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An analytical approach for estimating CO₂ and heat fluxes over the Amazonian region

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Abstract

Accurate assessments of the CO₂ fluxes between the terrestrial ecosystems and the atmosphere are pressingly needed for the climate change and carbon cycle studies. The Collatz et al. parameterization of leaf photosynthesis-stomatal conductance has been widely applied in land surface parameterization schemes for simulating the land surface CO₂ fluxes. The study in this paper developed an analytical solution approach for the Collatz et al.'s parameterization for stable solution and computational efficiency. This analytical approach is then applied to the simplified biosphere model (SSiB), enhancing its capability of simulating land surface CO₂ fluxes. The enhanced SSiB model is tested with field observation data sets from two Amazonian field experiments (ABRACOS missions and Manaus Eddy Covariance Study). Simulations of the land surface fluxes of latent heat, sensible heat and soil heat by the enhanced SSiB agree very well with observations with correlation coefficients being larger than 0.80. However, the correlation coefficient for the daily means of CO₂ fluxes is only 0.42 for the Manaus data set. A day-time “square wave” in the simulated CO₂ flux diurnal curves is found. The discrepancies between simulation and observation were found to be the results of incorrect parameter setup or improper leaf to canopy scaling strategy. A modification to the scaling strategy improves significantly the accuracy of the photosynthesis-stomatal conductance model.

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Keywords: Photosynthesis; Stomatal conductance; CO₂; Energy balance; Simplified biosphere model (SSiB); Analytical solution; ABRACOS; LBA

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,

such as albedo, surface roughness length, vegetation properties, and soil properties, could substantially alter terrestrial hydrologic system at global and regional scales (see reviews by Sellers et al., 1997; Kabat and Claussen, 2002). In these studies, biophysical models with different complexity have been developed. The project for intercomparison of land-surface parameterization scheme (PILPS, Henderson-Seller et al., 1993, 1995) has also been carried out to evaluate and improve the land surface parameterizations, and, therefore, to enhance the models' ability predicting the water cycle. In these models, however, empirical work

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45 had correlated stomatal conductance to the environ-
46 mental conditions independent from any consideration
47 of photosynthesis. By the late 1980s, scientific inter-
48 est on global change, particularly on the “greenhouse
49 effect” had promoted the development of more com-
50 plete models, which directly couple water and carbon
51 cycle processes (Sellers et al., 1997).

52 Increase in greenhouse gases, in particular CO₂,
53 has great impacts on global climate change. The po-
54 tential importance of land carbon cycle to the global
55 climate was suggested in Cox et al. (2000) who per-
56 formed future climate simulations with interactive
57 vegetation and ocean carbon cycles. Their simula-
58 tions produced significant climate warming caused by
59 climate-induced loss of Amazonian rainforests. Re-
60 cent studies have shown that terrestrial ecosystems,
61 especially tropical rain forest, may be an important
62 sink of atmospheric CO₂ (Tian et al., 2000; Schimel
63 et al., 2001). Regional studies based on in situ mea-
64 surements are consistent with carbon sinks associated
65 with tropical forests (Phillips et al., 1998). The Ama-
66 zon region contains the largest area of tropical forest
67 on Earth. Over the past 25 years, rapid development
68 has led to the destruction of over 500,000 km² of
69 forest in Brazil (Houghton et al., 2000), producing a
70 large source for atmospheric CO₂. Study has found
71 that the Amazonian region acted as a net source for
72 carbon in a range of 0.2–1.2 Pg year⁻¹ from 1992
73 to 1993 mainly because of the deforestation (Keller
74 et al., 2001). Since emissions from land clearing in
75 the tropics are thought to be large, there must be off-
76 setting sinks to balance these emissions. All of these
77 indicate a pressing need for accurate assessments of
78 the CO₂ fluxes between the terrestrial ecosystems and
79 the atmosphere.

80 Two efforts are required to address this need: one
81 is the observation of CO₂ fluxes between a terrestrial
82 ecosystem and the atmosphere in field for ground
83 truth; and the other is the development and validation
84 of models to understand the observed evidence and to
85 extrapolate the modeling results to the other regions.
86 The first effort has been made in many large-scale
87 field experiments, one of which is the Large-Scale
88 Biosphere-Atmosphere Experiment in Amazonia
89 (LBA, Keller et al., 1997). A number of other field
90 data sets have been collected in this region for analy-
91 ses and model validation. In the study of this paper,
92 the data from Anglo-Brazilian Amazonian Climate

Observation Study (ABRACOS, Gash et al., 1996) 93
and another measurement in central Amazonian rain 94
forest (Malhi et al., 1998) are used. 95

96 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- 99
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 CO₂ 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 compu- 120
tationally expensive and also may become numerically 121
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

127 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

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

149 The simplified biosphere model (SSiB) of Xue et al.
 150 (1991) has been evaluated by observational data from
 151 different vegetation types and different geographical
 152 location, and has been broadly used in global and re-
 153 gional climate studies, including the LBA (for exam-
 154 ple, Xue et al., 1996a; Chou et al., 2002). However,
 155 the current version of SSiB uses Jarvis' empirical ap-
 156 proach (Jarvis, 1976) for the formulation of stomatal
 157 conductance. It does not consider the photosynthetic
 158 activities of land surface vegetation and is thus unable
 159 to estimate land surface CO₂ fluxes for carbon cycling
 160 studies. In this paper, we attempt to enhance the SSiB
 161 model by deriving an analytical solution from Col-
 162 latz et al. model and to apply it to SSiB. Replacing
 163 the empirical stomatal resistance submodel in SSiB
 164 with Collatz et al. model, the SSiB model is then re-
 165 vised to have the CO₂ flux simulation capability. To
 166 test this extended capability of the SSiB model as a
 167 part of our effort within the LBA frame, we ran the
 168 model with the observational data from two large-scale
 169 field experiments held in Amazonian tropical forests.
 170 The output from the model is analyzed against their
 171 corresponding field observations. Discrepancies be-
 172 tween simulation and observation were found as a re-
 173 sult of incorrect parameter setup or improper leaf to
 174 canopy scaling strategy. A modification to the scal-
 175 ing strategy improves significantly the accuracy of the
 176 photosynthesis-stomatal conductance model. Finally,
 177 further improvement of the revised SSiB model is dis-
 178 cussed. It is important to note that the net CO₂ flux
 179 from the land surface is a function of both photosyn-
 180 thetic uptake and respiratory release by plants and de-
 181 composition. The latter is not addressed here and will
 182 be the focus of future updates to the model.

183 **2. Collatz et al. model**

184 The equations and parameterizations of plant pho-
 185 tosynthesis A_n and stomatal conductance g_s developed

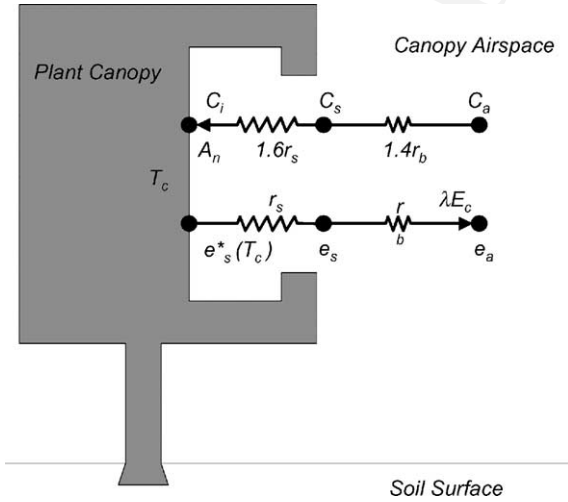


Fig. 1. Schematic diagram of Collatz' coupled photosynthesis-stomatal conductance model (canopy version in Sellers et al., 1996a). See Appendix A for symbol definition.

186 by Collatz et al. (1991) for C₃ plants and by Collatz
 187 et al. (1992) for C₄ plants are scaled up from leaf to
 188 canopy level in Sellers et al. (1996a). These equations
 189 have sound physiological bases and thorough descrip-
 190 tions to the interactive effects of environmental fac-
 191 tors and stomatal control of plant photosynthesis and
 192 transpiration. In the leaf to canopy scaling-up strat-
 193 egy used in Sellers et al. (1996a), a plant canopy is
 194 simplified as a “big leaf”. Fig. 1 is the schematic di-
 195 agram showing the exchanges of sensible heat, latent
 196 heat and CO₂ between atmosphere and the canopy in
 197 Collatz et al. model (1991, 1992). The formations of
 198 Sellers et al. (1996a) can be summarized in the fol-
 199 lowing five equations:

$$A_n = \frac{g_b}{1.4} \frac{C_a - C_s}{p} \quad (1) \quad 200$$

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

$$g_s = m \frac{pA_n e_s}{C_s e^*(T_c)} + bF \quad (3) \quad 202$$

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

$$g_s(e^*(T_c) - e_s) = g_b(e_s - e_a) \quad (5) \quad 204$$

205 The symbols in these equations are listed in Appendix
 206 A. Eq. (1) describes CO₂ transfer rate from canopy

airspace to leaf surface. Eq. (2) estimates CO₂ transfer rate from leaf surface to inside the stomata. Eq. (3) shows the relationship between stomatal conductance and photosynthesis at canopy scale based on Ball's (1988) stomatal conductance model. Eq. (4) is the leaf biochemical model that includes the leaf to canopy scaling approach of Sellers et al. (1992). Eq. (5) is the conservation equation for water transfer from inside stomata through stomata to the canopy airspace. The three limitations (W_c , W_e and W_s) of photosynthetic rate in Eq. (4) are computed as follows for C_3 plants:

$$W_c = V_{\max} \frac{C_i - \Gamma_*}{C_i + K_c(1 + O_i/K_o)} \Pi \quad (6)$$

$$W_e = \text{PAR}(1 - \omega\Pi)\varepsilon_3 \frac{C_i - \Gamma_*}{C_i + 2\Gamma_*} \Pi \left(\frac{\overline{G(\mu)}}{\mu} \right) \quad (7)$$

$$W_s = 0.5V_{\max}\Pi \quad (8)$$

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

$$W_c = V_{\max}\Pi \quad (9)$$

$$W_e = \text{PAR}(1 - \omega\Pi)\varepsilon_4\Pi \left(\frac{\overline{G(\mu)}}{\mu} \right) \quad (10)$$

$$W_s = V_{\max}2 \times 10^4 \frac{C_i}{p} \quad (11)$$

In these equations, the leaf to canopy scaling factor:

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

The inputs needed by these equations include PAR, T_a , T_c , e_a , C_a and g_b . The unknown variables are A_n , g_s , C_i , C_s and e_s (see Appendix A for symbol definitions).

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:

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

The expression for each A_i ($i = 1, 2, 3, 4, 5$) for C_3 and C_4 plants is listed in Table 1.

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

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

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

$$a_c C_i^2 + b_c C_i + c_c = 0 \quad (15)$$

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

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

$$A_n = A_1 C_i + A_5 \quad (16)$$

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

Fig. 2 is a flow chart of the above semi-analytical solution procedure. It starts from estimating the “leaf” surface water vapor pressure with the average of the canopy space water vapor pressure and the water vapor pressure insides the stomata. For any set of environmental conditions, the coefficients of Eq. (14) can be computed with the equations in Appendix B. Then an analytical solution of C_i can be obtained by analytically solving the cubic equation. Once the value of C_i corresponding to the set of the environmental conditions is obtained, the values of A_n , g_s , C_s and a new e_s can be obtained. The new e_s value is normally very close to its previous value. If not, the coefficients of Eq. (14) can be re-computed with the new e_s value and the steps to solve the cubic equation and to compute the values of A_n , g_s , C_s and e_s will be repeated. This procedure has two important aspects: (1) with the analytic approach, the physically and biologically unrealistic solutions are avoided. Under any specific environmental conditions, whether reasonable solutions of the model can be obtained depends on whether the

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

Plant type	Photosynthetic limitation	A_1	A_2	A_3	A_4	A_5
C_3	W_c	$V_{\max} \Pi$	Γ_*	1	$K_c(1 + O_i/K_o)$	$-R_d$
	W_e	$PAR(1 - \omega_{\Pi})\varepsilon_3 \Pi (\overline{G(\mu)})/\mu$	Γ_*	1	$2\Gamma_*$	$-R_d$
	W_s	$0.5V_{\max} \Pi$	0	1	0	$-R_d$
C_4	W_c	$V_{\max} \Pi$	0	1	0	$-R_d$
	W_e	$PAR(1 - \omega_{\Pi})\varepsilon_4 \Pi (\overline{G(\mu)})/\mu$	0	1	0	$-R_d$
	W_s	$2 \times 10^4 (V_{\max}/p) \Pi$	0	0	1	$-R_d$

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

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

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 r_b	50 s m ⁻¹
Rubisco maximum catalytic capacity V_{\max}	60 $\mu\text{mol m}^{-2} \text{s}^{-1}$
PAR extinction coefficient κ	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 ($W \text{ m}^{-2}$). This confirms the 303
 potential instability problem in iterations as claimed 304
 in Baldocchi (1994). 305

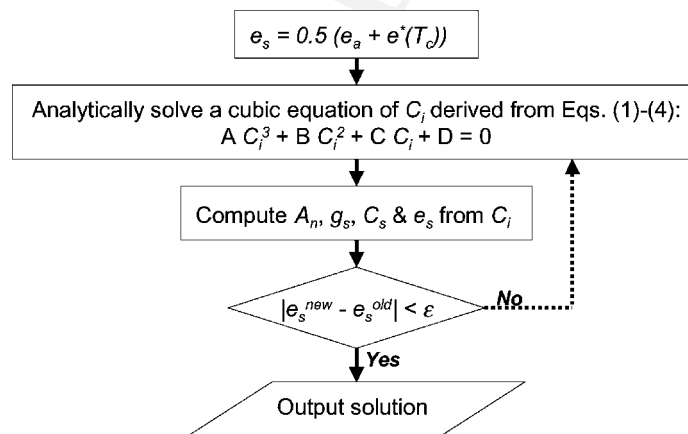


Fig. 2. The semi-analytical solution procedure for the Collatz et al. A_n-r_s coupled model.

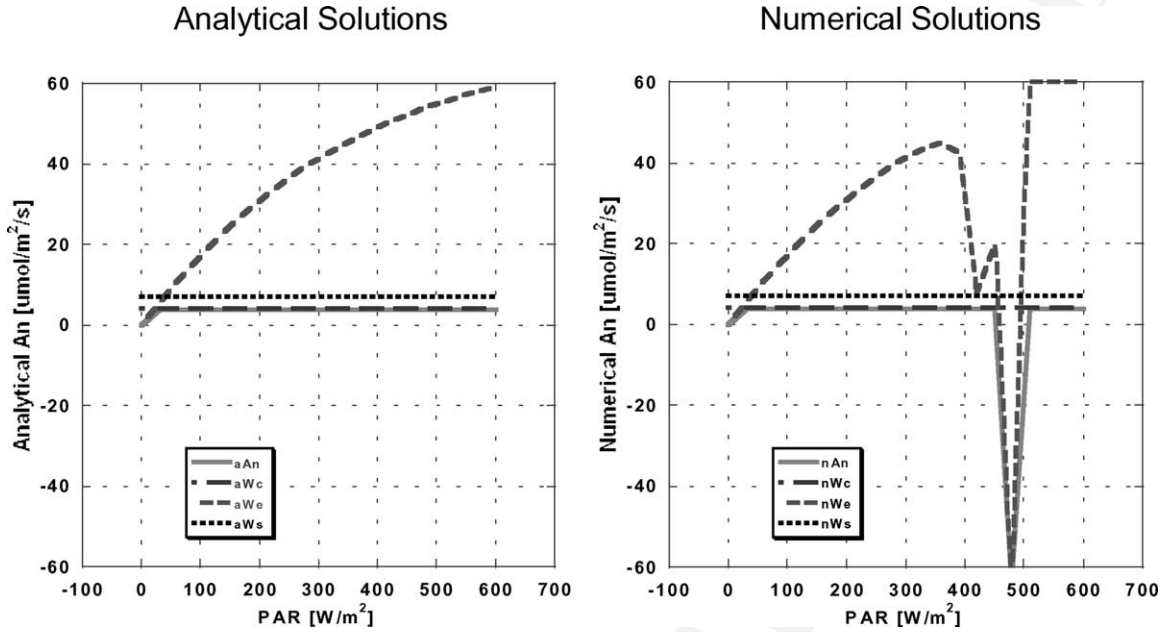


Fig. 3. Comparison between the analytical and numerical solution methods for the Collatz et al. A_n-r_s coupled model. The symbols aA_n , aW_c , aW_e , aW_s represent results from the analytical solution approach. The symbols nA_n , nW_c , nW_e , nW_s are the results from the numerical iteration method.

306 **4. Implementing Collatz et al. model in the**
 307 **simplified biosphere model (SSiB)**

308 Stomatas on plant leaves control both water vapor
 309 transfer from inside to outside and CO₂ transfer from
 310 outside to inside as indicated in Fig. 1. The original
 311 SSiB model (Xue et al., 1996a,b) simulates only the
 312 water vapor transfer by using the Jarvis' empirical ap-
 313 proach (Jarvis, 1976) to compute the stomatal resis-
 314 tance r_c to water vapor transfer. With the reasons stated
 315 previously, we enhance the SSiB model with the CO₂
 316 simulation capability by replacing the submodel of
 317 stomatal resistance in the original SSiB with the Col-
 318 latz et al. model introduced in the previous sections.

319 To compute the canopy resistance (the inverse of
 320 canopy stomatal conductance) with the photosyn-
 321 thesis-stomatal conductance model (Eqs. (1)–(5)), one
 322 needs to know the canopy airspace CO₂ concentration
 323 C_a . The value of C_a needs to be specified first, which
 324 is the product of the balance of CO₂ fluxes into and
 325 out of the canopy airspace. For a typical day-time,
 326 the influxes include the CO₂ transfer from the at-
 327 mosphere and from the soil surface into the canopy

airspace, namely F_{ca} and F_{cs} . The sink of the canopy
 328 airspace CO₂ is the canopy photosynthesis A_n . If F_{cs}
 329 and the CO₂ concentration of the atmosphere above
 330 the canopy, C_m , are known, then we have
 331

$$C_a = C_m - pr_a(A_n - F_{cs}) \quad (17) \quad 332$$

because
 333

$$F_{ca} = \frac{C_m - C_a}{pr_a} = A_n - F_{cs}. \quad (18) \quad 334$$

Eq. (18) can be used to simulate the CO₂ 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

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

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

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

Fig. 3 indicates that canopy net photosynthesis rate gets saturated when photosynthetically active radiation PAR is greater than about 50 ($W m^{-2}$). According to field measurements introduced in Section 6 and documentations in the literature (e.g. Thornley and Johnson, 1990), this saturation PAR level for most leaves is greater than 200 ($W m^{-2}$). One of the causes may be that implementation of the Collatz et al. model in the SSiB_2 model (Sellers et al., 1996a,b) assumes equal acceptance of PAR by all leaves within a canopy when the equations are integrated for all leaves in the canopy. In reality, only sunlit leaves in plant canopy receive direct PAR while shaded leaves receive diffusive PAR only. To consider this fact, we implement the Collatz et al. model for sunlit leaves and shaded leaves separately while the equation set (Eqs. (1)–(12)) and the analytical solution approach introduced previously are kept the same.

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_0 and the fraction of diffusive PAR is f_d , then

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

$$PAR_{dr} = \frac{(1 - f_d) PAR_0 \cos \theta_{ls}}{\sin \theta_s} \quad (21)$$

where θ_s is elevation angle of the sun and calculated from the time of day, the day of year and the latitude of observational site with the equation used in Campbell (1977, p. 55). The θ_{ls} is the mean angle between the leaf normal and the sunlight. We select $\theta_{ls} = 60^\circ$ for a canopy with spherical leaf angle distribution (Norman, 1982). Accordingly, the PAR received by the sunlit leaves $PAR_{slt} = PAR_{dr} = PAR_{df}$ while the PAR received by the shaded leaves $PAR_{shd} = PAR_{df}$.

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

$$F_{slt} = 2[1 - \exp(-0.5 F / \sin \theta_s)] \sin \theta_s \quad (22)$$

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

Using PAR_{slt} to run the analytical solution procedure for the Collatz et al. model introduced previously for a unit sunlit leaf (leaf area index = 1.0), one obtains the net photosynthesis rate A_{nslt} and stomatal conductance g_{slt} . Similarly using PAR_{shd} for a unit shaded leaf, one obtains A_{nshd} and g_{shd} . The canopy total net photosynthetic rate A_n and stomatal conductance are then computed as

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

$$g_c = \frac{1}{(F_{slt}/g_{slt}) + (F_{shd}/g_{shd})} \quad (24)$$

By this point, we have introduced three different versions of implementing the Collatz et al. model of plant photosynthesis and stomatal conductance: (1) the original implementation in SSiB_2 using iteration solution method; (2) a modified version using analytical solution method; and (3) another modified version using both the analytical solution method and the sunlit–shaded leaf separation scaling method. For this study of enhancing the SSiB for carbon simulation, we use field measurements to evaluate the following three versions of SSiB: (1) the original SSiB model using Jarvis' stomatal model (for convenience we will refer this version as SSiB_0); (2) the SSiB model using the Collatz et al. model in Sellers et al. (1996a) modified with the analytical solution method (referred to as SSiB_1); and (3) the SSiB model using the Collatz et al. model modified with the analytical solution method and the sunlit–shaded leaf separation scaling method (referred to as SSiB_2).

431 6. Field measurement data sets for model 432 evaluation

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

437 6.1. ABRACOS field experiment (1990 and 1991)

438 The ABRACOS is a comprehensive observational
439 study of land surface–atmosphere interactions in
440 large-scale clearings caused by tropical deforestation
441 (Shuttleworth et al., 1991). The main objective of
442 ABRACOS was to provide comparative data from ad-
443 jacent forested and cleared areas, and to provide rep-
444 resentative parameters and data from clearings for
445 GCM studies. The data used in this study were collec-
446 ted during the first two experimental seasons of
447 ABRACOS at the Fazenda Dimona ranch site
448 (02°19'S, 60°19'W), 100 km north of Manaus in
449 central Amazonia. Mission 1 was conducted from
450 4 October to 2 November 1990 and Mission 2 was
451 conducted from 29 June to 10 September 1991. Veg-
452 etation at the experiment site is mainly C₄ grass.
453 Further details of the ranch and the experimental site
454 are described by Wright et al. (1992), McWilliams
455 et al. (1993), and Bastable et al. (1993).

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

466 Three measurement systems, including a Campbell
467 Scientific Ltd. (UK) Bowen-ratio system, the Mk 2
468 'Hydra' Eddy correlation device, and a logarithmic
469 wind and scalar profile measurement rig were used to
470 estimate fluxes of water vapor and sensible heat. There
471 was excellent agreement between the three measure-
472 ment systems, the data from which were combined to
473 form a complete hourly time series record for each
474 experimental period. No CO₂ fluxes were measured
475 during ABRACOS. Therefore, this data set is used to

476 evaluate the model simulations of the water and en-
477 ergy budgets after introducing a complex photosyn-
478 thesis process, and to compare the model simulations
479 with two different stomatal conductance parameteri-
480 zations.

6.2. Manaus Eddy Covariance Study (1996)

481
482 Another data set used for this paper was obtained
483 from an Eddy Covariance Study which was conducted
484 from 6 July 1995 to 24 August 1996 in the Reserva
485 Biologica do Cuieiras (2°35'22"S, 60°6'55"W), some
486 60 km north of Manaus (Malhi et al., 1998). This is
487 part of a very extensive, continuous area of dense low-
488 land terra firm tropical rain forest. Vegetation of the
489 site is very similar to the site studied by Fan et al.
490 (1995). One of the primary focuses in the measure-
491 ment is to examine and describe the nature and mag-
492 nitude of the diurnal CO₂ flux and its relationship to
493 meteorological conditions (Williams et al., 1998). The
494 fluxes were measured in an Edisol Eddy covariance
495 system (Malhi et al., 1998). Meteorological data were
496 collected with an automatic weather station. The gas
497 analyzers were calibrated at least weekly using zero
498 and fixed concentration CO₂ and water vapor sam-
499 ples. Very little drift in analyzer concentration was
500 noted over a diurnal cycle or on a week-to-week ba-
501 sis. Real time data were collected as 10 min average.
502 Corrections were applied for the dampening of fluc-
503 tuations at high frequencies using the approach out-
504 lined by Moore (1986) and Moncrieff et al. (1997).
505 For the study in this paper, the data collected only
506 from late December 1995 to mid-January, 1996 were
507 used because of the better continuity and certainty of
508 biophysical parameters. For convenience, this data set
509 is called "Manaus data".

510 7. Results and discussion

511 The SSiB model will be used to study the impact
512 of land cover change in Amazonia region on the re-
513 gional climate and carbon balance using the Collatz
514 et al. photosynthesis and stomatal conductance model.
515 Thus, proper simulations in both carbon flux and heat
516 fluxes are necessary. The original SSiB model using
517 the empirical Jarvis stomatal model (SSiB.0) has pro-
518 duced reasonable simulations of heat fluxes in the

519 off-line tests for Amazon sites (e.g. Xue et al., 1991,
520 1996a). As the first step, we must check whether the
521 more realistic but more complex approach for simula-
522 tion of stomatal control is still able to yield reasonable
523 simulations in heat fluxes. Then we will evaluate how
524 the two modified SSiB versions (SSiB_1 and SSiB_2)
525 perform for the CO₂ flux simulations.

526 7.1. Simulation of heat fluxes (SSiB_0, SSiB_1 and 527 SSiB_2 versus observations)

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

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

Table 3
Vegetation parameters of the ABRACOS data set

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, <i>B</i>	6.9
Soil water potential at saturation (m)	-0.035
Porosity	0.59
Minimum stomatal resistance (sm ⁻¹)	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
<i>H</i>	SSiB_0	0.87	0.91	0.86
	SSiB_1	0.88	0.90	0.91
	SSiB_2	0.88	0.89	0.91
<i>LE</i>	SSiB_0	0.94	0.96	0.96
	SSiB_1	0.94	0.97	0.97
	SSiB_2	0.94	0.95	0.98
<i>G</i>	SSiB_0	0.83	0.91	0.91
	SSiB_1	0.82	0.90	0.73
	SSiB_2	0.82	0.83	0.84

544 are the comparisons between the observed and sim-
545 ulated daily means of latent heat, sensible heat and
546 soil heat fluxes for three versions of the SSiB model
547 (SSiB_0, SSiB_1 and SSiB_2). The correlation coeffi-
548 cients of the daily mean fluxes for the entire periods of
549 both M1 and M2 are listed in Table 4. The three ver-
550 sions of SSiB produce very similar simulations for the
551 three fluxes. Fig. 5a shows that in M2 the simulated
552 latent heat flux closely follows observations. The ob-
553 served latent heat fluxes dropped sharply several times
554 during M2 (3, 4, and 25 August and 2 September).
555 The model simulated these dramatic changes and re-
556 covered very well. In M1, although the three versions
557 of the model generally followed the trend, the sim-
558 ulations of the three heat fluxes fluctuated about the
559 observations (Fig. 4). In the early October, the mod-
560 els underestimated latent heat flux and overestimated
561 sensible heat flux by about 30%. But in the middle
562 October, the model overestimated latent heat flux
563 and underestimated sensible heat flux by about 20%.
564 These fluctuations might result from the biases of soil
565 heat flux simulations from their observations (Fig. 4c).
566 In general, the simulations of the heat fluxes from
567 the two modified SSiB versions (SSiB_1 and SSiB_2)
568 are very similar to those from the original SSiB
569 (SSiB_0).

570 For the Manus data set, detailed soil and vegetation
571 information was not available except that the vegeta-
572 tion cover of the study site is a continuous area of
573 dense lowland terra firm tropical rainforest and that
574 the leaf area index was 5–6 and canopy height 30 m
575 according to Malhi et al. (1998). In an off-line test,
576 it is important to have a proper set of vegetation and
577

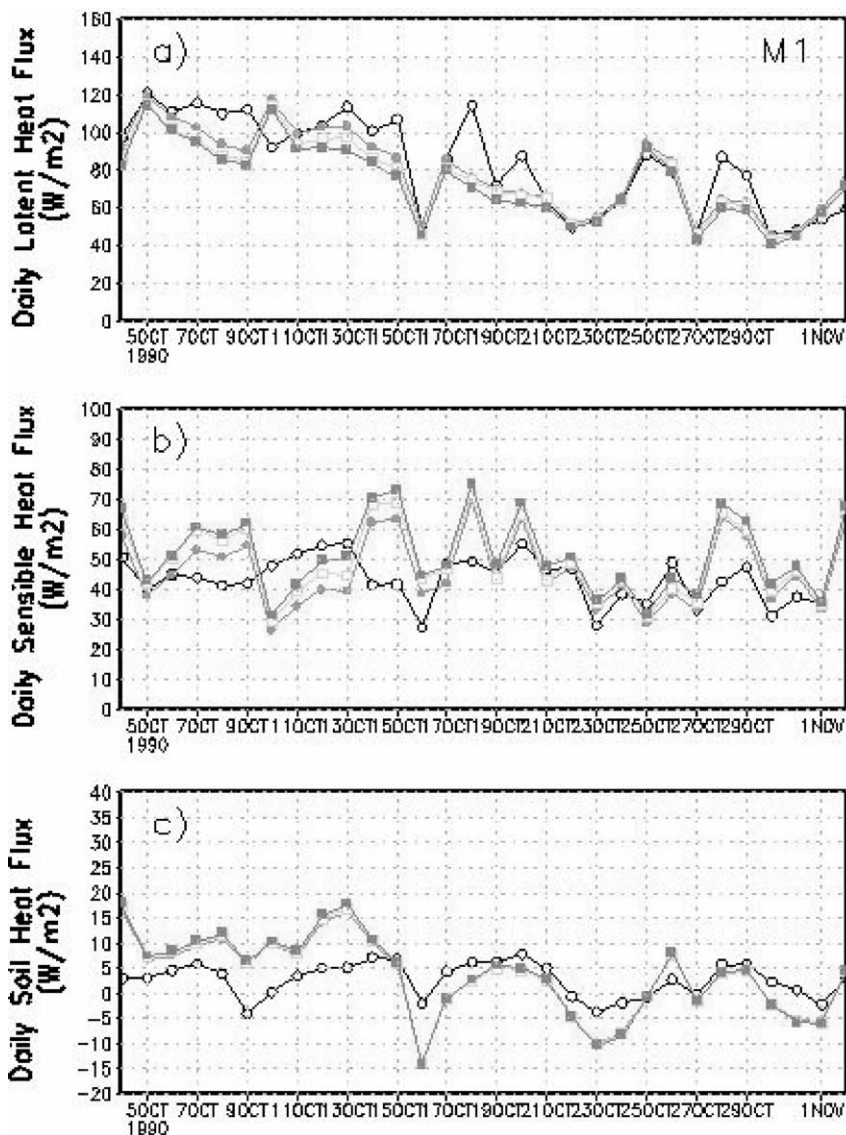


Fig. 4. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Mission 1 of the ABRACOS field experiment (line marked with open circles), the simulations of SSiB.0 (solid squares), the simulations of SSiB.1 (solid circles) and the simulations of SSiB.2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

577 soil parameters and it may cause systematic errors if
 578 these parameters are not setup correctly (Xue et al.,
 579 1996b; Xue et al., 1997). Because we have no mea-
 580 sured surface vegetation and soil information, we use
 581 the vegetation and soil parameters from a vegetation
 582 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 veg- 584
 etation type information to specify the land parame- 585
 ter values. Fig. 6 shows the result from three versions 586
 of SSiB. It is evident that all three versions are able 587
 to simulate the variability in latent heat, sensible heat 588

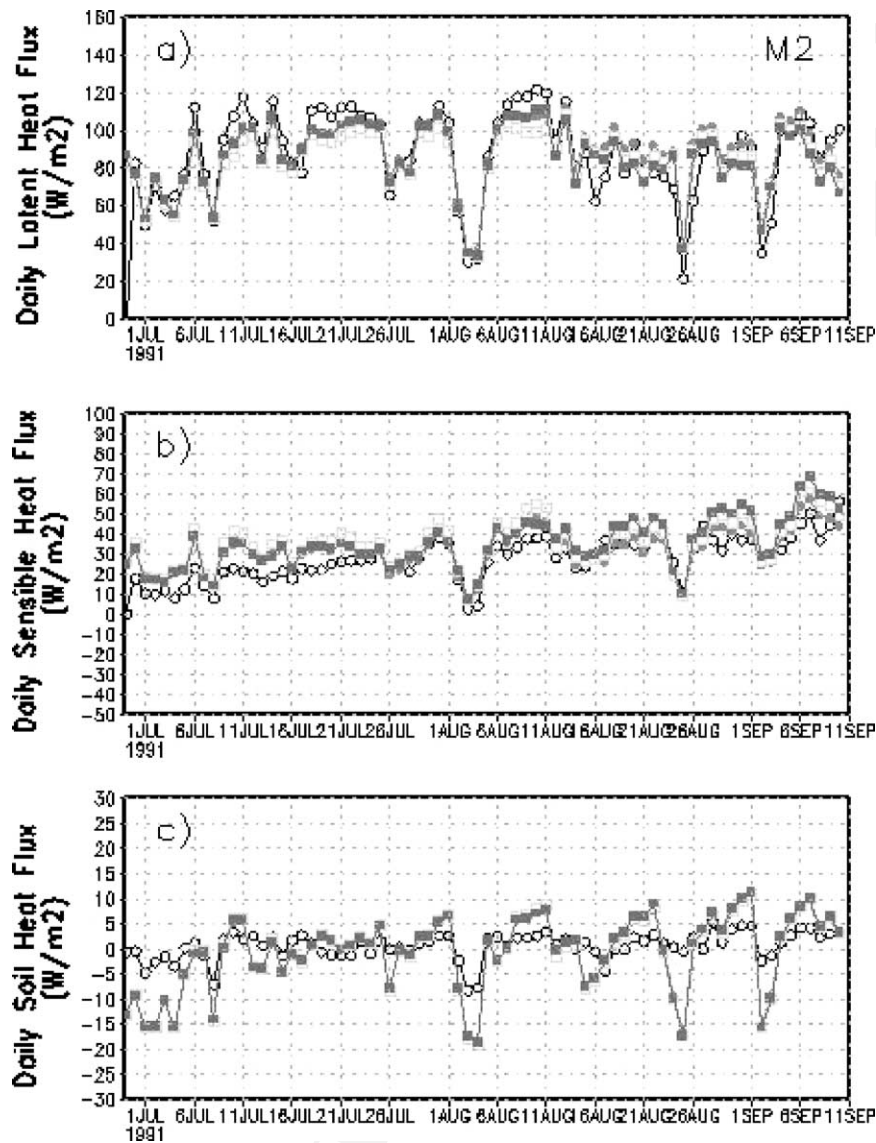


Fig. 5. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Mission 2 of the ABRACOS field experiment (line marked with open circles), the simulations of SSiB_0 (solid squares), the simulations of SSiB_1 (solid circles) and the simulations of SSiB_2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

589 and soil heat fluxes well. The correlations between the
 590 model outputs and the field observations are similar to
 591 the results for the ABRACOS data sets (Table 4). This
 592 result further indicates that the two modified versions
 593 of SSiB do not compromise the capability of the orig-
 594 inal SSiB in simulating the latent heat, sensible heat
 595 and soil heat fluxes.

7.2. Simulations of CO_2 flux (SSiB_1 and SSiB_2 versus observations) 596 597

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 per-
 600 form in CO_2 flux simulation is of the most concern.
 601

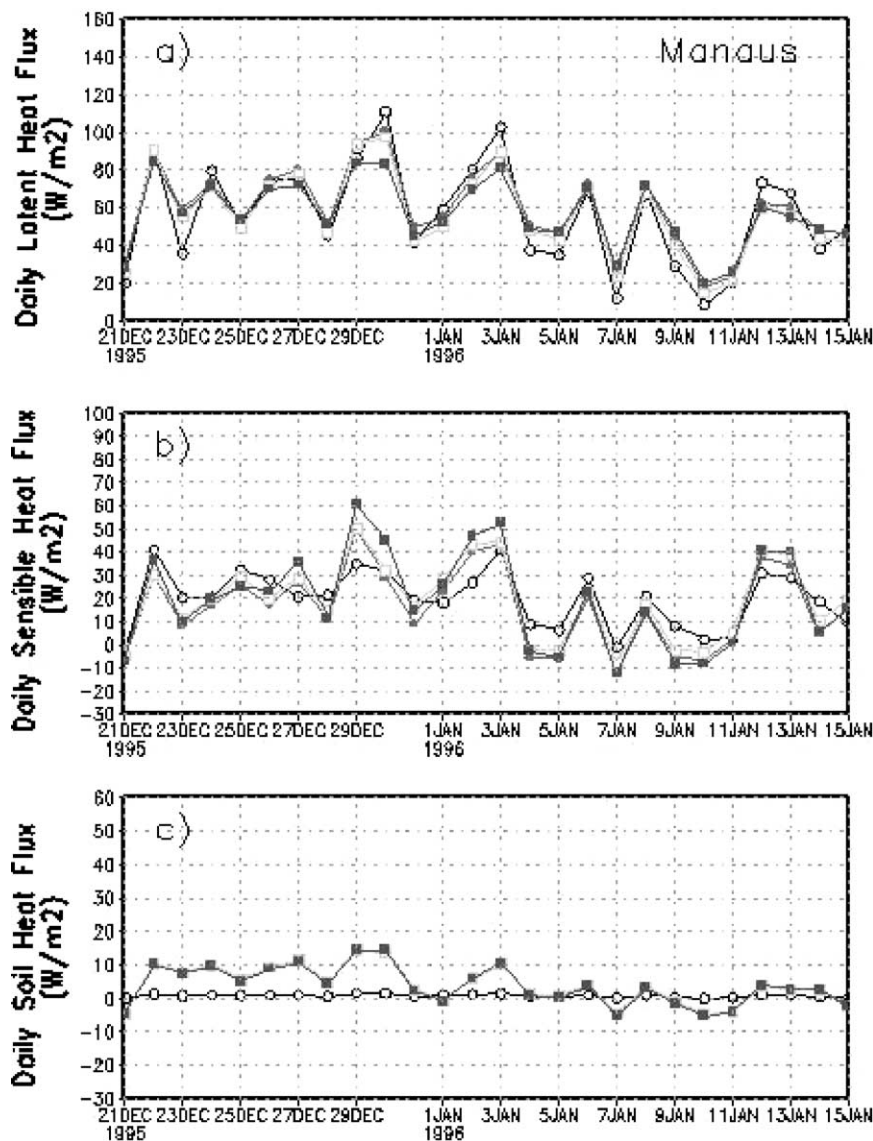


Fig. 6. The daily mean values of (a) latent heat flux, (b) sensible heat flux, and (c) soil heat flux obtained from the observations during the Eddy Covariance Study (line marked with open circles), the simulations of SSiB.0 (solid squares), the simulations of SSiB.1 (solid circles) and the simulations of SSiB.2 (open squares). If solid circles or open squares are not seen, they are overlaid by solid squares.

602 Using the only CO_2 flux measurements in the Manaus data set, we can find the answer to this question from the results demonstrated in the following figures.

606 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

609 circles) of the above canopy hourly CO_2 flux for the 26 days in the Manaus data set. The correlation coefficient between the hourly simulation and field observation is 0.73 for SSiB.1 and 0.84 for SSiB.2. Although both SSiB.1 and SSiB.2 simulated the diurnal cycles of the CO_2 flux, the simulations by SSiB.1, which uses the same leaf to canopy scaling

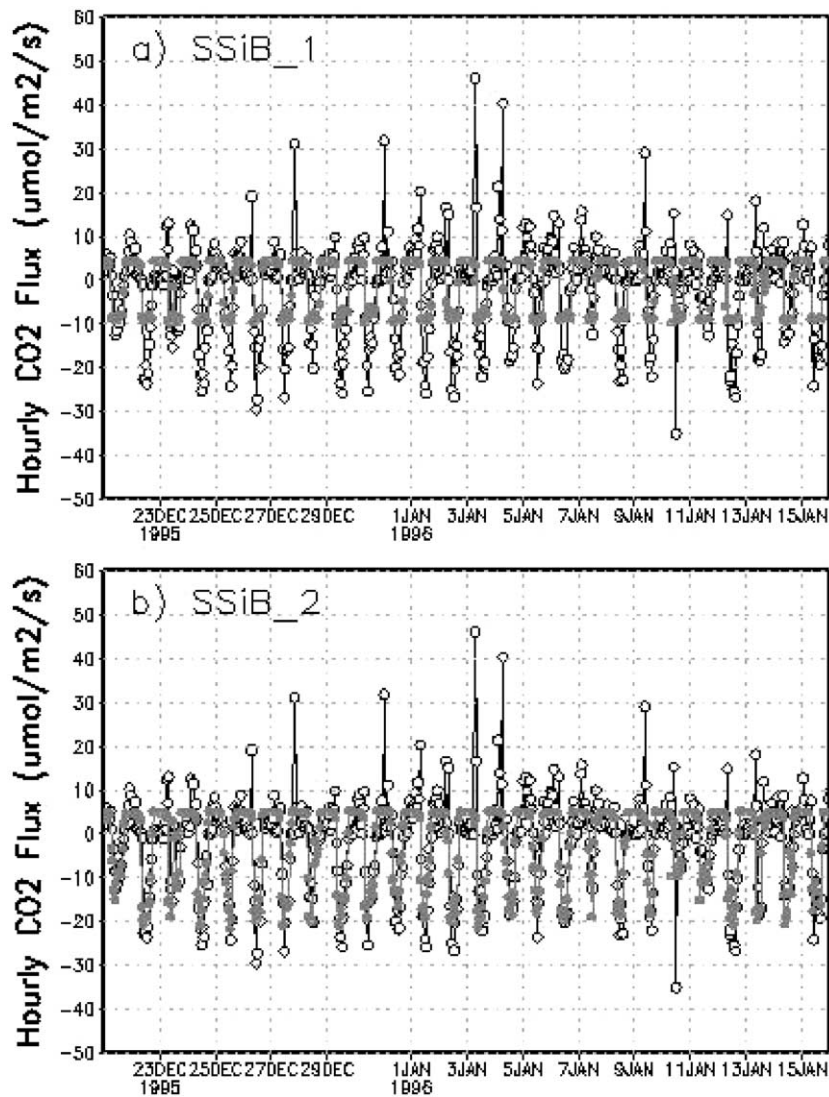


Fig. 7. The hourly above canopy CO₂ flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB.1; (b) for SSiB.2. Negative value means that CO₂ is transported from the above canopy atmosphere downward to the canopy.

616 strategy as in SSiB.2 (Sellers et al., 1996a), have very
 617 similar maximums during midday for all 26 days.
 618 The simulations by SSiB.2, which computes net pho-
 619 tosynthetic rate and stomatal conductance for sunlit
 620 and shaded leaves, respectively, have diurnal cycles
 621 varying mainly with incoming photosynthetically ac-
 622 tive radiation. The observed diurnal cycles of CO₂
 623 flux follow the PAR diurnal pattern. Thus, the SSiB.2

624 simulations have a higher correlation coefficient
 625 (0.84).

626 Fig. 8 is the diurnal cycles of the model simulations
 627 plotted against the field observations averaged over
 628 the 26 days. Despite general consistency of the sim-
 629 ulations of both SSiB.1 and SSiB.2 with observations,
 630 a noontime square wave in the simulations of SSiB.1
 631 is evident. To more clearly examine the difference in

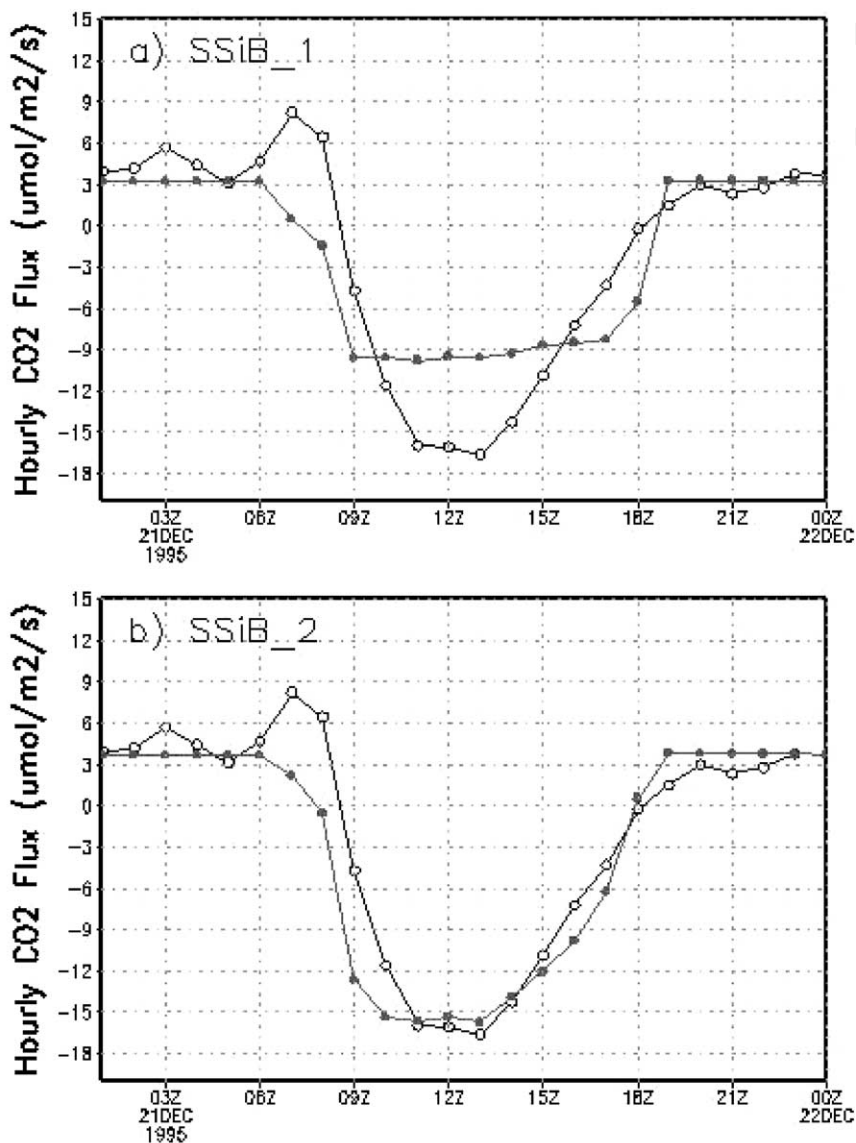


Fig. 8. The averaged diurnal curve of the above canopy CO₂ flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB-1; (b) SSiB-2. Negative value means that CO₂ is transported from the above canopy atmosphere downward to the canopy.

632 the CO₂ flux diurnal cycle simulations by SSiB-1 and
 633 SSiB-2, the simulated plant photosynthetic rate A_n
 634 and their three limitations (namely, the RuBP saturation
 635 limited rate W_c , the electron transportation limited
 636 rate W_e , and the sink limited rate W_s) averaged
 637 over the 26 days are plotted in Fig. 9 for SSiB-1 and
 638 Fig. 10 for SSiB-2. As in Eq. (4), the photosynthetic

rate A_n is the minimum of these three limitations ad- 639
 justed 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

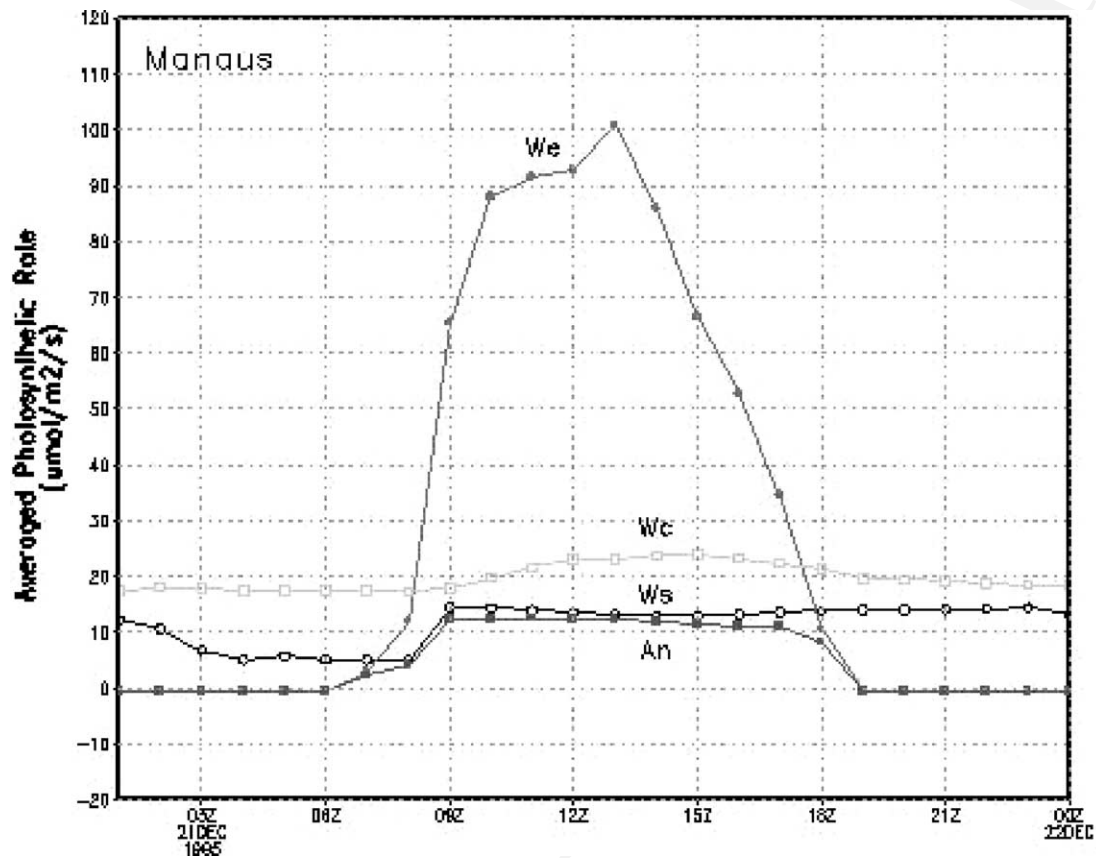


Fig. 9. The averaged diurnal curve of the canopy CO_2 photosynthetic rate and its three components simulated by Phost.1. Canopy net photosynthesis rate A_n is marked with solid squares. The Rubisco limitation W_c is open circles. The PAR limitation W_e is solid circles. The sink limitation W_s is open squares.

646 W_c and shows a day-time square wave. This day-time
 647 square wave is not consistent with observations well
 648 documented in the literature (Thornley and Johnson,
 649 1990). One of the reasons for this incorrect simulation
 650 by SSiB.1 in Fig. 9 may be that the parameters
 651 of the Collatz et al. model were setup incorrectly so
 652 that the simulations of W_c are too large or the com-
 653 puted values of W_c or W_s are too small. However,
 654 as stated in Section 5, an apparent reason for the in-
 655 correct simulation of SSiB.1 is the strategy of scal-
 656 ing the Collatz et al. model from leaf to canopy in
 657 Sellers et al. (1996a). The scaling-up method treats all
 658 leaves within the plant canopy the same way. This may
 659 have underestimated the light saturation phenomenon
 660 of plant leaves (Chen et al., 1999). This underestima-
 661 tion of light situation may have caused the simulation

of W_c 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.

Fig. 10 plots the daily above canopy CO_2 flux aver-
 ages of the model simulations and their field obser-
 vations. For SSiB.1, because of the unrealistic square
 wave in the diurnal variation of plant photosynthetic
 rate, the simulated daily above canopy CO_2 flux aver-
 ages (solid circles) do not match the observations
 well (open circles). For SSiB.2, its simulations (open
 squares) improve obviously over the simulation by
 SSiB.1. The correlation coefficient between the aver-
 ages of the simulated daily above canopy CO_2 flux
 and their corresponding observations is only 0.42 for

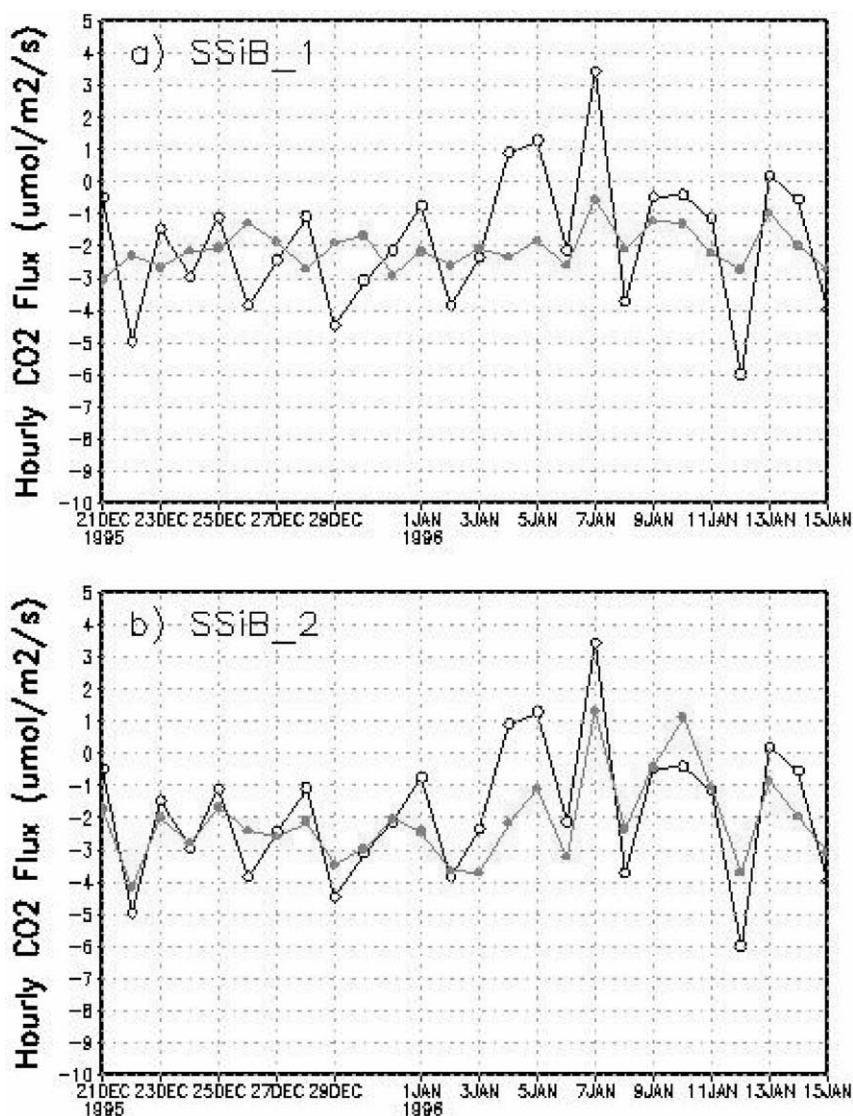


Fig. 10. The daily means of the above canopy CO_2 flux simulations (solid circles) and their field observations (open circles) for the 26-day data set from the Manaus Eddy Covariance Study: (a) for SSiB_1; (b) for SSiB_2. Negative value means that CO_2 is transported from the above canopy atmosphere downward to the canopy.

678 SSiB_1 and 0.80 for SSiB_2. In this paper, we set the
 679 soil respiration rate as a constant. It will be the fo-
 680 cus of further studies to improve the capability of the
 681 SSiB model in CO_2 flux simulations. With a more
 682 realistic simulation of F_{cs} in Eq. (18), the simula-
 683 tion result of F_{ca} by SSiB_2 is expected to be even
 684 better.

8. Conclusions

Using three data sets collected from two large-scale
 field experiments, this study aims to improve the so-
 lution experiment and scaling-up approach of the Collatz
 et al. model of plant photosynthesis and stomatal con-
 ductance in order to implement the model in the SSiB

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691 for CO₂ flux simulations. From the results obtained
692 we can make the following conclusions:

- 693 (1) The Collatz et al. model of plant photosynthe-
694 sis and stomatal conductance can solved with
695 a semi-analytic method, which brings with bet-
696 ter computational efficiency and stability for
697 the coupled land surface–atmosphere interaction
698 models.
699 (2) Implementation of the analytic solution approach
700 for CO₂ flux solution in the SSiB model produces
701 reasonable simulations of latent heat, sensible heat
702 and soil heat fluxes and enhances the SSiB into a
703 new generation model.
704 (3) The leaf to canopy scaling-up strategy used in
705 [Sellers et al. \(1996a\)](#) for the implementation of the
706 Collatz et al. model results in a day-time square
707 wave in the net photosynthetic rate simulations.
708 Considering the sunlit leaves and shaded leaves
separately in the Collatz et al. model implemen-

tation in the SSiB model improves the photosyn- 709
thesis and CO₂ flux simulations significantly. 710

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Appendix A. List of symbols with units and definition

Symbol	Units	Definition
A_n	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Net CO ₂ assimilation of the canopy
$A, A_i (i = 1, \dots, 7), a_c$		Interim variables for the analytic solutions
B, B_1, B_2, b_c		Interim variables for the analytic solutions
b	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Coefficient in Eq. (3) (0.01 for C ₃ , 0.04 for C ₄ vegetation)
C, c_c		Interim variables for the analytic solutions
C_a	Pa	CO ₂ concentration of the atmosphere
C_i	Pa	CO ₂ concentration inside plant leaves
C_s	Pa	CO ₂ concentration at leaf surface
C_1, C_2		Empirical coefficients of soil moisture adjustment factor, Eq. (19)
e_a	Pa	Water vapor pressure at the reference height
$e^*(T)$	Pa	Saturation vapor pressure at temperature T
e_s	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}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	CO ₂ flux above land surface
F_{cs}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	CO ₂ flux from the soil surface
F	$\text{m}^2 \text{m}^{-2}$	Canopy leaf area index
F_{shd}	$\text{m}^2 \text{m}^{-2}$	Shaded leaf area index
F_{slt}	$\text{m}^2 \text{m}^{-2}$	Sunlit leaf area index
f_d		Fraction of diffusive radiation in total radiation
$f(\psi)$		Adjustment factor to count for soil moisture effect

Appendix A. (Continued)

Symbol	Units	Definition
$G(\mu)$		Projection of leaves in direction of incoming radiation flux*
g_b	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Leaf boundary layer aerodynamic conductance
g_s	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Stomatal conductance to latent and sensible heat transfer
Γ^*	$\mu\text{mol mol}^{-1}$	The CO_2 compensation point of the leaves*
γ	Pa K^{-1}	Psychrometric constant
h_s		Relative humidity within the leaf surface boundary layer
K_c	$\mu\text{mol mol}^{-1}$	Michaelis-Menten competitive inhibition constant for CO_2^*
K_o	$\mu\text{mol mol}^{-1}$	Michaelis-Menten competitive inhibition constant for O_2^*
\bar{k}		Time-mean value of radiation extinction coefficient*
m		Coefficient in Eq. (3) (9 for C_3 , 4 for C_4 vegetation)
N		Canopy green leaf fraction
O_i	$\mu\text{mol mol}^{-1}$	Internal O_2 concentration of the leaves
P		Interim variables for the analytic solutions
PAR, PAR ₀	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Photosynthetically active radiation above the canopy
PAR _{dr}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Direct photosynthetically active radiation above the canopy
PAR _{df}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Diffusive photosynthetically active radiation above the canopy
PAR _{sht}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	PAR received by sunlit leaves
PAR _{shd}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	PAR received by shaded leaves
p	Pa	Air pressure
ψ	Pa	Soil water potential
Π		Leaf to canopy scaling factor (see Eq. (12))
Q		Interim variables for the analytic solutions
R_d	$\mu\text{mol m}^{-2} \text{s}^{-1}$	The dark respiration rate of the canopy
r_a		Aerodynamic resistance of the air above the canopy to the measurement height
ρc_p	$\text{J m}^{-3} \text{K}^{-1}$	Volumetric heat capacity of air
T_a	$^{\circ}\text{C}$	Air temperature at the reference height
T_c	$^{\circ}\text{C}$	Integrated leaf temperature of the canopy
θ_s	$^{\circ}$	Sun elevation angle
θ_{ls}	$^{\circ}$	Mean angle between leaf normal and sunlight
μ		Direction of incoming radiation flux
V_{max}	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Maximum RuBP carboxylation rate
V		Canopy cover fraction
W_c	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Rubisco-limited rate of CO_2 assimilation
W_e	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Electron transportation limited CO_2 assimilation rate
W_s	$\mu\text{mol m}^{-2} \text{s}^{-1}$	Product sink limited rate of CO_2 assimilation
$\omega\Pi$		Leaf-scattering coefficient for PAR (Sellers et al., 1996a)

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

727 In 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

730 $B = g_b p (A_6 ((1.6 - m h_s) B_1 + A_4 m h_s g_b)$
731 $+ A_3 A_7 m h_s g_b) + b F (A_4 B_1 g_b$
732 $+ A_3 B_2 g_b - B_1^2)$ (A.2)
733

734 $C = g_b p (A_6 (1.6 - m h_s) B_2 + A_7 (1.6 - m h_s) B_1$
735 $+ A_4 m h_s g_b) + b F (A_4 B_2 g_b - 2 B_1 B_2)$ (A.3)

736 $D = A_7 B_2 (1.6 - m h_s) g_b p - B_2^2 b F$ (A.4)

737 and

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

739 $A_7 = A_4 A_5 - A_1 A_2$ (A.6)

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

741 $B_2 = C_a g_b A_4 - 1.4 p A_7$ (A.8)

742 $h_s = e_s / e_s^* (T_c)$ (A.9)

743 If we define $P = (C/A) - (B^2/3A^2)$ and $Q =$
744 $(D/A) + (2B^3/27A^3) - (BC/3A^2)$, then the discrim-
745 inator of Eq. (14) is

746 $\Delta = \left(\frac{Q}{2}\right)^2 + \left(\frac{P}{3}\right)^3$ (A.10)

747 If $(\Delta \geq 0)$, the cubic Eq. (14) has only one valid solu-
748 tion. If $(\Delta < 0)$, Eq. (14) yields three roots. These
749 roots can be computed with equations listed in most
750 mathematical handbooks. The valid solution is the posi-
751 tive minimum of the three, that is

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

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

755 $a_c C_i^2 + b_c C_i + c_c = 0$ (A.12)

756 where

758 $a_c = g_b p A_1 (1.4 p A_1 (1.6 - m h_s) - m h_s g_b)$
759 $+ b F (1.4 p A_1 (1.4 p A_1 + g_b))$ (A.13)

$b_c = -g_b p A_1 1.4 p A_1 (C_a g_b - 1.4 p A_5)$ 761
 $+ A_5 g_b p (1.4 p A_1 (1.6 - m h_s) - m h_s g_b)$ 762
 $+ b F (2.8 p A_1 + g_b) (C_a g_b - 1.4 p A_5)$ (A.14) 763
764

$c_c = -g_b p A_5 (1.6 - m h_s) (C_a g_b - 1.4 p A_5)$ 765
 $+ b F (C_a g_b - 1.4 p A_5)^2$ (A.15) 766

The discriminator of Eq. (A.12) is

$\Delta_2 = b_c^2 - 4 a_c c_c$ (A.16) 768

When $(\Delta_2 \geq 0)$, 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

$C_i = \min(x_1, x_2)$ (A.17) 774

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

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