Appendix

Contents

[Cassava photosynthesis model 1](#_Toc6781709)

[Metabolic model 2](#_Toc6781710)

[Description 2](#_Toc6781711)

[Parameters and values 3](#_Toc6781712)

[Equations 14](#_Toc6781713)

[light reaction model 20](#_Toc6781714)

[Description and equations 20](#_Toc6781715)

[Parameters and value 21](#_Toc6781716)

[Rubisco activation 21](#_Toc6781717)

[Description 21](#_Toc6781718)

[Parameters and values 21](#_Toc6781719)

[Equations 22](#_Toc6781720)

[Dynamic stomatal conductance response 24](#_Toc6781721)

[Description and equations 24](#_Toc6781722)

[Parameters and values 25](#_Toc6781723)

[Cassava leaf model 25](#_Toc6781724)

[Description and equations 25](#_Toc6781725)

[Parameters and values 26](#_Toc6781726)

[Reference 27](#_Toc6781727)

# Cassava photosynthesis model

To estimate the influence of stomata and Rubisco response on dynamic photosynthesis rate, a cassava photosynthesis metabolic model was developed. The model was constructed based on the C3 photosynthesis model ([Zhu et al. 2007](#_ENREF_8)), a simplified light reaction model, a Rubisco activase model ([Mate et al. 1996](#_ENREF_4); [Zhu et al. 2013](#_ENREF_9)), and a dynamic stomatal conductance model ([Vialet-Chabrand et al. 2017](#_ENREF_6)). The model was implemented in MATLAB. Our prior model ([Zhu et al. 2007](#_ENREF_8)) is a general C3 photosynthesis model, which includes the reactions of the Calvin-Benson cycle and carbohydrate synthesis. In the model, the rate of change of the concentration of each metabolite over time is represented by ordinary differential equation (ODE):



where: *C* is metabolite concentration; *Vp* is the total rate of the reaction that produces *C*, and *Vu* is the total rate of *C* consumption. Rate equations of each reaction were developed based on standard Michaelis-Menten equations, except where the assumptions of this formulation were not met, notably in the case of Rubisco. The alternative equations to meet these situations followed [Zhu et al. (2007](#_ENREF_8)).

The model was parameterized using *Vcmax*, *Jmax*, *ki*, *kd*, Ball-Berry slope and intercept from measured photosynthetic and stomata parameters of cassava (Supplemental Table S4). The measured *Vcmax* was used as the maximum Rubisco activity in the metabolic model. *A*, transpiration (*T*), *ci*, and *gs* were estimated under various light conditions. The predicted water use efficiency (*WUE*) was calculated dividing *A* by *T*.

**Table S1 Input parameters of the cassava model**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Cultivar | Vcmax25 | Jmax25 | Kd(s-1) | Ki(s-1) | Ball Berry Slop | Intercept |
| Mbundumali | 100.1 | 169.4 | 0.0026 | 0.0017 | 5.50 | 0.079 |
| TME3 | 101.8 | 165.4 | 0.0017 | 0.0019 | 6.36 | 0.087 |
| TME419 | 107.8 | 167.6 | 0.0034 | 0.0022 | 5.32 | 0.078 |
| TME693 | 110.3 | 171.3 | 0.0011 | 0.0017 | 6.50 | 0.072 |
| TME7 | 104.8 | 163.4 | 0.0030 | 0.0020 | 5.80 | 0.070 |
| TMS01/1412 | 106.3 | 175.9 | 0.0035 | 0.0031 | 6.24 | 0.072 |
| TMS30001 | 117.2 | 169.7 | 0.0036 | 0.0018 | 6.43 | 0.047 |
| TMS30572 | 95.2 | 154.5 | 0.0010 | 0.0015 | 6.63 | 0.069 |
| TMS96/1632 | 102.7 | 163.2 | 0.0029 | 0.0019 | 5.48 | 0.110 |
| TMS98/0002 | 91.7 | 149.1 | 0.0039 | 0.0016 | 5.00 | 0.096 |
| TMS98/0581 | 99.3 | 148.7 | 0.0035 | 0.0021 | 7.29 | 0.068 |

# Metabolic model

## Description

Based on the C3 photosynthesis model (Zhu et al., 2007), the model equations and parameters were listed as follows. The subscripts of v1, v2 ……v131 correspond to the numbers in Zhu et al., (2007).

## Parameters and values

**Table S2** The Michaelis-Menten constants, inhibition constants and activation constants of the enzymes in the Calvin cycle, starch synthesis and triose phosphate export ([Zhu et al. 2007](#_ENREF_8)).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| RNa | Reaction | Parb | Value  (mM)c | Descriptiond |
| 1 | RuBP+CO2→2PGA | KM11 | 0.0115 | CO2 |
| 1 | RuBP+CO2→2PGA | KM12 | 0.222 | O2 |
| 1 | RuBP+CO2→2PGA | KM13 | 0.020 | RuBP |
| 1 | RuBP+CO2→2PGA | KI11 | 0.84 | PGA |
| 1 | RuBP+CO2→2PGA | KI12 | 0.04 | FBP |
| 1 | RuBP+CO2→2PGA | KI13 | 0.075 | SBP |
| 1 | RuBP+CO2→2PGA | KI14 | 0.9 | Pi |
| 1 | RuBP+CO2→2PGA | KI15 | 0.07 | NADPH |
| 2 | PGA+ATP ↔ADP + DPGA | KM21 | 0.240 | PGA |
| 2 | PGA+ATP ↔ADP + DPGA | KM22 | 0.390 | ATP |
| 2 | PGA+ATP ↔ADP + DPGA | KM23 | 0.23 | ADP |
| 2 | PGA+ATP↔ADP + DPGA | KE2 | 7.6  ×10-4 | Equ. Const. |
| 3 | DPGA+NADPH+H+ ↔GAP + Pi+NADP | KM31 | 0.004 | BPGA |
| 3 | DPGA+NADPH +H+ ↔GAP + Pi+NADP | KM32 | 0.100 | NADPH |
| 4 | DHAP ↔GAP | KE4 | 0.05 | Equ. Const. |
| 5 | GAP+DHAP ↔FBP | KM51 | 0.3 | GAP |
| 5 | GAP+DHAP ↔FBP | KM52 | 0.4 | DHAP |
| 5 | GAP+DHAP ↔FBP | KM53 | 0.02 | FBP |
| 5 | GAP+DHAP ↔FBP | KE5 | 7.1 | Equ. Const. |
| 6 | FBP→F6P+Pi | KM61 | 0.033 | FBP |
| 6 | FBP→F6P+Pi | KI61 | 0.7 | F6P |
| 6 | FBP→F6P+Pi | KI62 | 12 | Pi |
| 6 | FBP→F6P+Pi | KE6 | 6.7×105 | Equ Const. |
| 7 | F6P+GAP→E4P+Xu5P | KM71 | 0.1 | Xu5P |
| 7 | F6P+GAP→E4P+Xu5P | KM72 | 0.1 | GAP |
| 7 | F6P+GAP→E4P+Xu5P | KE7 | 10 | Equ. Const. |
| 8 | E4P+DHAP→SBP | KM8 | 0.02 | SBP |
| 8 | E4P+DHAP→SBP | KM81 | 0.4 | DHAP |
| 8 | E4P+DHAP→SBP | KM82 | 0.2 | E4P |
| 8 | E4P+DHAP→SBP | KE8 | 1.07 | Equ. Const. |
| 9 | SBP→S7P+Pi | KM9 | 0.05 | SBP |
| 9 | SBP→S7P+Pi | KI9 | 12 | Pi |
| 9 | SBP→S7P+Pi | KE9 | 6.7×105 | Equ. Const. |
| 10 | S7P+GAP→Ri5P+Xu5P | KM101 | 0.118 | P5P |
| 10 | S7P+GAP→Ri5P+Xu5P | KM102 | 0.072 | GAP |
| 10 | S7P+GAP→Ri5P+Xu5P | KM103 | 0.46 | S7P |
| 10 | S7P+GAP→Ri5P+Xu5P | KM104 | 1.54 | F6P |
| 10 | S7P+GAP→Ri5P+Xu5P | KE10 | 1.17 | Equ. Const. |
| 11 | Ri5P↔Ru5P | KE11 | 0.4 | Equ. Const. |
| 12 | Xu5P↔Ru5P | KE12 | 0.67 | Equ. Const. |
| 13 | Ru5P+ATP→RuBP+ADP | KM131 | 0.05 | Ru5P |
| 13 | Ru5P+ATP→RuBP+ADP | KM132 | 0.059 | ATP |
| 13 | Ru5P+ATP→RuBP+ADP | KI131 | 2 | PGA |
| 13 | Ru5P+ATP→RuBP+ADP | KI132 | 0.7 | RuBP |
| 13 | Ru5P+ATP→RuBP+ADP | KI133 | 4 | Pi |
| 13 | Ru5P+ATP→RuBP+ADP | KI134 | 2.5 | ADP |
| 13 | Ru5P+ATP→RuBP+ADP | KE13 | 0.4 | ADP |
| 13 | Ru5P+ATP→RuBP+ADP | KI135 | 6846 | Equ. Const. |
| 16 | ADP+Pi→ATP | KM161 | 0.014 | ADP |
| 16 | ADP+Pi→ATP | KM162 | 0.3 | Pi |
| 16 | ADP+Pi→ATP | KM163 | 0.3 | ATP |
| 16 | ADP+Pi→ATP | KE16 | 5.7 | Equ. Const. |
| 21 | F6P↔G6P | KE21 | 2.3 | Equ. Const. |
| 22 | G6P↔G1P | KE22 | 0.058 | Equ. Const. |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KM231 | 0.08 | G1P |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KM232 | 0.08 | ATP |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KA231 | 0.1 | PGA |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KA232 | 0.02 | F6P |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KA233 | 0.02 | FBP |
| 23 | G1P+ATP+Gn→PPi+ADP+Gn+1 | KI23 | 10 | ADP |
| 31 | Pext +DHAPi→Pi+DHAPo | KM311 | 0.077 | DHAP |
| 31 | Pext +DHAPi→Pi+DHAPo | KM312 | 0.63 | Pi |
| 31 | Pext +DHAPi→Pi+DHAPo | KM313 | 0.74 | Pext |
| 32 | Pext +PGAi→Pi+PGAo | KM32 | 0.25 | PGA |
| 33 | Pext +GAPi→Pi+GAPo | KM33 | 0.075 | GAP |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| RNa | Reaction | Param.b | Value (mM)c | Descriptiond |
| 112 | 2-PGCA +H2O 🡪 GCA + Pi | KM112 | 0.026 | PGCA |
| 112 | 2-PGCA +H2O 🡪 GCA + Pi | KI1121 | 94 | GCA, competitive with PGCA |
| 112 | 2-PGCA +H2O 🡪 GCA + Pi | KI1122 | 2.55 | Pi, competitive with PGCA |
| 113 | GCEA + ATP🡪 PGA + ADP | KM1131 | 0.21 | ATP |
| 113 | GCEA + ATP🡪 PGA + ADP | KM1132 | 0.25 | GCEA |
| 113 | GCEA + ATP🡪 PGA + ADP | KI113 | 0.36 | PGA, competitive with ATP |
| 113 | GCEA + ATP🡪 PGA + ADP | KE113 | 300 | Equil. Const. |
| 121 | GCAC+02🡪H2O2+GOAc | KM121 | 0.1 | GCAc |
| 122 | GOAc + SERc🡪 HPRc + GLYc | KM1221 | 0.15 | GOAc |
| 122 | GOAc + SERc🡪 HPRc + GLYc | KM1222 | 2.7 | SERc |
| 122 | GOAc + SERc🡪 HPRc + GLYc | KI1221 | 33 | GLYc, competitive with SERc |
| 122 | GOAc + SERc🡪 HPRc + GLYc | KE122 | 0.24 | Equil. Const. |
| 123 | HPRc + NADc🡪 NADHc + GCEAc | KM123 | 0.09 | HPRc |
| 123 | HPRc + NADc🡪 NADHc + GCEAc | KI123 | 12 | HPRc, self inibition |
| 123 | HPRc + NADc🡪 NADHc + GCEAc | KE123 | 2.5  ×105 | Equil. Const. |
| 124 | GOAc + GLUc🡪 KGc + GLYc | KM1241 | 0.15 | GOAc |
| 124 | GOAc + GLUc🡪 KGc + GLYc | KM1242 | 1.7 | GLUc |
| 124 | GOAc + GLUc🡪 KGc + GLYc | KI124 | 2 | GLYc competitive with GLU |
| 124 | GOAc + GLUc🡪 KGc + GLYc | KE124 | 607 | Equi. Const. |
| 131 | GLYc + NADc🡪 CO2 + NH3 + SERc +NADHc | KM1311 | 6 | GLYc |
| 131 | GLYc + NADc  🡪 CO2 + NH3 + SERc +NADHc | KI1311 | 4 | SERc, competitive with GLYc |
| 101a | GCEAc 🡪 GCEA | KM1011 | 0.39 | GCEA |
| 101a | GCEAc🡪GCEA | KI1011 | 0.28 | GCA, competitive with GCEA |
| 101b | GCA🡪GCAc | KM1012 | 0.2 | GCA |
| 101b | GCA🡪GCAc | KI1012 | 0.22 | GCEA, competitive with GCA |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| RNa | Reaction | Paramb | Value (mmol l-1)d | Descri-ptionc |
| 51 | DHAPc + PGAc ↔ FBPc | Km511 | .020 | FBPc |
| 51 | DHAPc + PGAc ↔ FBPc | Km512 | .300 | GAPc |
| 51 | DHAPc + PGAc ↔ FBPc | Km513 | .400 | DHAPc |
| 51 | DHAPc + PGAc ↔ FBPc | Km514 | .014 | SBPc |
| 51 | DHAPc + PGAc ↔ FBPc | KE51 | 12 |  |
| 52 | FBPc ↔ F6Pc + Pic | Km521 | .0025 | FBPc |
| 52 | FBPc ↔ F6Pc + Pic | KI521 | .7 | F6Pc |
| 52 | FBPc ↔ F6Pc + Pic | KI522 | 12 | Pic |
| 52 | FBPc ↔ F6Pc + Pic | KI523 | 7\*10-5 | F26BPc |
| 52 | FBPc ↔ F6Pc + Pic | KE52 | 6663 |  |
| 55 | G1Pc + UTPc↔GDPc +UDPGc | Km551 | .14 | G1Pc |
| 55 | G1Pc + UTPc↔GDPc +UDPGc | Km552 | .1 | UTPc |
| 55 | G1Pc + UTPc↔GDPc +UDPGc | Km553 | .11 | OPOPc |
| 55 | G1Pc + UTPc↔GDPc+UDPGc | Km554 | .12 | UDPGc |
| 55 | G1Pc + UTPc↔ GDPc+UDPGc | KE55 | 0.31 | Equi |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | Km561 | 0.8 | F6Pc |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | Km562 | 2.4 | UDPGc |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KI561 | .7 | UDPc |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KI562 | .8 | FBPc |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KI563 | 0.4 | SUCPc |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KI564 | 11 | Pic |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KI565 | 50 | Sucrose |
| 56 | UDPGc + F6Pc ↔ SUCPc + UDPc | KE56 | 10 | Equl. Const. |
| 57 | SUCPc ↔ Pic + SUCc | Km571 | .35 | SUCPc |
| 57 | SUCPc ↔ Pic + SUCc | Ki572 | 80 | SUCc |
| 57 | SUCPc ↔ Pic + SUCc | KE57 | 780 | Equil. Const. |
| 58 | F26BPc ↔ F6Pc + Pic | Km581 | .032 | F26BPc |
| 58 | F26BPc ↔ F6Pc + Pic | KI581 | .1 | F6Pc |
| 58 | F26BPc ↔ F6Pc + Pic | KI582 | .5 | Pic |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | Km591 | 0.5 | ATPc |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | Km592 | .021 | F26BPc |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | Km593 | 0.5 | F6Pc |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | KI591 | .16 | ADPc |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | KI592 | 0.7 | DHAPc |
| 59 | F6Pc + ATPc ↔ F26BPc + ADPc | KE59 | 590 |  |
| 60 | F6Pc + ATPc ↔ F26BPc + ADPc | Km601 | 0.042 | ADPc |
| 60 | F6Pc + ATPc ↔ F26BPc + ADPc | Km602 | 1.66 | ATPc |
| 60 | F6Pc + ATPc ↔ F26BPc + ADPc | Km603 | 0.28 | UDPc |
| 60 | F6Pc + ATPc ↔ F26BPc + ADPc | Km604 | 16 | UTPc |
| 60 | F6Pc + ATPc ↔ F26BPc + ADPc | KE60 | 16 | Equili. |
| 61 | SUCPc ↔ SUCc + Pic | KE61 | 1.2\*107 | Equili. |
| 62 | SUCc ↔ Sink | Km621 | 5 | Sucrose |

Table S3 The maximum rate of each enzyme (Vm) normalized on maximum Rubisco carboxylation activity (Vcmax).

|  |  |  |  |
| --- | --- | --- | --- |
| Maximum Velocity | Enzyme | Reaction | Vm/V1 |
| V1 | Rubisco | RuBP+CO2→2PGA | 1 |
| V2 | PGA Kinase | PGA+ATP → ADP + DPGA | 10.3 |
| V3 | GAP dehydragenase | DPGA+NADPH →GAP + Pi+NADP | 1.39 |
| V5 | FBP Aldolase | GAP+DHAP →FBP | 0.42 |
| V6 | FBPase | FBP→F6P+Pi | 0.25 |
| V7 | Transketolase | F6P+GAP→E4P+Xu5P | 1.07 |
| V8 | Aldolase | E4P+DHAP→SBP | 0.42 |
| V9 | SBPase | SBP→S7P+Pi | 0.11 |
| V10 | Transketolase | S7P+GAP→Ri5P+Xu5P | 1.07 |
| V13 | Ribulosebiphosphate kinase | Ru5P+ATP→RuBP+ADP | 3.71 |
| V16 | ATP synthase | ADP+Pi→ATP | 5.5 |
| V23 | ADP-glucose pyrophosphorylase and  Starch Synthase | ADPG+Gn→G(n+1)+ADP | 0.1 |
| V31 | Phosphate translocator | DHAPi→DHAPo | 0.3 |
| V32 | Phosphate translocator | PGAi→PGAo | 0.3 |
| V33 | Phosphate translocator | GAPi→GAPo | 0.3 |

|  |  |  |  |
| --- | --- | --- | --- |
| Max. Velocity | Enzyme  name | Reaction | Vm/V1 |
| V111 | Rubisco | RuBP + O2 → PGA + PGCA | 0.24 |
| V112 | Phosphoglycolate phosphatase | 2-PGCA +H2O → GCA + Pi | 18.0 |
| V113 | Glycerate kinase | GCEA + ATP → PGA + ADP | 1.96 |
| V121 | Glycolate oxidase | GCAC+02 → H2O2+GOAc | 0.45 |
| V122 | Serine glyoxylate aminotransferase | GOAc +SERc → HPRc + GLYc | 1.13 |
| V123 | NADH-hydroxypyruvate reductase | HPRc + NADc → NADHc + GCEAc | 3.44 |
| V124 | Glutamate glyoxylate aminotransferase (GGAT) | GOAc + GLUc → KGc + GLYc | 0.94 |
| V131 | Glycine decarboxylase | GLYc + NADc → CO2 + NH3 + SERc +NADHc | 0.86 |
| V1T | Glycerate/glycolate transporter | GCEAc ↔ GCEA | 0.4 |
| V2T | Glycerate/glycolate transporter | GCAc ↔ GCA | 0.4 |

|  |  |  |
| --- | --- | --- |
| Maximum Velocity | Reaction | Vm/V1 |
| V51 | DHAPc + PGAc ↔ FBPc | 0.037 |
| V52 | FBPc ↔ F6Pc + Pic | 0.022 |
| V55 | G1Pc + UTPc ↔ GDPc + UDPGc | 0.040 |
| V56 | UDPGc + F6Pc ↔ SUCPc + UDPc | 0.019 |
| V57 | SUCPc ↔ Pic + SUCc | 0.19 |
| V58 | F26BPc ↔ F6Pc + Pic | 0.007 |
| V59 | F6Pc + ATPc ↔ F26BPc + ADPc | 0.002 |
| V60 | ATPc + UDPc ↔ UTPc + ADPc | 1 |

Table S4 The initial concentrations of metabolites

|  |  |  |
| --- | --- | --- |
| Metabolite  name | location | Model default  (mmol l-1) |
| RuBP | Chl | 2.000 |
| PGA | Chl | 2.400 |
| DPGA | Chl | 0.0011 |
| GAP | Chl | 0.02 |
| DHAP | Chl | 0.48 |
| FBP | Chl | 0.670 |
| E4P | Chl | 0.050 |
| S7P | Chl | 2.0 |
| SBP | Chl | 0.30 |
| ATP | Chl | 0.68 |
| NADPH | Chl | 0.21 |
| CO2 | Chl | 0.012 |
| O2 | Chl | 0.26 |
| HexP | Chl | 2.2 |
| PenP | Chl | 0.25 |
| Pi | Chl | 5 |
| CP | Chl | 15 |
| CA | Chl | 1.5 |
| CN | Chl | 0.5 |
| Pext | Chl | 0.5 |

|  |  |  |  |
| --- | --- | --- | --- |
| **NADH** | Chl | | 0.22 |
| **NADHc** | Cyto | | 0.47 |
| **NAD** | Chl | | 0.08 |
| **NADc** | Cyt | | 0.02 |
| **ATP** | Chl | | 0.68 |
| **ATPc** | Cyt | | 0.36 |
| **ADP** | Chl | | 0.82 |
| **ADPc** | Cyt | | 0.64 |
| **GLUc** | Cyt | | 24 |
| **KGc** | Cyt | | 0.4 |
| **Pic** | Chl | | 5 |
| **SERc** | Cyt | | 7.5 |
| **GLYc** | Cyt | | 1.8 |
| **PGA** | Chl | | 4.3 |
| **GOAc** | Cyt | | 0.028 |
| **GCA** | Chl | | 0.36 |
| **GCAc** | Cyt | | 0.36 |
| **PGCA** | Chl | | 0.003 |
| **HPRc** | Cyt | | 0.004 |
| **GCEA** | Chl | | 0.18 |
| **GCEAc** | Cyt | | 0.18 |
|  | |  | |  |
| **TPc** | Cyt | | 2.3 |
| **FBPc** | Cyt | | 2 |
| **F26BPc** | Cyt | | 7×10-6 |
| **UTc** | Cyt | | 1 |
| **HexPc** | Cyt | | 6 |
| **UDPG** | Cyt | | 0.6 |
| **PTc** | Cyt | | 15 |
| **ATc** | Cyt | | 1 |

## Equations

The rate equations of the photosynthetic carbon metabolism (Zhu et al., 2007)



















Differential equations to describe rates of change in each intermediate of carbon metabolism.







# light reaction model

## Description and equations

The electron transport rate of the light reactions used in the model followed [von Caemmerer (2000](#_ENREF_7)):







where: *I2* is the light absorbed by *PSII*, *Jmax* is the maximum electron transport rate, θ is an empirical curvature factor (0.7 was assumed following the value in a C3 plant ([Evans 1989](#_ENREF_2))), β is 0.752 which is the convert constant of electron to ATP. α is leaf absorptance (0.85 after [von Caemmerer (2000](#_ENREF_7))), *f* corrects for spectral quality (0.15 according to [Evans (1987](#_ENREF_3)))*, VE\_ATPsyn*is the ATP synthesis rate calculated from Michaelis-Menten equation of ATP synthase.

## Parameters and value

Table S5 the parameters of light reaction model

|  |  |  |
| --- | --- | --- |
| parameters | Values | Reference |
| α | 0.85 | [von Caemmerer (2000](#_ENREF_7)) |
| β | 0.752 | [von Caemmerer (2000](#_ENREF_7)) |
| *f* | 0.15 | [Evans (1987](#_ENREF_3)) |
| *Jmax* | Table S1 |  |
| θ | 0.7 | ([Evans 1989](#_ENREF_2)) |

# Rubisco activation

## Description

The detailed model describing the reactions involved in Rubisco activation and deactivation (Zhu et al., 2012)

## Parameters and values

Table S6 The rate constants of the rubisco activation model (Zhu et al., 2013)

|  |  |  |
| --- | --- | --- |
| parameters | Values | Description |
| k1 | 1.5e-04 | The rate constant of the activation of the Rubisco bound with RuBP |
| kn1 | 1.6e-03 | The rate constant of E inactivation by binding of RuBP |
| km1 | 2 e-05 | The michaelis-menton constant for RuBP with E |
| Ke2 | 0.1 | Mate et al 1996 |
| Ke3 | 1.6 | Mate et al 1996 |
| k6 | 3.75 | Rubisco activity |
| kc | 0.016 | Michaelis-menton constant for CO2 |
| ko | 0.448 | Michaelis-menton constant for O2 |
| k7 | k6 \* 10 | The rate constant for ECM to ECMR |
| kr | 2 e-02 | he apparaent michaelis menton constant for RuBP |
| RAC | 0.006 | Rubisco activase activity |

Table S7 The initial concentrations of metabolites

|  |  |  |
| --- | --- | --- |
| parameters | Values | Description |
| ER | 0.8 | The concentration of inactive ER |
| Eaf | 0.2 | he total concentration of E, EC, AND ECM |
| ECMR | 0.2 | The concentration of ECMR |
| RuBP | 2 | The concentration RuB |

## Equations

CA = 1



























ET= ER+Eaf+ECMR

Percent = 1-ER/ET





# Dynamic stomatal conductance response

## Description and equations

Dynamic stomata conductance was calculated by the following ODE:



where: *gsteady* is calculated by the Ball-Berry model ([Ball et al. 1987](#_ENREF_1)); *k* is *ki* or *kd* calculated from measured stomata dynamics in cassava.

Ball-Berry model parameters for predicting stomatal conductance ([Ball et al. 1987](#_ENREF_1)) were obtained from light response curves measured in each one of the cultivars. The Ball-Berry model correlates stomatal conductance with net photosynthesis (*A*), relative humidity (*RHs*) and CO2 concentration at the leaf surface (*Ca*):



where: *g0* is the residual stomatal conductance when photosynthesis rate is zero, *m* is the slope of the relationship between *gs* and *A\*RHs/Ca*. *g0* and *m* were estimated by linear curve fitting.

## Parameters and values

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Cultivar | Kd(s-1) | Ki(s-1) | Ball Berry Slop(m) | Intercept(g0) |
| Mbundumali | 0.0026 | 0.0017 | 5.50 | 0.079 |
| TME3 | 0.0017 | 0.0019 | 6.36 | 0.087 |
| TME419 | 0.0034 | 0.0022 | 5.32 | 0.078 |
| TME693 | 0.0011 | 0.0017 | 6.50 | 0.072 |
| TME7 | 0.0030 | 0.0020 | 5.80 | 0.070 |
| TMS01/1412 | 0.0035 | 0.0031 | 6.24 | 0.072 |
| TMS30001 | 0.0036 | 0.0018 | 6.43 | 0.047 |
| TMS30572 | 0.0010 | 0.0015 | 6.63 | 0.069 |
| TMS96/1632 | 0.0029 | 0.0019 | 5.48 | 0.110 |
| TMS98/0002 | 0.0039 | 0.0016 | 5.00 | 0.096 |
| TMS98/0581 | 0.0035 | 0.0021 | 7.29 | 0.068 |

# Cassava leaf model

## Description and equations

At the leaf level, the metabolic model and Rubusco activase model was integrated with leaf level models of stomatal physiology, and energy balance based on the method of ([Nikolov et al. 1995](#_ENREF_5)).

**Leaf boundary layer conductance**

The leaf internal air space is assumed to be saturated and the saturation vapor pressure as a function of temperature:

The boundary layer conductance is given as:

**Leaf energy balance**

The leaf energy balance equation under steady state equilibrium

## Parameters and values

|  |  |  |
| --- | --- | --- |
| Environmental condition | value | Unit |
| Relative humidity | 0.6 |  |
| Leaf dimension | 0.06 | m |
| Wind speed (vw) | 5 | m s-1 |
| Temperature | 25 | oC |
| Atmospheric pressure | 101325 | Pa |
| Cp | 29.3 | J mol*−*1 *◦*C*−*1 |
| CLV | 44000.0 | J mole-1 |
| σ | 5.6697E-8 | W m-2K-4 |

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