Adaptation of 3-PG to novel species :
guidelines for data collection and parameter assignment

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Summary

There is growing interest worldwide in the use of the process-based model 3-PG as a forest management tool because (a) it is simple, and (b) it is freely available. This use will entail its adaptation to an increasing range of species, and even clones. The potential consequences of incorrect predictions by the model leading to something going badly wrong when it is used as a management tool, is of concern. This is particularly the case because it is difficult to simultaneously obtain above- and below-ground biomass data to properly test or parameterise 3-PG.

This report concerns the adaptation of 3-PG to novel species, and is based on my experience in estimating parameters for and applying 3-PG to *Eucalyptus globulus* and *E. grandis*, and estimating parameters for non-linear regression models and other process-based models.

I outline the structure of 3-PG, discuss the data required to adequately test its various components, and provide guidelines for the assignment of species-specific parameters. A proper appreciation of the subtleties of parameter assignment for 3-PG requires a basic description of its mathematical structure, which is given. I emphasise that: (a) in the first instance parameters should be assigned values based on direct measurement or by analogy with other species, (b) estimation of parameters by fitting model output to observed data should be done with care and a sound understanding of the structure of the model, (c) it is necessary to check that the final parameter values and all model outputs are biologically reasonable, and (d) predictions based on the assigned parameters should be always validated against independently observed data. Finally, I outline the development and application of software tools that aid parameter estimation in the context of 3-PG.

This document is a "work in progress", and will be updated as further experience is gained with parameterisation of 3-PG for a range of species and sets of available data.

Contents

1. Introduction

There is growing interest worldwide in the use of process-based models (PBMs) as tools for forest management. In Australia, PROMOD (Battaglia & Sands, 1997), CABALA (Battaglia *et al.*, 2004) and 3-PG (Landsberg & Waring, 1997) are widely used as an adjunct to traditional forest management tools by various agencies (research, government, commercial forestry and private consultants) for diagnostic services, decision making and economic analysis. In Brazil, Aracruz Cellulose is implementing 3-PG as the central component of a new GIS-based management system (Almeida *et al.*, 2003; Almeida *et al.*, 2004b), and in South Africa 3-PG is also being implemented as a forest management tool both through a project funded by the South African Government Innovation Fund (National Research Foundation, 2002) and the Institute for Commercial Forestry Research (ICFR).

It appears that the *de facto* PBM for use as a forest management tool is 3-PG. I believe this is not because it is technically superior to other models, but because (a) it is simple, and (b) it is freely available, whereas models such as PROMOD (originally) and CABALA (more recently) are not (Sands *et al.*, 2000). 3-PG is a generic, PBM of forest growth for which individual species are characterised by a set of species-specific parameters. It has been applied across a wide range of environments and species, including conifers and both evergreen and deciduous hardwoods.

The proposed use of 3-PG as a tool for forest management is predicated on the ability to reliably assign values for parameters characterising novel species. For instance, Aracruz intends to use 3-PG to differentiate between *Eucalyptus grandis* clones and hybrids, and the South African application requires its adaptation to a range of eucalypt, acacia, pine and other species. For most of these, even rudimentary parameter sets are not available.

The proliferation of species to which 3-PG is being applied, and the potential serious consequences of incorrect model predictions when it is used as a management tool, raises doubts I have about how 3-PG has and/or will be tested or parameterised. These arise partly because of a general lack of suitable data to properly test or parameterise the model, especially both above- and below-ground biomass data, and partly because testing and parameterisation might not been done within a proper understanding of the subtleties of even as simple a model as 3-PG. In only a few cases have parameters characterising a species been rigorously determined, and even then this has been largely by a process of trial and error, e.g. for *E. globulus* by Sands and Landsberg (2002).

As a first general rule, parameters for novel species should always be assigned by direct and independent measurement or by analogy with others species, as was largely the case with PROMOD (Battaglia & Sands, 1997) and CABALA (Battaglia *et al.*, 2004). Failing this, their values can be adjusted in order to optimise the fit of selected outputs to corresponding observed values, a process called *parameter estimation*. In this case, the use of software automating this optimisation will facilitate estimation. But uniformed use of such software can also result in disaster! It is often very easy to get a good fit to observed data for wrong reasons, especially if above- and below-ground observed biomass data are not simultaneously available.

A systematic protocol for assigning species-specific parameters can be facilitated through the use of a deeper understanding of 3-PG, the meaning of its parameters, and an understanding of the sensitivity of 3-PG outputs to these parameters (e.g. Sands & Landsberg, 2002). In particular, such understanding is essential to support the use of software tools for parameter estimation by optimising the fit of output to observed data.

Recent applications of 3-PG to *E. globulus* (Sands & Landsberg, 2002) and *E. grandis* (Almeida *et al.*, 2004a; Esprey *et al.*, 2004) attempted to provide rigour to model testing and parameter assignment. This report is based on my experience in these studies, and in estimating parameters for a range of other models. There is a wealth of additional experience in the literature. For example: general discussions in the context of modelling biological systems can be found in Haefner (1996), and in ground water research in Anderson & Woessner (1992) and Hill (1998), and some of the problems and pitfalls of parameter estimation in PBMs are highlighted by Hopkins (1996), and Sievänen & Burk (1993, 1994).

In this report I outline the structure of 3-PG, discuss the data required to adequately test its various components, and provide guidelines for the assignment of species-specific parameters. A proper appreciation of the subtleties of parameter assignment for 3-PG requires a basic description of its mathematical structure, which is given. I emphasise that: (a) in the first instance parameters should be assigned values based on direct measurement or by analogy with other species, (b) estimation of parameters by fitting model output to observed data should be done with care and a sound understanding of the structure of the model, (c) it is necessary to check that the final parameter values and all model outputs are biologically reasonable, and (d) predictions based on the assigned parameters should be always validated against independently observed data. Finally, I outline the development and application of software tools that aid parameter estimation in the context of 3-PG.

2. Overview of 3-PG

3-PG is a simple, process-based, stand-level model of forest growth developed by Landsberg and Waring (1997). It is a deliberate attempt to bridge the gap between mensuration-based growth and yield models, and process-based, carbon-balance models. It requires only readily available site and climatic data as inputs and predicts the time-course of stand development on a monthly basis in a form familiar to the forest manager, as well as various biomass pools, water use and available soil water. 3-PG can be applied to plantations or to even-aged, relatively homogeneous forests. It is a generic stand model since its structure is neither site nor species-specific, but it must be parameterised for individual species.

The model has found numerous applications for various species (e.g., Coops *et al.*, 2000; Landsberg *et al.*, 2001; Sands & Landsberg, 2002; Waring, 2000; Almeida *et al.*, 2004a; Dye *et al.*, 2004; Esprey *et al.*, 2004). A modified version, 3-PG Spatial, has been applied to study forest productivity across landscapes (e.g., Coops *et al.*, 1998a, 1998b).

A popular implementation of 3-PG is 3PGPJS (Sands, 2004). The interface is user-friendly, and based on a Microsoft Excel workbook that supplies all 3-PG input data and to which results are written, and an Excel add-in containing the 3PGPJS and 3-PG code written in Visual Basic for Applications. The input spreadsheets facilitate easy modification of site and climatic data, parameter values and run-time options. The use of normal spreadsheet operations for analysing and graphing 3-PG output gives added flexibility.

2.1 Model structure

The heart of 3-PG is five simple submodels: biomass production; allocation of biomass between foliage, roots and stems (including branches and bark); stem mortality; soil water balance; and a module to convert stem biomass into variables of interest to forest managers. Its state variables are the foliage, stem and root biomass pools, the stem numbers or stocking and the available soil water. The stem biomass pool includes bark and branches, although

3-PG can discount this for branch and bark by using a species- and age-dependent branch-and-bark fraction.

Additional information can be found in Landsberg and Waring (1997) and Sands and Landsberg (2002). Fig. 1 illustrates the structure of 3-PG, and Sec. 3 provides a detailed mathematical description of 3-PG. In this report, repeated terms are abbreviated by upper case letters, e.g. NPP for net primary production, whereas the mathematical description employs standard mathematical notation, e.g. P_n for NPP.

2.2   Data inputs

The climatic data required are monthly averages of daily total solar radiation, mean air temperature and daytime atmospheric vapour pressure deficit (VPD), monthly rainfall and irrigation, and frost days. 3-PG can use either actual monthly weather data or long-term monthly averages. Use of averaged data is common unless there is particular interest in specific events, such as droughts. Other inputs are factors describing the site: site latitude, a site fertility rating, maximum available soil water, and soil texture.

2.3   3-PG outputs

The primary 3-PG outputs are the state variables, and variables such as stand evapo-transpiration, net primary production (NPP), specific leaf area (SLA), and canopy leaf area index (LAI). It also provides stand-level outputs often used as inputs into management systems familiar to the forest manager, e.g. main-stem volume, mean annual volume increment (MAI), and mean diameter at breast height (DBH). Depending on how 3-PG is parameterised, DBH can be either the arithmetic or quadratic mean of single tree diameters, where the latter is preferred. Outputs from 3-PG can be either monthly or annual values.

2.4   Biomass production

Radiation intercepted by the canopy is determined from total incoming solar radiation and LAI through Beer's law. Gross primary production (GPP) is proportional to intercepted photosynthetically active radiation. The proportionality factor, called canopy quantum efficiency, takes into account environmental effects through multiplicative modifiers based on atmospheric VPD, available soil water, mean air temperature, frost days per month, site nutrition, and stand age. NPP is a constant fraction of GPP.

2.5   Biomass allocation

Allocation of NPP to roots is determined by growing conditions as expressed by available soil water, VPD and site fertility. The proportion of NPP allocated to roots increases when nutritional status and/or available soil water are low. Biomass allocation to foliage and stems depends on average tree size (i.e. DBH) in such a manner that allocation to foliage declines and that to stems increases as stands age. DBH is determined from the mean single-tree stem mass through an allometric relationship.
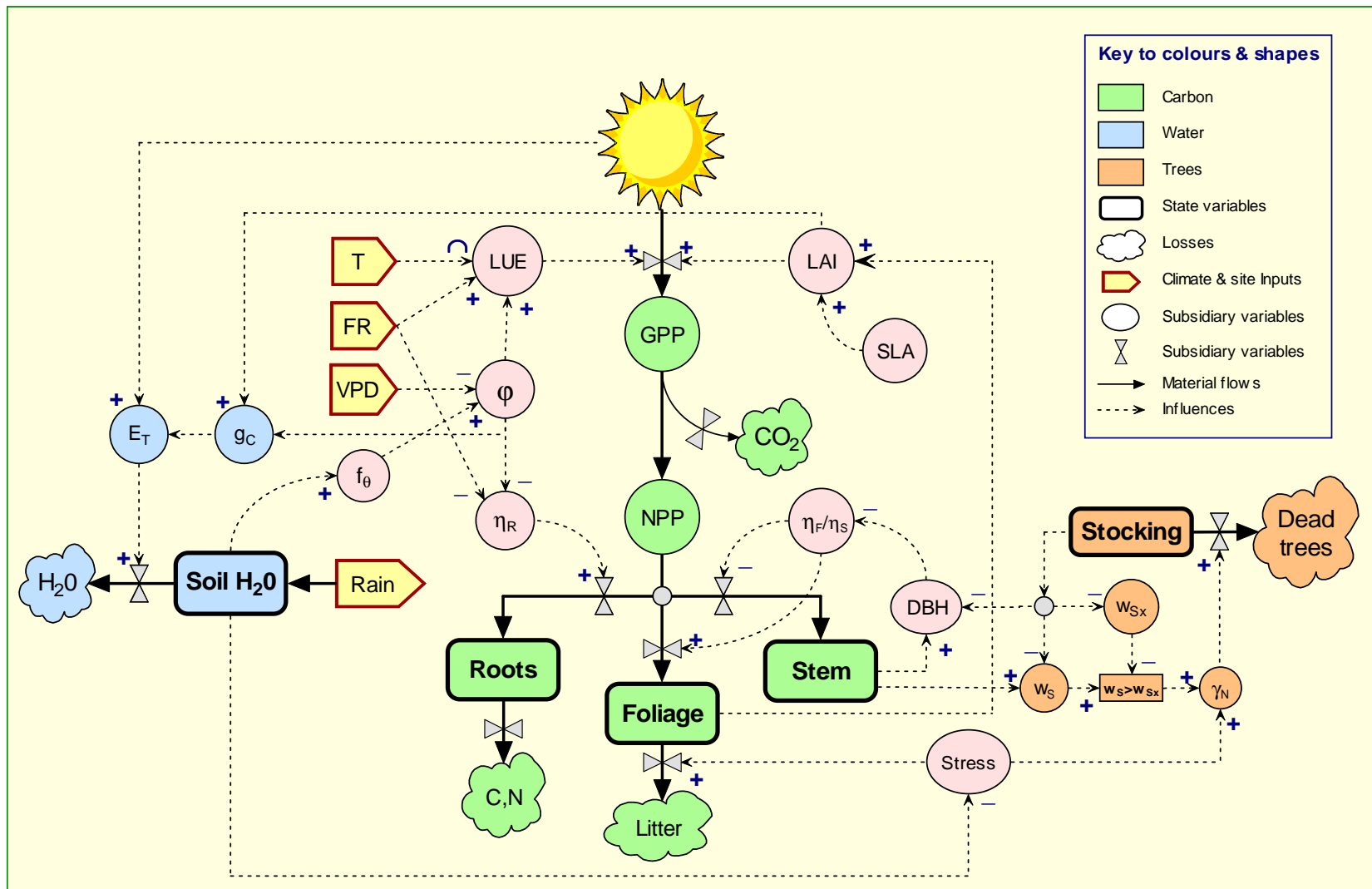
Figure 1. Basic structure of 3-PG and the causal influences of its variables and processes. Refer to Table 1 for the meaning of the symbols.

2.6 Stem mortality

An age dependent probability of tree death is applied monthly, and is potentially modified by long-term stress factors, e.g. water stress. Changes in stocking are also calculated using the self-thinning law to estimate an upper limit to the mean single-tree stem mass for the current stocking. If the current mean stem mass is greater than this limit, the population is reduced to a level consistent with the limit. Because suppressed trees die first, it is assumed that each tree removed has only a fraction of the biomass of the average tree.

2.7 Soil water balance

3-PG includes a single-layer soil-water-balance model working on a monthly time step. Rainfall (including irrigation) is balanced against evapotranspiration computed using the Penman-Monteith equation. Canopy rainfall interception is a fraction of rainfall, and depends on canopy LAI. Soil water in excess of the intrinsic soil-water holding capacity for the site is lost as runoff (or deep drainage). Canopy conductance is determined from canopy LAI and stomatal conductance. It increases with increasing LAI up to a maximum conductance, and is affected by VPD, available soil water and stand age.

2.8 Stand characteristics

Stand level characteristics such as stem volume, DBH, basal area, and MAI are computed from the biomass pools and stem numbers. The branch-and bark-fraction and basic density are explicitly age related. Allometric relationships in terms of stocking and DBH can be used to determine stem height, utilisable volume, etc.

3. Basic equations of 3-PG

This section lists the basic equations of 3-PG. Reference should be made to Landsberg and Waring (1997) and Sands and Landsberg (2002) for detailed justification of these. A complete list of symbols and units of all 3-PG variables and parameters are listed in Tables 1 and 2, respectively, with only the major variables defined below.

3.1 Basic symbol definitions

The required climatic input data are monthly averages of daily total solar radiation (Q MJ m^{-2} d^{-1}), mean air temperature (T_a °C) and day-time atmospheric VPD (D mbar), and monthly rainfall (R mm month^{-1}) and frost days (d_F month^{-1}).

The state variables of 3-PG are foliage, stem and root biomass (as dry matter; W_F, W_S and W_R t$_{DM}$ ha^{-1}), stem numbers or stocking (N trees ha^{-1}) and available soil water (θ_s mm). W_S includes bark and branches, but 3-PG can discount this for branch and bark through the age-dependent branch-and-bark fraction (p_{BB}). The basic unit of time (t) in the following description is a day, and the rate of change of the state variables with respect to time can be written as a set of coupled differential equations. However, because many of the relationships in 3-PG are better suited to a time step of a month rather than a day, 3-PG is usually implemented as a set of difference equations with a default time step of one month. The following description employs difference equations, and parameters in Appendix 2 with time in their units are conveniently given with the month as the temporal unit.

3-PG includes various internal variables, some of which are derived from the state variables, and others are explicitly age-dependent (Sec. 3.7). Stand means of the biomass pools are $w_i = 1000W_i/N$ (kg tree^{-1}), where the subscript i denotes F, S or R. Of particular importance are the stand leaf area index L (m^2 m^{-2}), and the measure B (cm) of tree size. The latter can be either the arithmetic mean DBH or the corresponding quadratic mean diameter (qDBH), where qDBH is preferred. In 3-PG, B is derived by inverting an allometric relationship between mean tree stem mass (i.e. w_S) and B. The choice of B as DBH or qDBH depends on which of these observations is used when 3-PG is parameterised. Other stand-level variables of significance to the forest manager are calculated from the state variables (Sec. 3.8).

3.2 Carbon balance

The carbon-balance equations of 3-PG are in essence those of McMurtrie and Wolf (1983). Let Δx be the change in any quantity x over a time interval of Δt days. The 3-PG carbon balance equations are then

$$\Delta W_F = \eta_F P_n - \gamma_F W_F \Delta t - m_F(W_F / N)\Delta N$$
$$\Delta W_R = \eta_R P_n - \gamma_R W_R \Delta t - m_R(W_R / N)\Delta N \tag{1}$$
$$\Delta W_S = \eta_S P_n - m_S(W_S / N)\Delta N \;,$$

where P_n (t ha^{-1} d^{-1}) is NPP, η_i is the fraction of NPP allocated to the ith pool, γ_F (d^{-1}) is the litterfall rate, γ_R (d^{-1}) is the root turnover rate, N is the stem number (trees ha^{-1}) and m_i is the fraction of the biomass per tree (W_i/N) in the ith pool that is lost when a tree dies. Death of trees is considered later (e.g. see Sec. 3.5).

The NPP is calculated from intercepted radiation, as determined by L and radiation incident above the canopy, through

$$P_n = 0.552\alpha_C Y(1 - e^{-kL/\zeta})\zeta \overline{Q}\Delta t \;, \tag{2}$$

where $\overline{Q}$ (MJ m^{-2} d^{-1}) is the mean daily solar radiation above the canopy over the time period Δt, ζ is the fractional ground cover by the canopy, α_C (mol mol^{-1}) is the canopy quantum efficiency modified by multipliers that take account of environmental effects (Sec. 3.3), k is the light extinction coefficient and Y is the (constant) ratio of NPP to GPP. The factor of 0.552 combines the conversion of total radiation into PAR (2.3 mol MJ^{-1}), of mol C into wood (24 g$_{DM}$ mol^{-1}), and g m^{-2} to t ha^{-1} (10^{-2}). Stand LAI is given by

$$L = 0.1\sigma W_F \tag{3}$$

where σ (m^2 kg^{-1}) is the age-dependent SLA and the factor 0.1 converts t ha^{-1} to kg m^{-2}.

3.3 Growth modifiers

Environmental effects on production are accounted for through dimensionless modifiers f_i ($0 \le f_i \le 1$) multiplicatively applied to the canopy quantum efficiency. These take into account the effects of mean air temperature (through f_T), frost days per month (through f_F), atmospheric VPD (through f_D), available soil water (through f_θ), site nutrition (through f_N), and stand age (through f_{age}). Then

$$\alpha_C = \alpha_{Cx}\varphi f_T f_F f_N$$
$$\varphi = f_{age} \min\{f_D, f_\theta\} \;, \tag{4}$$

where φ (known as PHYSMOD) also affects canopy conductance. In summary

$$f_T(T_a) = \left(\frac{T_a - T_{min}}{T_{opt} - T_{min}}\right)\left(\frac{T_{max} - T_a}{T_{max} - T_{opt}}\right)^{(T_{max} - T_{opt})/(T_{opt} - T_{min})}$$

$$f_F(d_f) = 1 - k_F(d_f/30)$$

$$f_N(FR) = 1 - (1 - f_{N0})(1 - FR)^{n_{fN}}$$

$$f_D(D) = e^{-k_D D} \tag{5}$$

$$f_\theta(\theta_S) = \frac{1}{1 + \left[(1 - \theta_S/\theta_{Sx})/c_\theta\right]^{n_\theta}}$$

$$f_{age}(t) = \frac{1}{1 + \left[(t/t_x)/r_{age}\right]^{n_{age}}}$$

where the dependent variables (T_a, d_F, etc) were defined earlier, and the various parameters (T_{min}, T_{opt}, etc) are summarised in Appendix 2. It is important to recognise that these parameters also need to be estimated or assigned values, and that the modifiers are multiplicative.

3.4 Biomass allocation

The biomass allocation ratios η_i are given by

$$\eta_R = \frac{\eta_{Rx}\eta_{Rn}}{\eta_{Rn} + (\eta_{Rx} - \eta_{Rn})m\varphi}$$

$$\eta_S = \frac{1 - \eta_R}{1 + p_{FS}} \tag{6}$$

$$\eta_F = p_{FS}\eta_S$$

where η_{Rn} and η_{Rx} are the minimum and maximum root allocation ratios, p_{FS} is the ratio of foliage:stem allocation, and m determines the effects of site fertility on allocation through

$$m = m_0 + (1 - m_o)FR \tag{7}$$

where m_0 is a parameter and FR ($0 \le FR \le 1$) is the site fertility rating.

The ratio p_{FS} is given by an allometric relationship with a measure of mean stem diameter B (e.g. quadratic mean diameter at breast height, in cm), itself obtained from an allometric relationship between B and mean stem mass w_S (i.e. stem+branch+bark, in kg):

$$p_{FS} = a_p B^{n_p}$$

$$w_S = a_S B^{n_S} \tag{8}$$

where the a's and n's are parameters. Sands and Landsberg (2002) showed how a_p and n_p are expressed in terms of the values p_2 and p_{20} of p_{FS} at $B = 2$ and 20 cm, and then used p_2 and p_{20} as parameters. From the second of Eqn (8) stem diameter is related to stand stem biomass and stocking through

$$B = (1000 W_S / a_S N)^{1/n_S} \tag{9}$$

since $w_S = 1000 W_S/N$, and the 1000 converts tonnes to kilograms.

3.5 Mortality

Tree mortality can be either density-independent (i.e. random or stress-induced), or density-dependent (i.e. through self-thinning). For each tree that dies, a fraction m_i of the mean biomass w_i in the ith biomass pool is removed. In general $m_i \leq 1$ because dieing trees are often suppressed. The values of m_i for density-dependent and density-independent mortality are assumed to be the same.

Density-independent mortality is represented by

$$\Delta N = -\gamma_N N \Delta t \tag{10}$$

where γ_N (d^{-1}) is the mortality rate. In the current version of 3-PG, γ_N is age-related; a later version of 3-PG will implement stress related effects on γ_N.

Density-dependent mortality is determined by applying the self-thinning rule (Landsberg & Waring, 1997) to ensure that the mean single-tree stem biomass w_S does not exceed the maximum permissible single-tree stem biomass w_{Sx} (kg tree^{-1}). The self-thinning rule gives w_{Sx} as a function of the current stem number

$$w_{Sx} = w_{Sx1000}(1000/N)^{n_N} , \tag{11}$$

where n_N is the exponent (usually 3/2) and w_{Sx1000} (kg tree^{-1}) is the value of w_{Sx} when the stem number is 1000 trees ha^{-1}. (If the stem number is 1000 trees ha^{-1}, then the total stand-level stem biomass at which self-thinning commences is about w_{Sx1000} t ha^{-1}). The need for self-thinning is checked at the end of each time step, and if $w_S > w_{Sx}$, then self-thinning is invoked as follows. If W_S^+ and N^+ are the stem biomass and stem numbers after self-thinning, then

$$W_S^+ = W_S - m_S(N - N^+)\frac{W_S}{N} , \tag{12}$$

and after self-thinning the stand must satisfy the self-thinning law, i.e.

$$\frac{W_S^+}{N^+} \leq w_{Sx1000}\left(1000/N^+\right)^{n_N} \times 10^{-3} . \tag{13}$$

Equations (12) & (13) are explicit equations for N^+ and W^+, and are solved iteratively to ensure the self-thinning law is satisfied for the new state.

3.6 Evapotranspiration and soil water balance

The soil water balance model in 3-PG operates on a monthly time step and is a balance between evapotranspiration E_T, rainfall R_P and irrigation R_I, all in mm month^{-1}, and makes allowance for canopy interception of rainfall. The water balance equation is

$$\Delta\theta_S = (1 - i_R)R_P + R_I - E_T , \tag{14}$$

where i_R is the fraction of rainfall intercepted, and subsequently evaporated from the canopy. Interception increases with canopy LAI up to maximum i_{Rx}:

$$i_R = i_{Rx} \min\{1, L/L_{ix}\} \tag{15}$$

where L_{ix} is the LAI at which interception is a maximum.

Any excess of θ_s over θ_{sx} is lost as run-off or deep soil drainage. Also, θ_s is bounded below by a minimum allowed available soil water θ_{sn} (mm). This is usually 0 but can be non-zero to

represent access to a water table or to simulate an irrigation strategy based on application of water when available soil water falls below a certain value.

Evapotranspiration is calculated using the Penman-Montieth equation, and depends on solar radiation, VPD and canopy conductance g_C (m s^{-1}). Canopy conductance is affected by stand age, VPD and soil water through the physiological modifier φ, and increases with increasing LAI up to a maximum g_{Cx} (m s^{-1}):

$$g_C = g_{Cx}\varphi \min\{1, L/L_{Cx}\}, \tag{16}$$

where L_{Cx} is the LAI at which conductance is a maximum. The Penman-Montieth equation contains various parameters that are physical in nature and have standard values, e.g. density of air and latent heat of vaporisation of water. It also takes into account the fact that transpiration occurs only during daylight hours, and the day length h (s d^{-1}) is calculated for the time of year and site latitude.

3.7   Age-dependent variables

Specific variables in 3-PG are age dependent and are given by empirical relationships whose parameters are certainly species specific. The variables in question are the specific leaf area σ, the leaf litterfall rate γ_F, stress-free density-independent mortality rate γ_N, the fraction of stem biomass in bark and branches p_{BB}, and basic density ρ (t m^{-3}).

Litterfall rate is given by

$$\gamma_F(t) = \frac{\gamma_{F1}\gamma_{F0}}{\gamma_{F0} + (\gamma_{F1} - \gamma_{F0})e^{-(t/t_{\gamma F})\ln(1+\gamma_{F1}/\gamma_{F0})}} \tag{17}$$

where γ_{F0} and γ_{F1} (d^{-1}) are litterfall rate at age 0 and for mature stands, and $t_{\gamma F}$ is the age at which the litterfall rate is $\frac{1}{2}(\gamma_{F0}+\gamma_{F1})$. The other age-dependent variables have a common functional form where only the parameters differ. Define the function f_e by

$$f_e(t; f_0, f_1, t_f, n) = f_1 + (f_0 - f_1)e^{-(\ln 2)(t/t_f)^n} \tag{18}$$

where f_0 and f_1 are the values of f_e when at age 0 and for mature stands, respectively, t_f is the age at which $f_e = \frac{1}{2}(f_0+f_1)$, and n is a constant (usually 1 or 2). Then

$$\begin{aligned}
\gamma_N(t) &= f(t; \gamma_{N0}, \gamma_{N1}, t_{\gamma N}, n_{\gamma N}) \\
\sigma(t) &= f(t; \sigma_0, \sigma_1, t_\sigma, 2) \\
p_{BB}(t) &= f(t; p_{BB0}, p_{BB1}, t_{BB}, 1) \\
\rho(t) &= f(t; \rho_0, \rho_1, t_\rho, 1)
\end{aligned} \tag{19}$$

and the meaning of the parameters is implied by the dependent variable and the definition (18) of the function f_e.

3.8   Stand-level variables

Stand-level variables such as stem diameter B (cm), basal area A (m^2 ha^{-1}), height H (m), and stem volume V_S (m^3 ha^{-1}) can be predicted by 3-PG from predicted stem mass and stocking using simple empirical relationships.

Mean stem diameter is obtained from Eqn (9), and basal area is then given by

$$A = \pi \left(B / 200 \right)^2 N \ . \tag{20}$$

Basal area estimated by Eqn (20) is unbiased when Eqn (8) is parameterised using observed quadratic mean diameter as B. Mean height can be estimated from the allometric relationship

$$H = a_H B^{n_{HB}} N^{n_{HN}} \ , \tag{21}$$

where the meaning of H (e.g. mean height, mean dominant height, etc) is determined solely by the data used for H when Eqn (21) is parameterised.

Stem volume can also be determined from an allometric relationship

$$V_S = a_V B^{n_{VB}} N^{n_{VN}} \ , \tag{22}$$

where the meaning of V_S (e.g. utilisable volume, total volume over or under bark, etc) is determined solely by the data used for V_S when Eqn (22) is parameterised. Alternatively, stand volume can be determined from total stem mass, basic density and the branch and bark fraction using

$$V_S = (1 - p_{BB}) W_S / \rho \tag{23}$$

where p_{BB} and ρ are given by the empirical relationships above. In general, use of Eqn (22) is recommended over Eqn (23) because of uncertainties due to unaccounted for age- and site-related effects on the prediction of p_{BB} and ρ.

4. Data required to test 3-PG

This Section outlines and makes recommendations on the type of data required to develop and test 3-PG, or to estimate species-specific parameters. Much of the required data goes beyond common practice for data collection, especially from commercial stands, but even some of it will be of great value when developing, parameterising or testing 3-PG – or similar process-based forest-growth models. Much of this data is preferred as a time-series from the same stand. In general, age-series data are not as suitable as time-series data as they come from different sites which often have distinct management and climatic histories.

The source of data typically required to test or parameterise 3-PG can be classified (B, F, L, M or P) as follows:

Data source class		Description
Biomass harvest	B	Data from direct measurement of harvested trees, e.g. biomass data (foliage, stem, root), leaf areas, wood density
Field data	F	Data not routinely obtained from an inventory assessment, e.g. from soil samples, litterfall traps, neutron probe moisture tubes, leaf area meter
Literature	L	Data obtained from the literature
Mensuration	M	Data from an inventory assessment, e.g. measured stem height and diameter, volume or other data inferred from statistical relationships
Physiological	P	Results of physiological experiments, e.g. gas-exchange analyses

This classification has been applied in Appendix 1 for 3-PG state variables and outputs, and Appendix 2 for 3-PG species-specific parameters.

4.1 Biomass production and partitioning

To parameterise or test 3-PG's prediction of biomass production, data should come from sites covering a range of site qualities (e.g. low, medium and high). It is highly desirable that good biomass data come from one or more sites that are not limited by either fertility or available soil water as this obviates the need to be concerned with two major growth modifiers, and also from sites that are limited by only water or only fertility. At least some of the individual items of data should comprise a significant time-series.

The required data include:

- site-specific data needed to run 3-PG (fertility rating, soil type, maximum available soil water)
- climate data needed to run 3-PG (monthly mean temperature, solar radiation, VPD and rainfall)
- time-series of the following pools:
  foliage: foliage biomass and/or leaf area index
  stem: stem biomass (including branches and bark) and/or volume and/or stand-mean stem diameter
  roots: root biomass
  litter: accumulated leaf litter over some period or periods

It is desirable but not essential that data are available for each pool at the same ages.

I recognize that root biomass data will be available only rarely. However, it is extremely desirable that observations of some measure of both foliage and stem are available. Growth of each pool is the product of NPP and the allocation fraction to that pool, and any combination of NPP and allocation to an unobserved pool can be consistent with observed pools because an error in predicting NPP can be compensated for by errors in the allocation fractions.

4.2 Effects of Spacing

To quantify the effects of stand stocking on stand properties, data should come from sites covering a range of site qualities (e.g. low, medium and high) and stocking (300–2400 trees ha^{-1}), and at a number of stand ages. It should include

- stand-means of current stocking, DBH (preferably quadratic mean DBH) and height
- total and utilisable stand volume, preferably obtained by direct measurement rather than from the application of volume equations
- total and utilisable stem mass (including and excluding branch and bark), which must be obtained by direct measurement rather than from the application of volume equations

4.3 Leaf litterfall

To quantify leaf litterfall, and especially effects of stress factors on litterfall, data covering an annual cycle with and without significant drought stress are required, including

- regular measurements of soil water availability and/or stress, e.g. available soil water, pre-dawn leaf water potential
- monthly accumulated litter production
- monthly measurement of foliage, e.g. actual leaf mass, or LAI and SLA.

4.4 Stem mortality

Time-series data on live stem numbers are required to test or parameterise stem mortality. To quantify the effects of stress factors on stem mortality, these data are required covering extended growth periods with and without significant drought stress, including

- measurements of soil water stress, e.g. available soil water, pre-dawn leaf water potential
- stand-mean stem heights and diameters, or other data suitable to check 3-PG's predictions of growth.

4.5 Evapotranspiration and stand water use

To test the predictions of canopy transpiration and stand water use, growth data and available soil water are required covering extended growth periods. In addition to the basic growth data listed above, the data should include

- regular measurements of available soil water, and/or sap-flow measurements over an annual cycle
- measurements of canopy stomatal conductance under conditions of high or low soil water stress.

If 3-PG is known to accurately predict stand growth under conditions where water is not limiting growth, it is possible to base a test and/or parameterisation of the soil water submodel on the above observations alone.

5. Assigning species-specific values to 3-PG parameters

Individual species in 3-PG are characterised by a set of species-specific parameters. The use of 3-PG for forest management is predicated on the ability to obtain reliable estimates for parameters characterising several eucalypt, acacia, pine and other species. Although 3-PG has been applied to a wide range of species, including conifers and hardwoods, in only a few cases have the species-specific parameters been rigorously determined, and this has been largely by a process of trial and error, e.g. see Sands and Landsberg (2002).

As a first general rule, parameter values should always be assigned by direct measurement, or by analogy with other species. Failing this, parameters can be estimated by adjusting their values to optimise the fit of 3-PG output to observed data. In this case, software for fitting model output to observed data is highly desirable (Sec. 7). A systematic protocol for assigning species-specific parameters can be based on a sound understanding of 3-PG, the meaning of its parameters, and knowledge of the sensitivity of its outputs to species-specific parameters. Such understanding is essential to support the application of numerical techniques for parameter estimation by optimising the fit of output to observed data. This Section provides guidelines on the assignment or estimation of 3-PG species-specific parameters.

5.1 Classification of parameters

Whenever possible, parameters should be assigned values by observation, either directly as the result of some experimental measurement, or indirectly, e.g. by regression analysis of experimental data. In other cases, the value of a parameter for one species can be assigned to another closely related species, based on an understanding of the comparative physiology of the species, or when a sensitivity analysis has shown that model output is insensitive to that parameter. Estimation by adjusting parameter values to optimise the fit between observed and predicted data is effective, but should only be the last choice, and should bear in mind any *a priori* knowledge, e.g. the range of values parameters can take (MacFarlane *et al.*, 2000).

These observations are reflected in the classification of parameters by their *estimation class* (D, O or E):

Estimation class		Description
Default	D	The parameter can be assigned some generic value, e.g. based on work with other species, or from *a priori* knowledge
Observed	O	The parameter can be directly measured, e.g. via gas-exchange analysis, or determined by analysis of experimental data, e.g. by regression analysis
Estimated	E	The parameter can only be estimated indirectly, e.g. by adjusting its value to optimise the fit of some output to observed data

This classification is not unique, but serves as a formal guide as to how a particular parameter might be assigned a value.

Sensitivity analysis of key model outputs (e.g. LAI, DBH) to the species-specific parameters in the model (Battaglia & Sands, 1998; Esprey *et al.*, 2004) provides a classification of parameters according to the accuracy with which they must be assigned. These *sensitivity classes* (L, M or H) are

Sensitivity class		Description
Low	L	Outputs are essentially independent of the parameter value
Medium	M	Outputs depend moderately on the parameter value
High	H	Outputs depend strongly on the parameter value, or their sensitivity varies significantly across sites

Although parameter sensitivity depends on the basic parameter set in use and on the stand age, the sensitivities are usually robust.

Appendix 2 lists all 3-PG parameters and assigns them to one of the above classes. These reflect current judgement for *E. globulus* and *E. grandis* and are not meant to be cast in concrete, but will provide guidance for parameter estimation for a range of species. The following comments further illustrate these assignments:

- Examples of estimation class D are constants such as the psychometric constant appearing in the Penman-Monteith equation, a molecular weight for wood, and the light interception coefficient *k*. The first two are either standard physical or stoichiometric quantities, and clearly independent of the species. On the other hand,

k is determined primarily by the leaf angle distribution in the canopy, and is usually assigned a value simply on that basis. (However, it can also be inferred from observations of canopy LAI and light transmission, assuming Beer's law applies.)

- Insensitive parameters (sensitivity class L) can safely be assigned a value common to other species. This is particularly helpful when the parameters are not experimentally accessible. (They could also be given an estimation class D.)

- Parameters representing processes that are experimentally accessible should be assigned values based on direct observation (estimation class O), irrespective of their sensitivity class, e.g. stomatal conductance can be measured by gas-exchange analysis. Also, the coefficient and power in an allometric relationship can be obtained by linear regression of *ln*-transformed variables, although nonlinear regression against untransformed data is to be preferred.

- Parameters that cannot be measured assigned values directly, and especially those that must also be determined accurately (e.g. of sensitivity class H), have to be estimated by varying their values to give an optimal fit of model output to observed data (i.e. are of estimation class E). Examples are maximum canopy quantum efficiency and parameters determining biomass partitioning.

5.2 General guidelines for assigning parameters

It is imperative that the assignment of parameter values, and in particular parameter estimation, be performed with a good understanding of the model. Such an understanding soundly guided work on *E. globulus* (Sands & Landsberg, 2002) and *E. grandis* (Almeida *et al.*, 2004a).

The following is an overview of the general process of parameter assignment, and some of the issues that might arise:

- First assign values to all parameters that can be directly observed, or can safely be given default values or by analogy with other species.

- Of the remaining parameters, identify those that can not be estimated by fitting to observed data, e.g. because suitable data is not available, and reconsider these with a view to assigning them default values.

- In some cases a parameter might be calculated using another model, e.g. the canopy production model of Sands (Sands, 1995, 1996) could be used to calculate canopy quantum efficiency from photosynthetic light response data.

- Estimate the remaining parameters by fitting model output to appropriate observed data, taking into account any *a priori* information, e.g. on the permissible range for the parameters. This may be by either manually adjusting parameter values, or by using appropriate software, or both, and it may be an iterative process.

- It is important the fit be based on observations of as many distinct variables as possible, and from sites covering a wide range of conditions.

- There is no point in basing a fit on observed data that are correlated, e.g. stem volume, stem biomass and DBH and usually highly correlated.

When a parameter set has been established, some basic checks must be performed on both the parameters and the subsequent outputs of the model:

- Check that all parameter values are biophysically or biologically reasonable.

- Perform at least a basic sensitivity analysis of observed and assigned values in the context of the final parameter set. If they are of low sensitivity, then they should not need to be considered further, whereas the values of sensitive parameters should be checked that they are biologically reasonable.

- Verify that the behaviour of all outputs is reasonable, especially those not used in the estimation process, e.g. canopy LAI is often predicted to be very high early in canopy development. Should an output behave unreasonably, repeat the estimation with a bound placed on the offending output.

5.3 Guidelines for estimating parameters

Parameter estimation is a systematic process in which the fit of model outputs to observed data is optimised. This process may be manual, or automated through the use of software. The quality of the fit is measured by the merit function (Φ) such that smaller values for Φ indicate a better fit between predictions and observations. Typically, Φ is a weighted sum-of-squares of the differences between observed and predicted data items, and may include a penalty that increases Φ when parameter bounds have been violated.

In geometrical terms, estimation is equivalent to searching for the lowest point in a complex, multi-dimensional landscape. This process rarely goes as smoothly as desired and can be quite slow, essentially because this landscape is complex. Sometimes this landscape has long contorted valleys with each step in the process jumping from side-to-side, or the landscape can be flat with the optimum poorly determined. Also, there is no guarantee that the solution is in fact the best – optimisation will only reach a local optimum, and can easily miss a saddle in the landscape leading to a deeper valley.

Common reasons for slow progress are: poor initial parameter values, too many parameters are being estimated simultaneously, groups of parameters are highly correlated, or the process attempts to assign unreasonable values to parameters. The following guidelines can help resolve some of these issues:

- Automated parameter estimation requires initial guesses for the parameters in question. A manual attempt to assign parameter values can provide initial values suitable for the automated process – and aid an understanding of the process.

- A successful estimation should be repeated with different initial parameter values. This will highlight the robustness of the estimated parameter set, and possibly avoid convergence to a local minimum of Φ.

- If the values of distinct variables used in the fitting process have a wide range, then different weights may have to be assigned to each variable. For instance, LAI typically is less than 6, stem biomass exceeds 100 m^3 ha^{-1}, and stocking can exceed 1000 trees ha^{-1}. Weights inversely proportional to the observed mean for each variable will give more equal weight to the variables.

- If the errors associated with different observations have a wide range, then different weights may have to be assigned to different observations. For instance, stem biomass is heteroscedastic, and over a typical rotation can vary over a factor of 100. Thus observations late in the rotation (when W_S is large) will carry more weight than those early in the rotation. Weights inversely proportional to the observed value will give more equal weight to each observation.

- It is advisable to simultaneously use data spanning a wide range of site conditions. However, an initial estimation based on a single or few sites can quickly highlight

problems such as correlation between parameters, or parameters or model output variables going out of range.

- Software packages for estimation provide confidence intervals or standard errors for the estimated parameters. If the confidence interval is large it is often worth fixing the parameter mid-range to reduce the number of parameters being estimated.

- If the confidence interval encompasses the value of a parameter which in practice turns some process or effect off, consider repeating the estimation with the parameter fixed at that particular value.

- Software packages for estimation also provide the correlation matrix between parameter estimates. If two or more parameters are highly correlated, estimation can often be aided by fixing one mid-range and estimating the others.

- A difficult estimation can often be aided by successively estimating groups of parameters. It is then worth trying to refine the entire parameter set by estimating all the parameters with their new values as initial values for the full estimation.

Parameter estimation by optimising the fit between observed values and predicted model outputs is a powerful, but often abused, technique. Application of software packages for estimation can readily lead to erroneous results! To avoid this

- parameter estimation must be tempered by judgement,

- should be undertaken only with a sound understanding of the model and the role each parameter plays, and

- the resulting parameter sets and model predictions must be carefully checked for biological reality.

Finally, it is important to perform a sensitivity analysis once a set of parameters have been determined, and to compare the results from this with known or inferred errors, or with the predicted confidence intervals on each parameter.

6. Parameter estimation for 3-PG

Wherever possible parameters are assigned by direct measurement, or by analogy with other species. This Section is devoted largely to the process of estimating parameters by fitting 3-PG outputs to observed data. Reference is made to the mathematical description of 3-PG given in Sec. 3. The notation is as used in Sec. 3 and as listed in Tables 1 and 2.

6.1   Available data and parameter estimation

Ideally, parameter estimation should be based on observed values of all the state variables, i.e. W_F, W_S, W_R, N and θ_s. This is because these are the primary variables predicted by the model, and are most strongly tied to its internal dynamics. However, surrogates are often available for stem and foliage biomass data (Sec. 6.2).

The set of parameters that can be uniquely estimated depends strongly on the available data. Some examples

- NPP is the product of intercepted radiation, α_{Cx}, Y and the growth modifiers f_i; see Eqns (2), (4). Thus, if the sites whose data are used have similar conditions, the various f_i will have similar values and it will not be possible to separate α_{Cx} from parameters in the f_i by fitting model output to observed data at these sites.

- Growth of any biomass pool is the product of NPP and the allocation ratio. If the only observed data are for the foliage and stem biomass pools, it is not possible to estimate both α_C and the root allocation ratio η_R (in the sense of estimating the parameters characterising these quantities). In reality, only the product of $\alpha_C(1 - \eta_R)$ can be estimated in the absence of root biomass data, and the only way to estimate α_C is to assume a value for η_R; see Eqns (1), (6).

- On the other hand, if root biomass data are also available, $\alpha_C \eta_R$ can also be estimated, and hence α_C and η_R are both obtained. Thus, to independently estimate α_{Cx} and parameters characterising biomass allocation (i.e. p_2, p_{20}, η_{Rn}, η_{Rx}), observed values of foliage, stem and root biomass data are required.

- Since the foliage pool is affected by litterfall, the values of the parameters in γ_F will affect the estimated parameters in the foliage:stem allocation ratio p_{FS}. Thus sound estimation of p_{FS} also requires observed litterfall data (accumulated or monthly)

- Similarly, γ_R affects the parameters in the root allocation ratio η_R. As it is unlikely that fine-root turnover data are available, a generic value is assigned to γ_R.

- In the absence of above- and below-ground biomass data, it is difficult or impossible to separate effects of site fertility on NPP from its effects on above:below-ground biomass allocation; see Eqns (4)-(7). Hence it will be impossible to separate the effects of site fertility rating on α_C (through the modifier f_N) from its effects on root biomass allocation (through m).

Parameter estimation for PBMs will often yield a good fit of outputs to observed data for the wrong reasons, e.g. see Hopkins (1996). This is especially the case with 3-PG if data on foliage, stem and root biomass are not simultaneously available. For this reason, the resulting parameter sets and model predictions must be carefully checked for biological reality.

6.2   Surrogate data for stem and foliage biomass

Biomass data are not routinely measured in forestry trials. Common surrogates for stem bioamss are DBH, stem height or volume. LAI is a surrogate for foliage biomass. There is no simple surrogate for root biomass.

LAI is an acceptable surrogate for foliage biomass, especially if SLA is also available or is reliably predicted, because of the direct relationship Eqn (3) between them. Because DBH is calculated in 3-PG by inverting the allometric relationship Eqn (8) between w_S and B, it is a suitable surrogate for stem biomass. So fitting predicted values of B to observations of DBH is an acceptable way to estimate the parameters characterising biomass production and allocation. However, it is essential that a_S and n_S have been assigned directly from observed w_S as a function of B, not estimated as part of the fitting process.

Volume and height can also be predicted in 3-PG from allometric relationships with B, so observed height and volume are also suitable surrogates for stem biomass, subject to the above comments on assignment of a_S and n_S. However, if volume is predicted as the product of stem mass, basic density and branch and bark fraction using Eqn (23), the often poorly predicted values for ρ and p_{BB} give rise to uncertainties in the resulting parameter estimates.

6.3   Interacting parameter groups

There is a high degree of interaction in the effects of groups of 3-PG parameters on the behaviour of 3-PG. If parameters are estimated in groups, as is often the case with manual

estimation, currently assigned values for one group of parameters will affect values for another group yet to be assigned. For this reason, manual estimation of parameters can be a tedious, iterative process. Software packages for estimation do allow one to estimate many parameters simultaneously, and hence avoid this problem. However, I often base an initial assignment of values to groups of related parameters on a simple manual manipulation.

Three interacting parameter groups are (a) maximum canopy quantum efficiency α_{Cx}, (b) parameters controlling biomass allocation (i.e. p_2, p_{20}, η_{Rn}, η_{Rx}) and (c) those controlling the growth modifiers f_i. These groups interact because growth of each biomass pool is the product of NPP and the corresponding allocation ratio; see Eqns (1)-(4). The goal is to find values for α_{Cx}, p_2, p_{20}, η_{Rn} and η_{Rx} that apply to all stands, irrespective of the degree of limitation, and for the parameters characterising the f_i.

Groups (a) and (b) strongly interact, and can be uniquely estimated if biomass data from all pools are available at sites free of major growth limitations. Group (c) interacts with the others to a lesser extent, and their estimation requires data from sites with significant growth limitations. However, site fertility usually does not vary significantly during a rotation, and unless growth data is available from a range of sites with widely varying fertility, including sites free of fertility limitations, the product $\alpha_{Cx}f_N$ cannot be separated into α_{Cx} and the effect f_N of site fertility on NPP.

As noted in Sec. 6.1, the parameters determining biomass allocation strongly interact with the parameters in γ_F, and with γ_R itself. Further, if there is significant tree mortality, they also interact with parameters in γ_N.

Another feature 3-PG has in common with other PBMs is that parameters often group together to affect an output (e.g., see Sievänen & Burk, 1993, 1994; Sands & Landsberg, 2002). For example, NPP is proportional to the product of α_{Cx}, Y, the molecular weight of wood, and the conversion of total solar radiation to PAR, and the valued estimated for α_{Cx} is affected by the values for the others. Also, 3-PG calculates stem volume from W_S, ρ and p_{BB}, see Eqn (23), so it is determined by products of a number of often poorly known parameters.

6.4   Estimation based on observed GPP

Observed values of GPP and LAI from a range of sites can be used to estimate α_{Cx} and the parameters in the f_i (e.g. Stape *et al.*, 2004). For each site, calculate α_C by dividing GPP by the light intercepted by the canopy; see Eqn (2). A good approximation for α_{Cx} will be the maximum of these α_C, or their average over sites at which production is believed to be unlimited. The ratio α_C / α_{Cx} is then the product of the various f_i, and this data can be used to assign parameters in the f_i.

6.5 Biomass production and allocation

When estimating the parameters α_{Cx}, p_2, p_{20}, η_{Rn} and η_{Rx} characterising biomass production and allocation it is important to disentangle the effects of the growth modifiers f_i from α_{Cx} so the estimated values apply to all sites. I suggest three alternative approaches, and if applied manually, these may need some iteration in the parameter assignment process. It is assumed that those parameters that are not being estimated have sound values.

1) If biomass data are available from stands where production is not limited by site factors (especially nutrition or soil water), most or all $f_i = 1$ and values estimated for α_{Cx}, p_2, p_{20}, η_{Rn} and η_{Rx} by fitting to the observed biomass data will apply to all sites.

2) Assign plausible values to the parameters characterising the f_i and then use biomass data from any stands (with or without known limitations) to estimate α_{Cx}, p_2, p_{20}, η_{Rn} and η_{Rx} by fitting to the observed biomass data. The parameters in the f_i may then need to be adjusted iteratively along with these parameters.

3) Set all $f_i = 1$, e.g. by suitable temporary parameter assignments, and then estimate values of p_2, p_{20}, η_{Rn} and η_{Rx} common to all sites and site-specific values of α_{Cx} for each site. The site-specific values of α_{Cx} are then used as data to assign or estimate values for the parameters characterising the f_i, and to the true, i.e. site non-specific, value of α_{Cx} (see Sec. 6.6).

Other data can sometimes be used in lieu of stem or foliage biomass data when estimating these parameters (see Sec. 6.2).

The parameters a_S and n_S in the allometric relationship between stem mass and diameter should preferably be assigned directly from observed stem biomass data obtained through biomass harvests, rather than by fitting 3-PG output to observed B. If both observed stem biomass data and observed DBH are available, it might be possible to simultaneously estimate the allocation and allometric parameters. However, I expect their estimates will show significant correlation.

6.6 Limitations to productivity

Determination of the parameters characterising the productivity modifiers f_i can also proceed in various ways, e.g.:

1) Some parameters can be observed directly. An example is the parameter k_D in the modifier f_D. This modifier affects conductance multiplicatively; see Eqns (4), (16). Hence, measurements of stomatal conductance under various conditions can be used to determine how f_D depends on VPD. This will then suggest a value for k_D.

2) Another approach assumes p_2, p_{20}, η_{Rn} and η_{Rx} have been assigned values that apply at all sites, and site-specific values for α_{Cx} have been obtained at sites for which there are known limitations to production by using α_{Cx} to optimise the fit to observed biomass data separately at each site. By examining how these site-specific values for α_{Cx} depend on the site factors, it is possible to assign the parameters characterising one or more of the modifiers f_i, as well as a site-independent value for α_{Cx}. Sands and Landsberg (2002) used this approach to parameterise the temperature modifier f_T.

After assigning values to the parameters in the productivity modifiers f_i in this way, it is advisable to then re-estimate α_{Cx}, p_2, p_{20}, η_{Rn} and η_{Rx}.

6.7 Stem mortality

If stem numbers are not accurately predicted, B as given by Eqn (9) will be in error. It follows that estimated parameters characterising biomass allocation will also be in error. Two simple approaches for resolving this problem are:

1) In the case of short rotation plantations, if there are early deaths and stem numbers are subsequently stable, set the initial stem number at the stable value and mortality to 0.

2) The parameters in the stem mortality model (e.g. γ_{N0} and γ_{N1} for random death, and w_{Sx1000} for self-thinning) can be assigned values more or less by inspection so that the overall pattern of stem mortality is reproduced.

Otherwise, the mortality parameters can be estimated by fitting predicted N to observed stem numbers. It is important to be aware of possible significant site-effects (e.g. due to drought stress) on stem mortality, as these effects are currently not predicted by 3-PG.

6.8 Litterfall and root turnover

The parameters characterising the litterfall rate γ_F are important because litterfall affects foliage biomass, and hence can bias the determination of the parameters characterising the foliage:stem allocation ratio. Litterfall varies seasonally, and in response to possible site-effects (e.g. drought stress). Since the current version of 3-PG does not model seasonal or stress-induced variations in the litterfall rate, I recommend the use of litterfall data accumulated over an extended period and an average leaf biomass for that period to estimate a possibly age-dependent value of γ_F as in Eqn. (17).

Root turnover γ_R is also a problem as it affects the root biomass pool. Hence, if root biomass data are available and the partitioning parameters η_{Rn} and η_{Rx} are estimated by fitting to root data, their values will be affected by γ_R. In the lack of other information, γ_R is given a default value (e.g. 0.015 month^{-1}).

6.9 Soil water and evapotranspiration

At present I have no direct experience assigning parameters in the water balance submodel. I expect this will be a challenging process because whereas 3-PG uses a monthly time-step, actual soil water content can vary markedly on a daily time scale depending on the distribution of rainfall within the month. I suggest deriving from the observed soil water data a variable that more closely matches a 3-PG water-use related output, and then fitting the derived data to that output. Two examples would be monthly average available soil water, or monthly or annual transpiration.

6.10 Use of monthly or annual increments

If canopy leaf area index and monthly (or annual) increments in stem biomass are available, α_{Cx}, p_2 and p_{20} could be estimated by fitting predicted increments to the observed increments; see Eqns (1), (6). Also, if monthly increments are used, it must be appreciated that 3-PG assumes that respiration, represented by Y, is constant, whereas in reality it varies seasonally. This may introduce bias, because production is governed by the product $\alpha_{Cx}Y$.

7. Parameter estimation software

Parameter estimation for process-based models is greatly facilitated by the use of software that implements a technique for minimising the merit function Φ, usually the residual sum-of squares, by adjusting the values of nominated parameters. This section discusses the application of such software for parameter estimation in the context of 3-PG.

Several distinct algorithms are available for minimising Φ by varying selected parameters. Examples are the Simplex method (e.g. Nelder & Mead, 1965; Press *et al.*, 1987), the Marquardt algorithm (e.g. Marquardt, 1963; Draper & Smith, 1981), and so-called evolutionary or genetic algorithms (e.g. Wang, 1997; Goldberg, 1989). Since Φ is in general a non-linear function of the parameters of the model, parameter estimation by fitting model outputs to observed data is an example of generalised non-linear regression.

All advanced statistical packages, e.g. SAS, GenStat, S-Plus, provide implementations of one or more of the above algorithms for generalised non-linear regression. However, they require the model to be written in the particular macro language of the package, and do not couple in a simple way to models in other languages.

The freeware package PEST (Parameter ESTtimation; Doherty, 2002) provides a powerful and robust implementation of the Marquardt algorithm. Although developed for applications in ground water research, it is claimed to be "model independent", provided that the model in question is implemented as an executable file (.EXE file) and communicates with the user solely through text files. It has a long history as a DOS-oriented program applied in conjunction with models that are also DOS-oriented, but can be run under a Windows environment through the use of the so-called "command window". All input and output files for PEST and the model must be standard ASCII text files. The user has to develop a series of "PEST control files" that are read by PEST and describe the format of the model's input, output and parameter files, and the details of the estimation to be performed.

Early attempts to use PEST to estimate parameters in 3-PG used a separate implementation of 3-PG as an executable file with text files for input and output. In that case the user no longer had immediate access to the power of the commonly used spreadsheet implementation of 3-PG (i.e. 3PGPJS) for application of the newly determined parameters or analysis of results.

Excel provides the Solver add-in which optimises a nominated cell by varying the contents of other cells. This can be used for parameter estimation when the model is entirely coded in the spreadsheet cells, possibly with simple functions coded as macros. Although 3-PG could be implemented this way it is a tedious process and yields code that is difficult to maintain. So 3PGPJS is not, and hence Solver can not be used for parameter estimation with the full model. Other third party Excel add-ins, e.g. Evolver (Palisade Corporation, 2003), and the Solver DLL (Frontline Systems, 1999), could be used to apply sophisticated optimisation techniques in the context of spreadsheet-based implementations such as 3PGPJS. These packages are being evaluated as part of an on-going project examining tools for parameter estimation in spreadsheet-based models. However, as commercial packages, they are not freeware and require specific licences for use.

Larry Tooke, a consultant for a project to develop the use of 3-PG as a management tool in South African forestry (National Research Foundation, 2002), made a major innovation by developing a spreadsheet-based technique that allows the use of PEST with spreadsheet-based models. This tool allows parameter estimation for any Excel-based model and takes away the drudgery of setting up the PEST control files. In addition, it gives confidence limits or standard errors on the parameter estimates, and the correlation between estimates. These are invaluable additional results from the estimation that are not readily available from manual estimations, or from applications of the Excel Solver add-in.

Further work on this tool, to be called PESTXL, is ongoing. As part of the afore-mentioned project, I am developing a user-friendly interface and "wizard" that will allow the 3PGPJS user to access and apply PEST without knowledge of, or the need to see, PESTXL. The result will be a tool that can be used with any Excel-based model, not just 3PGPJS. With PESTXL, the power of PEST is available, along with the versatility and convenience of a spreadsheet environment, e.g. the 3PGPJS interface. A separate report on the structure and potential applications of PESTXL will be prepared.

PESTXL will be available as freeware.

8. Concluding remarks

Although these guidelines were written with 3-PG specifically in mind, they are relevant to other process-based forest growth models. They are also not meant to be the "last word" on the issue of parameter assignment and estimation in a 3-PG context. In particular, there is a wealth of experience "out there" pertinent to parameter estimation to be explored, and the present guidelines will inevitably be enhanced as more experience is gained through adapting 3-PG to diverse species. I invite readers to share their experiences with me.

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Appendix 1:   Names and descriptions of 3-PG input and output variables

This table lists the major 3-PG input and output variables. Data class (Biomass, Field, Mensuration, Physiological, Literature) refers to the broad classification of data sources required to supply the required input data or to test output data. Details are given in Sec. 3.

Description	Symbol and 3PGPJS name		Units	Data class	Comments
Site and management attributes					
Soil class		SoilClass	-	F	Based on texture: sand, sandy loam, clay loam or clay
Fertility rating	FR	FR	-	F	Difficult to quantify; based on experience or calibration
Maximum available soil water	θ_{sx}	maxASW	mm	F	Based on soil texture and soil water holding capacity
Minimum available soil water	θ_{sn}	minASW	mm	F	Usually zero, but used to emulate access to water table
Climatic factors					
Day length (sunrise to sunset)	h	DayLength	s d^{-1}	L	Calculated from basic theory
Mean number of frost days per month	d_F	FrostDays	d month^{-1}	F	
Mean daily incident solar radiation	Q	SolarRad	MJ m^{-2} d^{-1}	F	Climatic data is either observed, obtained from climatic data
Mean daily temperature	T_a	Tav	°C	F	bases or inferred from climatic generators
Mean day-time VPD	D	VPD	mbar	F	
Mean monthly precipitation	R_P	Rain	mm month^{-1}	F	
Applied irrigation	R_I	Irrig	mm month^{-1}	F	From known irrigation schedule
Stand attributes					
Stand age	t	StandAge	yr		
Stand stocking	N	StemNo	trees ha^{-1}	M	
Stand basal area	A	BasArea	m^2 ha^{-1}	M	
Stand volume excluding branch & bark	V	StandVol	m^3 ha^{-1}	M	All of these have their standard meaning and can be obtained
Stand-based mean DBH	B	avDBH	cm	M	as the result of routine mensuration
Mean annual volume increment		MAI	m^3 ha^{-1} yr^{-1}	M	
Peak MAI of stand to the current stand age		MAIx	m^3 ha^{-1} yr^{-1}	M	
Stand age at which MAI peaked		ageMAIx	yr	M	
Long-term average stem biomass growth rate		ltStemGR	kg ha^{-1} yr^{-1}	B	Based on biomass measurements several years apart

Description	Symbol and 3PGPJS name		Units	Data class	Comments
Canopy attributes					
Specific leaf area	σ	SLA	$m^2\ kg^{-1}$	B	Requires weighed leaf mass and measured leaf area
Fraction of ground area covered by canopy	ζ	CanCover	-	F	Measurements of crown dimensions
Canopy LAI	L	LAI	$m^2\ m^{-2}$	F	From leaf area meters such as LICOR
Peak canopy LAI up to the current stand age		LAIx	$m^2\ m^{-2}$	F	From time-series of LAI measurements
Stand age at which LAI peaked		ageLAIx	yr	F	
Biomass pools					
Foliage biomass	W_F	WF	$t_{DM}\ ha^{-1}$	B	
Root biomass	W_R	WR	$t_{DM}\ ha^{-1}$	B	
Stem biomass, including branches and bark	W_S	WS	$t_{DM}\ ha^{-1}$	B	All of these must be obtained from destructive biomass
Total biomass		TotalW	$t_{DM}\ ha^{-1}$	B	harvests
Mean stem biomass per tree	w_S	AvStemMass	kg_{DM}/tree	B	
Basic density	ρ	Density	$t_{DM}\ m^{-3}$	B	
Fraction of stem biomass as branch and bark	p_{BB}	fracBB		B	
Accumulated litter fall		TotalLitter	$t_{DM}\ ha^{-1}$	F	Obtained from litterfall traps
Growth modifiers					
Age dependent modifier	f_{age}	fAge	-		
VPD dependent modifier	f_D	fVPD	-		
Temperature dependent modifier	f_T	fTemp	-		
Frost dependent modifier	f_F	fFrost	-		These can't be directly measured
Soil water dependent modifier	f_θ	fSW	-		
Nutrition dependent modifier	f_N	fNutr	-		
Physiological modifier of canopy conductance	φ	PhysMod	-		

Description	Symbol and 3PGPJS name		Units	Data class	Comments
Biomass production and allocation					
Gross primary production in current period	P_g	GPP	t_{DM} ha^{-1}	B	Very difficult to measure
Net primary production in current period	P_n	NPP	t_{DM} ha^{-1}	B	
Total solar radiation intercepted by canopy		RadInt	MJ m^{-2} month^{-1}	F	Measurement of transmitted radiation using light sensors
Canopy quantum efficiency after modifiers	α_C	alphaC	mol mol^{-1}	B, P	Hard to measure. Possibly predict using a canopy production
Light utilisation efficiency based on total biomass	ε	Epsilon	g_{DM} MJ^{-1}	B, P	model, e.g. Sands (1995, 1996)
Light utilisation efficiency based on stem biomass	ε_S	StemEpsilon	g_{DM} MJ^{-1}	F, B	Inferred from biomass or volume increments and Q_{int}
Stem volume increment in current period		CVI	m^3 ha^{-1}	M	Often based on DBH increments or repeated inventories
FR modifier of root biomass allocation	m	m	-	B	
Fraction of NPP allocated to roots	η_R	pR	-	B	Infer from carbon budget based on frequent detailed biomass
Fraction of NPP allocated to stems	η_S	pS	-	B	harvests including respiration and litterfall
Fraction of NPP allocated to foliage	η_F	pF	-	B	
Ratio of foliage to stem biomass allocation	p_{FS}	pFS	-	B	
Current leaf litterfall rate	γ_F	gammaF	month^{-1}	F	From litter traps
Litter fall in current period		Litter	t_{DM} ha^{-1}	F	
Stem mortality					
Max. mean tree stem mass at current stocking	w_{Sx}	wSmax	kg tree^{-1}	M, B	Inferred from largest tree if mortality is density-dependent
Density independent mortality rate	γ_N	gammaN	month^{-1}	M	Inferred from repeated stem counts
Number of stems dying in current period		Mortality	trees ha^{-1}	M	

Description	Symbol and 3PGPJS name	Units	Data class	Comments
Water use				
"Supplemental" irrigation to maintain $\theta_s \geq \theta_{sn}$	supIrrig	mm		Can't be measured
Fraction of rainfall intercepted by canopy	i_R fRainInt	-	F	Hard to measure, requires knowledge of stem flow
Rainfall intercepted by canopy in current period	RainInt	mm	F	Hard to measure, requires knowledge of stem flow
Canopy conductance	g_C CanCond	m s^{-1}	P	Gas exchange data, infer from detailed models
Water use efficiency	ω WUE	gDM mm^{-1}	M, F	Can be inferred from biomass increments, water use
Evapotranspiration rate in current period	E_T EvapTransp	mm	F	Could be estimated directly from sap flow data
Monthly transpiration rate in current period	Transp	mm	F	
Available soil water	θ_s ASW	mm	F	Neutron moisture tubes or TDR data

Appendix 2: 3-PG parameter names, units, default values and classification for parameter estimation

The parameter values listed are for *E. globulus* and taken from Sands and Landsberg (2002). The sensitivity classes (Low, Medium and High) and estimation classes (Default, Observed and Estimated) are described in Sec. 4.1, and data source classes (Literature, Mensuration, Biomass, Field and Physiological) are explained in Sec.3. The assigned sensitivity class is based on data from Esprey et al (2004) for *E. grandis*.

Description	Symbol and 3PGPJS name		Units	Value for *E. globulus*	Site / species specific	Sensitivity class	Estimation class	Data source class	Data requirements and comments
Biomass partitioning and turnover									
Allometric relationships & partitioning									
Ratio of foliage:stem partitioning at B = 2 cm	p_2	pFS2	-	1	Species	H	E	B	Foliage biomass or LAI, stem biomass or DBH
Ratio of foliage:stem partitioning at B = 20 cm	p_{20}	pFS20	-	0.15	Species	H	E		
Constant in stem mass v diam. relationship	a_S	stemConst	-	0.095	Species	M	O	B	Stem biomass and DBH at contrasting sites
Power in stem mass v diam. relationship	n_S	stemPower	-	2.4	Species	H	O	B	
Maximum fraction of NPP to roots	η_{Rx}	pRx	-	0.8	Species	M	O/E	B/L	Ideally below and above ground biomass data
Minimum fraction of NPP to roots	η_{Rn}	pRn	-	0.25	Species	M	O/E		or *a priori* allocation ratios
Litterfall & root turnover									
Litterfall rate at t = 0	γ_{F0}	gammaF0	month^{-1}	0.027	Both	L	D		
Litterfall rate for mature stands	γ_{F1}	gammaF1	month^{-1}	0.001	Both	H	O	F	Observed litterfall, SLA and LAI
Age at which litterfall rate has median value	$t_{\gamma F}$	tgammaF	month	12	Both	L	E/D		
Average monthly root turnover rate	γ_R	Rttover	month^{-1}	0.015	Both	L	D	L	General understanding of root turnover rates
Growth modifiers									
Temperature modifier									
Minimum temperature for growth	T_{min}	Tmin	°C	8.5	Species	L	D		Growth data from extreme temperature sites (warm and cold).
Optimum temperature for growth	T_{opt}	Topt	°C	16	Species	M	E	B/M	
Maximum temperature for growth	T_{max}	Tmax	°C	40	Species	L	D		
Frost modifier									
Number of days production lost for each frost day	k_F	kF	days	0	Species	L	D	B/M	Growth data from very cold sites

Description	Symbol	3PGPJS name	Units	Value for *E. globulus*	Site / species specific	Sensitivity class	Estimation class	Data source class	Data requirements and comments
Fertility modifiers									
Value of m when $FR = 0$	m_0	m0	-	0	Species	?	O		Good growth data from sites unlimited by
Value of f_N when $FR = 0$	f_{N0}	fN0	-	1	Species	M	O	M/B	fertility and soil water stress AND sites limited
Power of $(1-FR)$ in f_N	n_{fN}	fNn	-	0	Species	L	O		fertility.
VPD modifier									
Defines stomatal response to VPD	k_D	CoeffCond	mbar	0.05	Species	L	D	P	Conductance data from gas exchange analyses
Soil water modifier									
Moisture ratio deficit which gives $f_\theta = 0.5$	c_θ	SWconst	-	0.7	Site	H	D	F	Soil water retention data from soils of different
Power of moisture ratio deficit in f_θ	n_θ	SWpower	-	9	Site	L	D		textures.
Age modifier									
Maximum stand age used to compute relative age	t_x	MaxAge	yr	50	Species	L	D		Growth data covering long time periods; not
Power of relative age in f_{age}	n_{age}	nAge	-	4	Species	L	D	B/M	relevant for short rotations
Relative age to give $f_{age} = 0.5$	r_{age}	rAge	-	0.95	Species	L	D		
Conductance									
Maximum canopy conductance	g_{Cx}	MaxCond	m s^{-1}	0.02	Species	H	O/E	P	Conductance data from gas exchange analyses
Canopy LAI for maximum canopy conductance	L_{Cx}	LAIgcx	m^2 m^{-2}	3.33	Species	L	D	L	Empirical data
Canopy boundary layer conductance	g_B	BLcond	m s^{-1}	0.2	Both	L	D	L	General understanding of canopy energy balance
Stem mortality and self-thinning									
Seedling mortality rate ($t = 0$)	γ_{N0}	gammaN0	yr^{-1}	0	Species	?	O		
Mortality rate for older stands (large t)	γ_{N1}	gammaNx	yr^{-1}	0	Species	?	O	M	Time series of stem numbers when no density
Age at which $\gamma_N = \frac{1}{2}(\gamma_{N0}+\gamma_{N1})$	$t_{\gamma N}$	tgammaN	yr	2	Species	?	O		dependent mortality
Shape of mortality response	$n_{\gamma N}$	ngammaN	-	1	Species	?	O		
Maximum stem mass per tree at 1000 trees/ha	w_{Sx1000}	wSx1000	kg/tree	300	Species	L	D	M	Time-series of stem numbers
Power in self thinning law	n_N	thinPower	-	3/2	Species	L	D	L	Based on theoretical scaling laws & observation
Fractions of mean foliage, root and stem biomass pools per tree on each dying tree	m_F	mF	-	0	Species	L	D		Based on observation of stands undergoing self
	m_R	mR	-	0.2	Species	L	D	F	thinning
	m_S	mS	-	0.2	Species	L	D		

Canopy structure and processes

Description	Symbol	3PG$_{PJS}$ name	Units	Value for *E. globulus*	Site / species specific	Sensit-ivity class	Estim-ation class	Data source class	Data requirements and comments
Specific leaf area									
Specific leaf area at stand age 0	σ_0	SLA0	m^2 kg^{-1}	11	Species	L			
Specific leaf area for mature aged stands	σ_1	SLA1	m^2 kg^{-1}	4	Species	H	O	B	Observed SLA for young and mature crops
Age at which specific leaf area = ½(σ_0+σ_1)	t_σ	tSLA	yr	2.5	Species	L			
Rainfall interception									
Maximum fraction of rainfall intercepted by canopy	i_{Rx}	MaxIntcptn	-	0.15	Both	M	D		Requires data on rainfall above and below canopy and stem flow
LAI for maximum rainfall interception	L_{ix}	LAImax-Intcptn	m^2 m^{-2}	0	Species	L	D	F/L	
Light interception, production and respiration									
Extinction coefficient for PAR absorption by canopy	k	k	-	0.5	Species	M	D	O	Light interception data, leaf angle distribution
Age at full canopy cover	t_c	fullCanAge	yr	0	Species	M		F	Observation of canopy development
Maximum canopy quantum efficiency	α_{Cx}	alpha	-	0.06	Species	H	E	B/M	Growth data with no fertility or water limitation
Ratio NPP/GPP	Y	Y	-	0.47	None	H	D	L	Based on Waring et al (1998)
Wood and stand properties									
Branch & bark fraction									
Branch and bark fraction at stand age 0	p_{BB0}	fracBB0	-	0.75	Species	L	O		
Branch and bark fraction for mature aged stands	p_{BB1}	fracBB1	-	0.15	Species	L	O	B	Observed branch, bark and stem biomass data
Age at which p_{BB} = ½(p_{BB0}+ p_{BB1})	t_{BB}	tBB	yr	2	Species	L	O		
Basic density									
Minimum basic density – for young trees	ρ_0		t m^{-3}	0.5	Both	H	O		
Maximum basic density – for older trees	ρ_1	rhoMax	t m^{-3}	0.5	Both	H	O	B	Observed wood density over varying aged trees and sites
Age at which ρ = ½ density of old and young trees	t_ρ	tRho	yr	4	Both	M	O		

Description	Symbol	3PGPJS name	Units	Value for *E. globulus*	Site / species specific	Sensitivity class	Estimation class	Data source class	Data requirements and comments
Stem height allometric relationship									
Constant in stem height relationship	a_H	aH	-	0	Species	?	O		
Power of DBH in stem height relationship	n_{HB}	nHB	-	0	Species	?	O	M	Observed height and diameter data
Power of stocking in stem height relationship	n_{HN}	nHN	-	0	Species	?	O		
Stem volume allometric relationship									
Constant in stem volume relationship	a_V	aV	-	0	Species	?	O		
Power of DBH in stem volume relationship	n_{VB}	nVB	-	0	Species	?	O	M	Observed height and diameter data
Power of stocking in stem volume relationship	n_{VN}	nVN	-	0	Species	?	O		
Conversion factors									
Intercept of net radiation *v* solar radiation relationship	Q_a	Qa	W m^{-2}	-90		H	D		
Slope of net radiation *v* solar radiation relationship	Q_b	Qb	-	0.8		H	D		
Molecular weight of dry matter		gDM_mol	gm mol^{-1}	24		H	D	L/P	Obtained from literature and physiological experiments
Conversion of solar radiation to PAR		molPAR_MJ	mol MJ^{-1}	2.3		H	D		