $W_c$  or  $W_s$  are too small. However, 653 as stated in Section 5, an apparent reason for the in-654 correct simulation of SSiB\_1 is the strategy of scal-655 656 ing the Collatz et al. model from leaf to canopy in Sellers et al. (1996a). The scaling-up method treats all 657 leaves within the plant canopy the same way. This may 658 have underestimated the light saturation phenomenon 659 of plant leaves (Chen et al., 1999). This underestima-660 tion of light situation may have caused the simulation 661

of  $W_e$  being too high. SSiB\_2 attempts to avoid this problem by implementing the Collatz et al. model to sunlit leaves and shaded leaves separately. The results shown in Figs. 7b and 8b from SSiB\_2 demonstrated significant improvement. 666

Fig. 10 plots the daily above canopy  $CO_2$  flux av-667 erages of the model simulations and their field obser-668 vations. For SSiB\_1, because of the unrealistic square 669 wave in the diurnal variation of plant photosynthetic 670 rate, the simulated daily above canopy CO<sub>2</sub> flux av-671 erages (solid circles) do not match the observations 672 well (open circles). For SSiB\_2, its simulations (open 673 squares) improve obviously over the simulation by 674 SSiB\_1. The correlation coefficient between the aver-675 ages of the simulated daily above canopy CO<sub>2</sub> flux 676 and their corresponding observations is only 0.42 for 677

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Fig. 10. The daily means of the above canopy  $CO_2$  flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB\_1; (b) for SSiB\_2. Negative value means that  $CO_2$  is transported from the above canopy atmosphere downward to the canopy.

SSiB\_1 and 0.80 for SSiB\_2. In this paper, we set the soil respiration rate as a constant. It will be the focus of further studies to improve the capability of the SSiB model in CO<sub>2</sub> flux simulations. With a more realistic simulation of  $F_{cs}$  in Eq. (18), the simulation result of  $F_{ca}$  by SSiB\_2 is expected to be even better.

#### 8. Conclusions

685

Using three data sets collected from two large-scale 686 field experiments, this study aims to improve the solution method and scaling-up approach of the Collatz 688 et al. model of plant photosynthesis and stomatal conductance in order to implement the model in the SSiB 690

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for  $CO_2$  flux simulations. From the results obtained we can make the following conclusions: tation in the SSiB model improves the photosynthesis and  $CO_2$  flux simulations significantly. 710

(1) The Collatz et al. model of plant photosynthe sis and stomatal conductance can solved with
 a semi-analytic method, which brings with bet ter computational efficiency and stability for
 the coupled land surface-atmosphere interaction
 models.

 (2) Implementation of the analytic solution approach for CO<sub>2</sub> flux solution in the SSiB model produces reasonable simulations of latent heat, sensible heat and soil heat fluxes and enhances the SSiB into a new generation model.

(3) The leaf to canopy scaling-up strategy used in Sellers et al. (1996a) for the implementation of the Collatz et al. model results in a day-time square wave in the net photosynthetic rate simulations. Considering the sunlit leaves and shaded leaves separately in the Collatz et al. model implemen-

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Symbol	Units	Definition
$\overline{A_n}$	$\mu mol m^{-2} s^{-1}$	Net $CO_2$ assimilation of the canopy
$A, A_i \ (i = 1, \ldots, 7), a_c$		Interim variables for the analytic solutions
$B, B_1, B_2, b_c$		Interim variables for the analytic solutions
b	$\mu$ mol m $^{-2}$ s $^{-1}$	Coefficient in Eq. $(3)$ (0.01 for C <sub>3</sub> , 0.04 for C <sub>4</sub> vegetation)
C, <i>c</i> <sub>c</sub>		Interim variables for the analytic solutions
$C_{\mathrm{a}}$	Ра	$CO_2$ concentration of the atmosphere
Ci	Ра	$CO_2$ concentration inside plant leaves
Cs	Ра	$CO_2$ concentration at leaf surface
$C_1, C_2$		Empirical coefficients of soil moisture adjustment factor,
		Eq. (19)
ea	Pa	Water vapor pressure at the reference height
$e^*(T)$	Pa	Saturation vapor pressure at temperature $T$
es	Pa	Water vapor pressure at leaf surface
$\varepsilon_3/\varepsilon_4$	$mol mol^{-1}$	Intrinsic quantum efficiency of leaf photosynthesis for
		$C_3/C_4$ plant*
$F_{ca}$	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	$CO_2$ flux above land surface
F <sub>cs</sub>	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	$CO_2$ flux from the soil surface
F	$m^2 m^{-2}$	Canopy leaf area index
$F_{\rm shd}$	$m^2 m^{-2}$	Shaded leaf area index
$F_{\rm slt}$	$m^2 m^{-2}$	Sunlit leaf area index
fd		Fraction of diffusive radiation in total radiation
$f(\psi)$		Adjustment factor to count for soil moisture effect
J N I /		5

Appendix A. List of symbols with units and definition

17

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Symbol	Units	Definition
$\overline{G(\mu)}$		Projection of leaves in direction of incoming radiation flux*
<i>g</i> <sub>b</sub>	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	Leaf boundary layer aerodynamic conductance
g <sub>s</sub>	$\mu mol m^{-2} s^{-1}$	Stomatal conductance to latent and sensible heat transfer
$\Gamma_{*}$	$\mu$ mol mol <sup>-1</sup>	The CO <sub>2</sub> compensation point of the leaves*
- ↑ 1/	$Pa K^{-1}$	Psychometric constant
h.		Relative humidity within the leaf surface boundary layer
K.	umol mol <sup>-1</sup>	Michaelis-Menten competitive inhibition constant for
nc	µmor mor	$CO_2^*$
Ko	$\mu mol mol^{-1}$	Michaelis–Menten competitive inhibition constant for $O_2^*$
$\overline{k}$		Time-mean value of radiation extinction coefficient*
т		Coefficient in Eq. $(3)$ (9 for C <sub>3</sub> , 4 for C <sub>4</sub> vegetation)
Ν		Canopy green leaf fraction
<i>O</i> i	$\mu$ mol mol <sup>-1</sup>	Internal $O_2$ concentration of the leaves
P		Interim variables for the analytic solutions
PAR. $PAR_0$	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	Photosynthetically active radiation above the canopy
PARdr	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	Direct photosynthetically active radiation above the
u		canopy
PAR <sub>df</sub>	$\mu molm^{-2}s^{-1}$	Diffusive photosynthetically active radiation above the canopy
PAR <sub>s1t</sub>	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	PAR received by sunlit leaves
PAR <sub>shd</sub>	$\mu mol m^{-2} s^{-1}$	PAR received by shaded leaves
n	Pa	Air pressure
Р V	Pa	Soil water potential
Π		Leaf to canopy scaling factor (see Eq. (12))
0		Interim variables for the analytic solutions
$\tilde{R}_{\rm d}$	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	The dark respiration rate of the canopy
r <sub>o</sub>		Aerodynamic resistance of the air above the canopy to
- a		the measurement height
0Cn	$J m^{-3} K^{-1}$	Volumetric heat capacity of air
рер T <sub>o</sub>	°C	Air temperature at the reference height
$T_{a}$	°Č	Integrated leaf temperature of the canopy
$\theta_{c}$	•	Sun elevation angle
$\theta_{1c}$	0	Mean angle between leaf normal and sunlight
		Direction of incoming radiation flux
μα V	$mol m^{-2} s^{-1}$	Maximum RuBP carboxylation rate
v max V		Capopy cover fraction
, W	$mol m^{-2} s^{-1}$	Rubisco-limited rate of CO <sub>2</sub> assimilation
W	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	Electron transportation limited CO <sub>2</sub> assimilation rate
we W	$\mu$ mol m <sup>-2</sup> s <sup>-1</sup>	Product sink limited rote of CO <sub>2</sub> assimilation
w <sub>s</sub>	µmorm s	L a f souttering coefficient for DAP (Sollars et al. 1006c)
$\omega_{\Pi}$		Lear-scattering coefficient for PAR (Sellers et al., 1996a)

### Appendix A. (Continued)

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#### 726 Appendix B. Analytical solutions of Eq. (14)

728 
$$A = A_3 A_6 m h_s g_b^2 p + A_3 B_1 b g_b F$$
 (A.1)  
729 (A.1)

730 
$$B = g_{b}p(A_{6}((1.6 - mh_{s})B_{1} + A_{4}mh_{s}g_{b})$$
  
731 
$$+A_{3}A_{7}mh_{s}g_{b}) + bF(A_{4}B_{1}g_{b}$$
  
732 
$$+A_{3}B_{2}g_{b} - B_{1}^{2})$$
(A.2)  
733

734 
$$C = g_b p(A_6(1.6 - mh_s)B_2 + A_7(1.6 - mh_s)B_1$$
  
735  $+A_4mh_sg_b) + bF(A_4B_2g_b - 2B_1B_2)$  (A.3)

736 
$$D = A_7 B_2 (1.6 - mh_s) g_b p - B_2^2 bF$$
 (A.4)

738 
$$A_6 = A_1 + A_3 A_5$$
 (A.5)

739 
$$A_7 = A_4 A_5 - A_1 A_2 \tag{A.6}$$

740 
$$B_1 = C_a g_b A_3 - 1.4 p A_6$$
 (A.7)

741 
$$B_2 = C_a g_b A_4 - 1.4 p A_7 \tag{A.8}$$

742 
$$h_{\rm s} = e_{\rm s}/e_{\rm s}^*(T_{\rm c})$$
 (A.9)

743 If we define  $P = (C/A) - (B^2/3A^2)$  and  $Q = (D/A) + (2B^3/27A^3) - (BC/3A^2)$ , then the discrim-745 inator of Eq. (14) is

$$\Delta = \left(\frac{Q}{2}\right)^2 + \left(\frac{P}{3}\right)^3 \tag{A.10}$$

147 If  $(\Delta \ge 0)$ , the cubic Eq. (14) has only one valid solution. If  $(\Delta < 0)$ , Eq. (14) yields three roots. These roots can be computed with equations listed in most mathematical handbooks. The valid solution is the positive minimum of the three, that is

752 
$$C_i = \min(x_1, x_2, x_3)$$
 (A.11)

If  $A_1 \neq 0$  and  $A_3 = 0$  in Eq. (13), Eq. (14) becomes the following quadratic equation:

755 
$$a_{\rm c}C_{\rm i}^2 + b_{\rm c}C_{\rm i} + c_{\rm c} = 0$$
 (A.12)

756 where

758 
$$a_{\rm c} = g_{\rm b}pA_1(1.4pA_1(1.6 - mh_{\rm s}) - mh_{\rm s}g_{\rm b})$$
  
759  $+bF(1.4pA_1(1.4pA_1 + g_{\rm b}))$  (A.13)

$$b_{\rm c} = -g_{\rm b}pA_1 1.4pA_1 (C_{\rm a}g_{\rm b} - 1.4pA_5)$$
761

$$+A_5g_bp(1.4pA_1(1.6 - mh_s) - mh_sg_b)$$
 762

$$+bF(2.8pA_1 + g_b)(C_ag_b - 1.4pA_5)$$
 (A.14) 763  
764

$$c_{\rm c} = -g_{\rm b}pA_5(1.6 - mh_{\rm s})(C_{\rm a}g_{\rm b} - 1.4pA_5)$$
<sup>765</sup>

$$+bF(C_ag_b - 1.4pA_5)^2$$
 (A.15) 766

The discriminator of Eq. 
$$(A.12)$$
 is

$$\Delta_2 = b_{\rm c}^2 - 4a_{\rm c}c_{\rm c} \tag{A.16}$$

When  $(\Delta_2 \ge 0)$ , the quadratic equation has two roots. 769 These two roots can be computed with equations listed 770 in most mathematical handbooks. The minimum of 771 them is the valid value for  $C_i$  if it is greater than zero, 772 that is 773

$$C_{\rm i} = \min(x_1, x_2)$$
 (A.17) 774

If  $\Delta_2 < 0$ , then the equation has no valid solutions. 775

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