Modelling and monitoring forest evapotranspiration. Behaviour, concepts and parameters
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Citation for published version (APA):
Modelling and Monitoring Forest Evapotranspiration

Behaviour, Concepts and Parameters

Stefan Dekker
Modelling and Monitoring
Forest Evapotranspiration
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ACADEMISCH PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Universiteit van Amsterdam, op gezag van de Rector Magnificus prof. dr. J.J.M. Franse ten overstaan van een door het College voor Promoties ingestelde commissie, in het openbaar te verdedigen in de Aula der Universiteit op dinsdag 24 oktober 2000 te 14h00 uur

door Stefan Cornelis Dekker

geboren te Middelburg
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Faculteit natuurwetenschappen, wiskunde en informatica

Dekker, Stefan C.

Modelling and monitoring forest evapotranspiration: behaviour, concepts and parameters / S.C. Dekker
Thesis Universiteit van Amsterdam – With ref. – With summary in Dutch.
NUG1:819
Subject headings: modelling; hydrology; transpiration

This study was carried out at the Netherlands Centre for Geo-Ecological Research (ICG), Department of Physical Geography and Soil Science, Institute of Biodiversity and Ecosystem Dynamics (IBED), Faculty of Science, Universiteit van Amsterdam, The Netherlands. The research was supported by the Earth Life Sciences and Research Council (ALW) with financial aid from the Netherlands Organisation for Scientific Research (NWO).
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Voorwoord

Vier jaar geleden begon ik als OIO met de gedachte dat een promotiebaan hard en eenzaam werken zou zijn. Op het eind op wachtgeld worstelen aan de laatste hoofdstukken. Er waren vele vragen en onzekerheden: zou ik moeten monitoren in Speuld en Appelscha? In hoeverre zou ik mijn eigen weg moeten kiezen en op welke vlakken zou ik kunnen samenwerken?

Nu, vier jaar later, kan ik alleen maar zeggen dat het fantastisch was. Geen worstelingen, geen individueel gezwoeg. Ik had al snel het idee dat de hele wereld bezig was met boshydrologie. Eigenlijk is het zelfs jammer dat het boekje af is. Ik heb genoten van deze onderzoekstijd en kijk terug op een leuke samenwerking binnen een enthousiaste onderzoeksgroep. Tijdens mijn promotieonderzoek had ik alle vrijheid en mogelijkheden die je als promovendus maar wensen kan. Hiervoor, maar natuurlijk ook vanwege het feit dat hier het eindresultaat voor u ligt, wil ik een aantal mensen bedanken.

Ten eerste wil ik mijn co-promotor Willem Bouten noemen. Willem, je was voor mij de ideale begeleider zowel op wetenschappelijk gebied als persoonlijk. Je was altijd enthousiast, kritisch en je hebt een visie over het leiden van een onderzoeks groep die mij erg aanspreekt. Zonder jouw enthousiasme en openheid was ik zeker minder gemotiveerd geweest en was ik niet verder gegaan in de universitaire wereld. Mijn promotor Koos Verstraten wil ik bedanken voor zijn positieve houding en het vertrouwen in mijn werk.

Een promotieonderzoek kan op verschillende manieren uitgevoerd worden: individueel of juist gezamenlijk. Om samen te kunnen werken met medeonderzoekers moeten ze gemotiveerd zijn en zich kunnen inleven in jouw probleemstelling. Vanwege hun enthousiasme voor mijn onderzoek wil ik de volgende mensen bedanken. Fred Bosveld van het KNMI had altijd tijd voor mij en deelde met mij een grote interesse in parameters. Aan hem dank ik de meteorologische data die gebruikt zijn in dit proefschrift. Daarnaast bedank ik Marcel Schaan van het Salinity lab die mij heeft geholpen met het ‘bootstrappen’ en de neurale netwerken. John Tenhunen and Eva Falge from the University of Bayreuth, thank you for teaching me how to work with plant physiological models.


Mijn kamergenoten Guda van der Lee, Albrecht Weerts en later Boris Jansen wil ik extra bedanken voor de zeer goede sfeer op onze kamer en het oplossen van kleine en grote problemen. Hoewel onze onderzoeken ver uit elkaar lagen, bleek al snel dat er grote overeenkomsten in uitkomst en problemen waren tussen een zuurstofprofiel in een slipplaat en tijdreeksen van transpiratiemetingen.

Ten slotte bedank ik Patrick Boogaart voor de goede (wetenschappelijke) gesprekken in de kroeg en tijdens congressen. Mijn ouders dank ik voor het feit dat ze mij gestimuleerd hebben door te leren.

Koosje, bedankt voor alles! Je hebt zelfs meegeleefd in voor jou totaal oninteressante problemen over inverse modellering, misfits van modellen en unieke of eigenlijk niet-unieke schattingen van parameters. Door jouw opmerkingen is het mij altijd gelukt relativerend tegen mijn onderzoek aan te kijken.

Juni 2000
Stefan Dekker
1. GENERAL INTRODUCTION

Mathematical models are univocal descriptions of our concepts. They represent our perception of the true world and they are essential tools in hydrological and ecological studies to assess ecosystem responses during changes of environmental conditions or to assess the behaviour of the system. Confidence in these models is gained by comparing model results with observations. To achieve this confidence, a variety of tests with different purposes and terminologies, but all dealing with the comparison of model results with observations, are nowadays accepted. As a result, modellers claim that a model test is performed while any reference to the criteria is mostly not given.

1.1 TERMINOLOGY

In the last decade, a debate in literature over model testing in ecology and earth sciences has started (e.g. Janssen and Heuberger, 1995; Konikow and Bredehoeft, 1992; Oreskes et al., 1994; Rykiel, 1994; Rykiel, 1996). Rastetter (1996) pointed out that the essence of the debate is the problem of induction (Popper), which is the problem of extrapolating from the specific to the general. No tests can establish the general validity of the model. Main reasons that we cannot establish the truth are (i) that some parameters or variables can only be established on a specific scale and therefore are incompletely known, (ii) that model concepts are simplicities of the true world and are developed with different perceptions and different aims and (iii) that all variables and observations are measured in a specific context with their own assumptions and inferences.

A summary of the different purposes and terminologies of the model tests, used in the debate, is given here. The authors agree with the definition of calibration, as the process to estimate model parameters and constants to improve the agreement between model output and observations (Janssen and Heuberger, 1995; Konikow and Bredehoeft, 1992; Oreskes et al., 1994; Rykiel, 1996). However, the purpose of calibration is not clear at all. A good match does not prove the validity of the model because the solution can be non-unique (Konikow and Bredehoeft, 1992; Oreskes et al., 1994) and the model can compensate calibration errors due to a wrong parameterisation (Konikow and Bredehoeft, 1992). Therefore, Janssen and Heuberger (1995) suggest a calibration process, in which the evaluation of the model is incorporated. They discerned three major aspects: (i) the assessment of the ability of the model to reproduce the system behaviour, (ii) the assessment of the suitability of the model for the intended use, and (iii) the assessment of
the robustness of the estimated model parameters for different parts of the data set. They pointed out that the uncertainty in the model parameters should be adequately accounted for in further model applications.

In contrast to calibration, many different definitions of verification and validation are proposed in the used literature and references therein. Based on definitions in dictionaries, verification means 'the act to prove to be true or accurate or to ascertain the accuracy of truth'. Validation, as defined in the dictionary, means 'the establishment of legitimacy, in terms of arguments and methods'. A first reason that many different definitions exist is that the verification and validation are synonyms in ordinary language and denote both the establishment of truth. Oreskes et al. (1994) use the definitions from the dictionary and point out that verification (truth) is only possible in closed systems in which all components of the system are established independently and are known to be correct. Because natural systems are never closed, verification is impossible. Because of the synonyms in ordinary language, the same discussion about the establishment of the truth was found for validation.

A second, maybe more important reason that causes the confusion about the terminologies of verification and validation is that different purposes can be found why model results are compared with measurements and why a model must be verified or validated. For instance, one intended goal of verification or validation is to gain confidence in the model's ability to make reliable predictions (Konikow and Bredehoeft, 1992). Another goal is to establish the truth of the model concept, in the perspective that models are hypotheses, which can only be falsified. Because models are developed with different purposes, different perceptions and in different contexts, a model concept can be 'true' in the context of one perception.

Due to the impossibility of establishing the truth, Konikow and Bredehoeft (1992) and Oreskes et al. (1994) pose that verification and validation are impossible. Rykiel (1996) pointed out that validation is a process that can be decomposed in several components. As a result, the terms verification and validation are misleading and should be abandoned in favour of more meaningful terms. A more technical definition of verification is a demonstration that the modelling formalism is correct. Konikow and Bredehoeft (1992) and Oreskes et al. (1994) use for this definition 'verification of numerical solutions'. Konikow and Bredehoeft (1992) pose terms as sensitivity testing, benchmarking or history matching. Oreskes et al. (1994) re-use the term confirmation, which was proposed by the logical positivists. A model can be confirmed by observations, if these observations can be
shown to be true. Rykieł (1996) uses the term credibility and qualification, in which credibility is a sufficient degree of belief in the model for its intended purpose. Therefore, credibility is a subjective qualitative judgement, and cannot be quantified in any absolute sense. Qualification assesses the domain over which a model may properly be used.

1.2 MODEL BEHAVIOUR, CONCEPTS AND PARAMETERS

From the above discussion, it is clear that models cannot be used to establish the truth. Nevertheless, many other purposes consist to use and develop models. From a scientific point of view, models can be used to improve the insight in the processes, to extrapolate in time and space or to determine variables, which cannot be directly measured. To achieve these goals, confidence must be gained in the model concepts and model parameters. In figure 1.1, an outline is given to find out how to gain this confidence. The start of this outline is always the comparison of the model behaviour with the system behaviour. With this comparison model concepts or values of model parameters can be evaluated. In this thesis different methodologies are developed and used to improve the understanding of the model concepts in terms of cause-effect relationships and to improve the interpretation of the model parameters in terms of system properties.

System behaviour – Model behaviour

A model concept or values of model parameters can only be evaluated by comparing model results with measurements. As a consequence, we must always link the system behaviour, e.g. the measurements, to the model behaviour. Model results are compared to measurements to confirm the model concept or the value of the model parameter. However, confirmation of a model by measurements can be very easy and is dependent on the range and kind of the measurements. The result of confirmation is often a statement as average, well or good. To make confirmation more valuable, Reckhow (1983) point out that ‘the modeller must apply (i) a variety of tests, e.g. using the same variations in conditions as the calibration was performed, (ii) a statistical criterion for goodness of fit and (iii) an error analysis in both the predictions and observations’. Nevertheless, confirmation is a subjective measure and a good model result, only enhances our confidence in the model concept or the model parameters.
Figure 1.1: Outline to find out how to gain confidence in models: Model concepts or values of model parameters are always evaluated by comparing model results to measurements, e.g. comparing the model behaviour to the system behaviour. The understanding of the model concept can be improved by a focus on cause-effect relationships and the interpretation of the model parameters can be improved in terms of system properties.

As a result of the subjective judging of the confirmation step, the same results can either enhance the confidence in the model concept or model parameters or can stimulate the development of new model concepts or new model parameterisations. To improve this stimulation, we must not focus on similarities but rather on discrepancies (e.g. falsification, or an analysis of residuals) between model results and measurements.

Model concepts – Cause-Effect relationships

Several model concepts, using different processes, can give equal results. The choice of the processes and variables, included in the model concept, are related to the modellers own perception and to the specific aim of the model. As shown in Figure 1.1, a model concept can be improved by incorporating cause-effect relationships. With a focus on
discrepancies, the residuals between model results and measurements can be compared with input variables to identify missing variables or processes. These missing variables and processes with identifiable physical basis can give information on cause-effect relationships. If two or more model concepts are available, the discrepancies between the model results can also improve our understanding of the processes.

**Model Parameters – System properties**

In general, models contain parameters, which need to be identified. In many cases the parameters cannot be measured independently and can only be calibrated by a comparison of model results and measurements. The aim of calibration is the fit. However, a good fit does not guarantee the uniqueness of the parameter values and does not contribute to the interpretation of the model parameter in terms of system properties. Only a unique parameter estimate with high accuracy can contribute to the understanding of the system and can be used for extrapolation in time and space. With transfer functions these parameter estimates can be linked to system properties.

The parameter identification methodologies presented in this thesis will focus on the uniqueness of the parameters. Classical parameter identification approaches aim to find an optimal model-to-data fit by minimising the total data set with one objective function, for instance the Sum of Squared Errors (SSE). A major problem of parameter identification is that systematic model errors can be compensated by calibration errors in which parameters become non-unique fit-parameters without any physical meaning. The remaining residuals, between model results and measurements, are caused by random and systematic measurement errors and model inaccuracies and may contain information to improve the parameter estimates. With residual analysis, patterns can be explored to trace systematic effects due to wrong model parameter estimates. If fit-parameters are identified by calibration, than parameter estimates can vary by using different objective functions (Janssen and Heuberger, 1995). It is also known that the identification of the parameters is dependent on the range and distribution of the data (e.g. (Gupta and Sorooshian, 1985; Gupta et al., 1998; Kuczera, 1982; Musters and Bouten, 2000; Sorooshian et al., 1983; Yapo et al., 1998)) and dependent on extreme values (Finsterle and Najita, 1998; Legates and McCabe, 1999). This means that parameter identification problems will not simply disappear with the availability of more measurements. It also means that relevant information must be extracted from the total data set to identify the parameters. Once these conditions are selected, parameter values and accuracies can be estimated. The
accuracy of the parameter value is dependent on both model and measurement errors.

Parameter identification will suffer less from the problems of non-uniqueness by using independent parameters. These parameters can either be derived from literature or by calibration only by using another type of measurements than used with the model evaluation.

1.3 EVAPOTRANSPIRATION

In this thesis, several methodologies are developed and used to improve the understanding of forest evapotranspiration model concepts and to improve the interpretation of the model parameters.

The energy and water exchange at the earth surface play an important role in climate and climate change research (Shuttleworth, 1995). So-called Soil Vegetation Atmosphere Transfer (SVAT) processes describe this exchange and are incorporated in atmospheric Global Circulation Models (GCM) and global change models. The grid-sizes of these global models are in the order of 100-300 km².

The major issues in SVAT research deal with (1) plot scale research on SVAT processes and (2) how to scale these SVAT processes to regional scales and to global change time scales. Scaling in space can be done by aggregation of parameters or by aggregation of model output (e.g. Rastetter et al., 1992), (Kabat et al., 1997), (Heuvelink and Pebesma, 1999). With scaling in time more feedback mechanisms must be taken in the plot scale model, such as growth and nutrient availability. A major problem in model evaluation is that the evaluation measurements are collected at smaller spatial and temporal scales than the model predictions.

This study deals with plot scale research of forest evapotranspiration processes. Evaporation of intercepted rain is an important hydrological process in forests. Water budget studies show that the evaporation of intercepted rain amounts 10- 50 % of the total rainfall (e.g. Calder, 1998; Wijk et al., 2000). In general, the model concept of a water bucket of stored water in the canopy that can evaporate or drain is rather well understood. Evaporation of intercepted rainfall is normally considered to be a physical process by using the energy balance and aerodynamic transport equations of Penman (1948). In most studies, the water retention characteristics of the canopy are not known, while evaporation, canopy water storage and drainage are dependent to it. To estimate these processes, the model is calibrated to measurements. In most studies only throughfall is
measured, while the other processes are derived from the calibrated values.

In contrast to evaporation, there is no consensus about the concepts of the process of transpiration. From all different types of process oriented forest transpiration models, four different perspectives were found: the cooling of leaves, the assimilation of CO₂, the energy balance (combined with bulk stomatal conductance) and the water balance. Transpiration of forests can be measured at different spatial scales. At the leaf level, porometers and gas-exchange chambers are used to find plant-physiological mechanisms under changes of environmental conditions. At the tree level, two techniques are generally used: sapflow (Köstner et al., 1998) and soil water content measurements (Musters et al., 2000). At the stand level, eddy-correlation techniques are used and for larger areas remote sensing techniques can be useful for obtaining information of parameters for land-surface interactions (Running et al., 1989). Due to the different model concepts, problems related to transpiration are even broader than with the process of evaporation of intercepted water.

1.4 ORGANISATION OF THE THESIS

The chapters 2 to 6 are integral copies of manuscripts that are published, submitted or will be submitted in relevant scientific journals. In each chapter information on models, measurements and research site, relevant for that manuscript is given. Consequently, duplication sometimes occurs.

All half-hourly micro-meteorological measurements used in this thesis for both 1989 and 1995 were measured by the KNMI (Bosveld et al., 1998; Bosveld 1999). All soil water, throughfall and water storage measurements were measured by the UvA (Bouten et al., 1996; Tikta and Bouten, 1994)

In chapter 2, three forest transpiration model concepts are compared: leaf cooling, CO₂ assimilation and the combined energy and water balance. The purpose of the chapter is to find similarities and discrepancies for transpiration fluxes of half hourly periods and to find improvements of descriptions of forest transpiration processes.

Chapter 3 describes the gas-exchange of CO₂ and H₂O at the leaf and stand scale. Photosynthesis measurements with gas exchange chambers are used to calibrate the Farquhar/Ball leaf scale model. This calibrated CO₂ leaf model is scaled up to the canopy level by a three-dimensional light interception model in order to estimate CO₂ photosynthesis, transpiration and water use efficiency. Modelled canopy transpiration is
independently confirmed to sapflow measurements. So independent parameters are used to simulate stand fluxes. Finally the residual, between model results and measurements are used to identify variables and processes, which were not considered in the original model.

In chapter 4 and 5, the information content of measurements is used to identify unique parameters with high accuracy. In this thesis, the Parameter Identification Method based on Localisation of Information (PIAILI) was further developed and was partly based on the work of Musters and Bouten (2000) and Vrugt et al. (2000). Different objective functions with high information content are used by PAILI to identify the various parameters. The selected conditions can be used to improve the physical meaning of the various parameters. In chapter 4, forest transpiration is modelled with the Single Big Leaf (SBL) model concept, based on the Penman-Monteith equation. The model contains many calibration parameters and mathematical forms of response functions. With calibration, the model parameters are optimised to fit the latent heat eddy correlation measurements. However, time series of environmental conditions determining forest transpiration contain periods with coupled conditions and redundant information while other conditions are hardly measured. In this chapter, measurements with high information content are selected by PAILI. The accuracy and parameter estimates are calculated by using only these selected measurements. The aim of chapter 5 is to identify model parameters of a rainfall interception model by using throughfall and canopy storage measurements. Throughfall, canopy storage and evaporation processes are all dependent of each other. With PAILI, conditions are selected with highest information yielding unique parameters with high accuracy. As soon the selection criteria are known to identify the parameters, true measurements were used.

In chapter 6, an analysis of the residuals between model results and measurements is performed with Artificial Neural Networks (ANNs). Random and systematic measurement errors and model inaccuracies cause these residuals. ANNs are used to explore patterns in the residuals to find model inaccuracies. Only systematic errors with an identifiable physical basis are used to further improve the existing SBL model. Model improvement may consist of incorporation of additional environmental variables, not considered in the original model or an improved model parameterisation.

Finally, in chapter 7, some remarks are given about modelling and monitoring and some suggestions are made for future forest evapotranspiration research to improve the understanding of the cause-effect relationships and to improve the interpretation of the parameters in terms of system properties.
REFERENCES


2. MODELLING FOREST TRANSPIRATION FROM DIFFERENT PERSPECTIVES

ABSTRACT

Forest transpiration models have been developed in different disciplines such as plant physiology, ecology, meteorology, hydrology and soil science. In the present study, three different kinds of model perspectives for transpiration control are used: leaf cooling, CO₂ assimilation and the combined energy and water balance. All three process-oriented models are calibrated on measurements in a Douglas fir stand in the Netherlands. The performances of these models are equally good, although they have different complexities, different numbers of calibration parameters (ranging from 1 to 6) and the models are calibrated on different measurements (eddy correlation at canopy level or CO₂ measurements at leaf level). The resemblance of the model results is caused by the calibration procedure and by the high impact of radiation in all three cases. Significant discrepancies become apparent when differences between model responses are examined and when specific (short) periods are selected when input variables are uncoupled. The main differences between the models are caused by another formulation of leaf area index and vapour pressure deficit (D). Considerable differences in simulated transpiration occur in the afternoon due to the diurnal hysteresis between D and radiation.

2.1 INTRODUCTION

For many decades models describing forest transpiration have been developed in many scientific disciplines such as plant physiology, ecology, meteorology, hydrology and soil science. Each of these disciplines applies its own methodology and studies transpiration at its own specific level of interest, resulting in a large diversity of forest transpiration models. Other reasons for this large diversity are the different aims of the models, different spatial and temporal scales, and the availability of data to parameterise the models.

From all different kind of process oriented forest transpiration models, we found four different perspectives: the cooling of leaves, the assimilation of CO₂, the energy balance (combined with bulk stomatal conductance) and the water balance.

Praza et al. (1994) have presented a model based on cooling of leaves by air and evaporation, while the leaves are warmed by radiation. The advantage of this model is that it is based only on global radiation and temperature, which are easy to measure.

The second cluster of transpiration models covers models based on CO₂ assimilation. If stomata are open, gas exchange of CO₂ and H₂O takes place. Most models are based on Farquhar's model (Farquhar et al., 1980) combined with an empirical relationship to calculate stomatal conductance (Ball et al., 1987; Leuning, 1995). At the leaf scale, model parameters are species dependent. Because leaf assimilation is a non-linear function of radiation, it is necessary to simulate the radiation regime in the canopy (Castro and Fetcher, 1998; Cescatti, 1997; Falge et al., 1997; Wang and Jarvis, 1990).

The third group are the models based on the energy balance, which sometimes are enlarged with a stomatal conductance model. Models based on the energy balance are mostly derived from the Penman equation. Priestly and Taylor (Priestly and Taylor, 1972) have shown that transpiration is a rather conservative variable, which can be determined primarily by the available energy. Combined with temperature and vapour pressure deficit (D) they obtained good results for well-watered vegetation. Makkink (1957) demonstrated a simplified form of the Penman equation, which depends only on radiation and temperature. Usually the models contain several parameters, which are dependent on species, site and scale. Monteith (1965) enlarged the Penman model with a stomatal conductance model. In many cases, the leaf is described as a single big leaf where canopy conductance is composed of the bulk stomatal conductance (gᵢ) and the remaining conductance when the stomata are closed (gₒ). Bulk stomatal conductance is often modelled as a product of reducing functions of leaf area index (LAI), D, radiation, temperature and soil water status (Bosveld and Bouten, 1992; Jarvis et al., 1976; Stewart, 1988).

The last group includes models based on the water balance, which are mostly used in catchment studies where the streamflow behaviour is related to the catchment properties (McCulloch and Robinson, 1993). In these models root water uptake is determined by a potential transpiration calculated from atmospheric conditions and a reducing function which depends on the soil water availability. Soil physicists calculate the root water uptake by solving the Richards' equation, which is extended with a sink term for root water uptake (Ball et al., 1987; Clothier and Green, 1997).

Comparisons between models of evaporation and transpiration have been made by Barr et al. (1997), Garatuza-Payan et al. (1998) and Bosveld and Bouten (1992) who all
compared models based on the energy balance or combined energy balance and stomatal conductance models. Price and Black (1989) compared a CO₂ assimilation model with the Penman-Monteith model, although they could not parameterise the more complex CO₂ assimilation model because of a lack of data.

The purpose of this study is to find similarities and discrepancies in simulated transpiration fluxes at half-hourly periods of completely different forest transpiration models to find improvements of descriptions of forest transpiration processes. Three model concepts, leaf cooling, CO₂ assimilation and a combination of cluster 3 and 4, e.g. energy balance and water balance, are selected and are all calibrated on a Douglas fir stand (*Pseudotsuga menziesii*) in the Netherlands. These models have different perspectives, different complexities and they are calibrated on different types of measurements.

2.2 MATERIALS AND METHODS

Research site

The research site, Speuld, is located in a 2.5 ha Douglas fir forest in the central Netherlands, near Garderen. The forest is dense with 780 trees ha⁻¹ without understorey and planted in 1962. Average tree height between is 21.6 m, lowest living whorl 10.4 m, mean diameter at breast height is 0.249 m and the single sided leaf area, including stem area, ranging from 9.0 m² m⁻² to 12.0 m² m⁻² in summer (Jans et al., 1994). The soil is a well-drained Typic Dystrochrept (Soil survey staff, USDA, 1975) with a distinct forest floor of 5 cm, on heterogeneous ice-pushed sandy loam and loamy sand textured river deposits. The water table is at a depth of 40 m throughout the year. The 30-year average rainfall is 834 mm y⁻¹ and is evenly distributed over the year, mean potential evapotranspiration is about 712 mm y⁻¹. Yearly transpiration reduction by water stress is low (about 5 %), although short periods with considerable drought stress occur (Tiktak and Bouten, 1994).

Measurements

Half-hourly measurements of meteorological driving variables were measured by the Royal Meteorological Institute of the Netherlands (KNMI) on a 36 m high guyed mast. Short wave incoming radiation was measured with a CM11 Kipp solarimeter. Temperature and humidity were measured with ventilated and shielded dry bulb and wet bulb sensors at 18 m above the forest floor. Wind speed was measured with a three cup-anemometer at
18 m above the forest floor. Over 43 days, eddy correlation of water vapour flux was measured 30 m above the forest floor with a fast response Ly-α hygrometer and a sonic anemometer-thermometer system (Bosveld et al., 1998).

Model choices and calibration

Three selected models were calibrated on the Douglas fir stand. Comparison between model results and measurements was based on eddy correlation measurements. Because the eddy correlation technique measures total evapotranspiration, only periods with a dry canopy were selected. Forest floor evaporation was fairly constant during the year at about 0.15 mm d⁻¹ (Schaap and Bouten, 1997). Models and measurements are compared after adding the forest floor evaporation fluxes to the calculated transpiration fluxes.

Leaf cooling model

The leaf cooling (LC) model of Prazak (Prazak et al., 1994) was chosen. This model calculates transpiration on basis of the requirement of water for cooling the canopy. Trees are simultaneously warmed by incident solar radiation and cooled by ambient air and by transpiration. Global radiation and temperature are the driving variables. Properties of the forest are expressed in two calibration parameters for the effective absorptivity of the radiation and the effective thickness of the leaves.

The model was calibrated on eddy correlation measurements. Optimum canopy temperature was set constant at 25°C. The two calibration parameters were optimised by an inverse modelling approach and found at 0.211 (-) for the effective absorptivity and 0.16 mm for the effective thickness of the leaves. Explained variances between the measurements and model results is $R^2 = 0.777$ and standard deviation of the error is 30.3 W m⁻². Because the true thickness of a needle is about 1 mm we conclude that both parameters are calibration parameters and do not have any physiological or physical meaning.

$CO_2$ assimilation model

The $CO_2$ assimilation (Assim) model we have chosen is the frequently used Farquhar model (Farquhar et al., 1980), which describes photosynthesis at the leaf scale. Combined with the stomatal conductance model of Ball et al. (1987), photosynthesis and transpiration are modelled at the leaf scale. No energy balance is included in this model. To obtain canopy fluxes, this leaf model is scaled using the three-dimensional light
interception model Standflux (Falge et al., 1997).

Driving variables are photosynthetically active radiation (PAR), temperature, $D$ and wind speed. System variables are detailed LAI and stand characteristics to scale from leaf to stand. Net photosynthesis is calculated with temperature response functions and transpiration is calculated from the calculated stomatal conductance and the $D$ gradient.

Three parameters of the leaf model were calibrated on measured CO$_2$ fluxes at the leaf level using CO$_2$ gas exchange chamber measurements (Dekker et al., 2000) and scaled up by the use of detailed stand characteristics (Jans et al., 1994). Dekker et al. (2000) found that an extra temperature response function must be included in Ball’s model to obtain realistic canopy fluxes. The explained variance between model results and measurements is $R^2 = 0.804$ and standard deviation is $30.1$ W m$^{-2}$

*Combined energy balance with stomatal conductance and water balance model*

The Single Big Leaf (SBL) model we used is based on the Penman-Monteith equation (Monteith, 1965) where stomatal conductance is modelled as a product of reducing functions. It is assumed that the environmental factors that influence stomatal conductance ($g_i$) are day number of the year to calculate a seasonal trend of LAI, $D$, solar radiation, air temperature and soil water pressure head. The seasonal trend of LAI is caused by shoot growth and needle fall, where new needles may have a different stomatal conductance. To calculate the soil water pressure head a detailed soil water model (Tiktak and Bouten, 1994) was coupled to this model.

Driving variables are net radiation, global radiation, temperature, $D$, wind speed and precipitation. System variables are LAI and soil properties. For every response function (LAI, $D$, solar radiation, air temperature and soil water pressure) one parameter was optimised. Together with $g_i, ref$ this results into 6 calibration parameters. Calibration was performed by Bosveld and Bouten (1992). The soil water model was calibrated on soil water measurements, measured with TDR (Tiktak and Bouten, 1994), and the response functions were calibrated on latent heat fluxes measured with eddy correlation during dry canopy. The explained variance between model results and measurements is $R^2 = 0.834$ and standard deviation is $28.1$ W m$^{-2}$.
2.3 RESULTS AND DISCUSSION

Model output comparison

Large differences in predicted transpiration between models were expected with the use of completely different model concepts. During the analysis, however, comparable explained variances and standard deviations between models and measurements at half-hourly

![Graphs showing model output comparison](image)

**Figure 2.1**: Comparing modelled and measured transpiration on 30 minutes interval base. Modelled transpiration was added with a forest floor evaporation model. Explained variances and standard deviations are: LC ($R^2 = 0.796$, $\sigma = 30.3 \text{ W m}^{-2}$), Assim ($R^2 = 0.804$, $\sigma = 30.1 \text{ W m}^{-2}$), SBL ($R^2 = 0.855$, $\sigma = 28.1 \text{ W m}^{-2}$). Dashed lines are 1:1 line, curved lines are fitted functions. Figure 2.1D shows the non-linearity of the measurements if an extra noise of 30 W m$^{-2}$ is added to the measurements.
basis were found (Figure 2.1A-2.1C). The fact that the Single Big Leaf (SBL) model produces slightly better results is not surprising because of the use of six parameters. As shown in Figure 2.1, maximum-modelled transpiration is about 190 W m$^{-2}$ in all cases, whereas some measurements are somewhat higher than 200 W m$^{-2}$. These high measurements are not related to a wet canopy. In some cases a somewhat higher flux may be caused by a wet forest floor, although values of more than 25 W m$^{-2}$ for forest floor evaporation were never established. High measured fluxes are also related to a higher noise of the measurements. In all three models a non-linearity is found, represented by the fitted curved line shown in Figure 2.1. The differences in non-linearity between the models are small. This non-linearity can be caused by two reasons, (i) a missing link in the model or (ii) the fact that the model error is nearby zero while the error in the measurement is large. If an extra noise of 30 W m$^{-2}$, which equals the error between model and measurement, is randomly added to the measurements and plotted against the true measurements, an identical non-linearity is found (Figure 2.1D). This means that the non-linearity found in Figure 2.1, can be explained by the one-sided noise at the x-axis. In addition of similarities of explained variances between models and measurements of the selected periods, model results of a total year are also almost identical. Annual totals for the LC, Assim and SBL are respectively, 310, 315 and 304 mm. The latter includes a reduction in annual transpiration of 20 mm as a result of soil water stress. Figure 2.2

![Figure 2.2: Thirty day moving average of modelled forest transpiration in mm day$^{-1}$](image)

Figure 2.2: Thirty day moving average of modelled forest transpiration in mm day$^{-1}$
shows the 30-day moving average transpiration of the three models. Their dynamics are comparable although deviations of 20\% occur around day 150. These deviations are caused mainly by including a LAI function over the growing season in the Assim and the SBL models. Differences between these two models are caused by the different impact of the LAI variation. Light extinction in the three-dimensional canopy model of the Assim model is very strong because of the high LAI. A 30\% reduction of LAI reduces transpiration by only 10\%, whereas the SBL model is calibrated to a 40\% variation in transpiration during the growing season.

On a half-hourly basis, explained variances and standard deviations between the models are for LC - Assim, SBL - LC and SBL - Assim respectively $R^2 = 0.836, 0.897$ and $0.861$. With all these similarities we cannot reject any one of the model concepts. This is not surprising because all these model types are still used in many studies. There are two reasons for these similarities. The first reason is the calibration procedure. For all three models, the final calibration was based on eddy correlation measurements. Although the idea of the Assim model is that calibration is not necessary, we used the extra temperature calibration to have comparable results between the models in terms of explained variances.

The second reason is the conservative behaviour of transpiration to radiation. A linear regression between eddy correlation measurements minus forest floor evaporation and global radiation of the total period, including the drought stress periods leads to $R^2 = 0.765$ and a standard deviation of 31.2 W m$^{-2}$ (Figure 2.3), which is comparable to the model results. It means that any calibrated model is able to describe transpiration to an acceptable level as long as radiation is included in the model. Because of strong correlation between input variables, for instance temperature is correlated with $D$ and radiation, a mean response is easy to find and gives reasonable estimates. Short periods when these correlation are uncoupled are very rare and hardly influence the overall fit criteria.

The magnitude of the uncertainties in the measurements also make it difficult to choose between the models. A standard deviation of the eddy correlation measurements of 21 W m$^{-2}$ at half-hourly intervals was calculated for atmospheric statistics. Owing to variation of the footprint and the fact that the buffer capacity for vapour below the measurement level is about 15 W m$^{-2}$, the uncertainty range is even wider. Because standard deviations between model results and measurements are 30.3, 30.1 and 28.1 W m$^{-2}$ on average half-hourly basis, better estimates are not directly foreseen.
Figure 2.3: Linear regression equation between global radiation \( (R_g) \) and eddy correlation measurements.

Discrepancies

From the above analysis we conclude that all models are able to describe transpiration, mainly because of the strong correlations between radiation, temperature and \( D \) at ambient environmental conditions. This means that more observations during ambient conditions will not lead to a validation of one type of model. However, observations outside the range of calibration, for instance during manipulation experiments, may give misleading results if conditions are changed in an unnatural way. Therefore, to compare the models' performance it is better to focus on periods where discrepancies occur. To do this, periods are selected when input variables were uncoupled.

Several techniques can be used to find periods with uncoupled input variables. For instance, in Figure 2.4A, when for four days model outputs are selected where the \( D \) ranged between 10 and 30 mbar. Largest deviations between the models occur in the afternoon where the Assim model shows a delay for all days. Observations between 14.00 and 19.00 hour are selected in a subset. Explained variances between model and measurements of this subset are for LC, Assim and SBL respectively \( R^2 = 0.717, 0.690 \) and 0.784. This delay is caused by the time lag of \( D \) with respect to global radiation (Figure 2.4b). Because the Assim model is most sensitive to \( D \), the transpiration is delayed.
Figure 2.4: (A) The model results and eddy correlation measurements of 4 selected days with different vapour pressure deficit $(D)$. (B) The delayed diurnal dynamics of $D$ and global radiation $(R_g)$ during these selected days.

Hysteresis between $D$ and radiation is shown in Figure 2.5, where the same four days are plotted. Several researchers have reported diurnal clockwise hysteresis of measured leaf stomatal conductance (Pereira et al., 1987; Takagi et al., 1998). Because leaf stomatal conductance cannot be compared with bulk canopy stomatal conductance, we compare transpiration rates. Figure 2.6 shows the average deviation between measurements and model results plotted against $D$. The largest deviation occurs between 10-20 mbar for the Assim model, although the Assim model gives better estimates at high and low $D$. 

26
Figure 2.5: Clockwise hysteresis between global radiation ($R_g$) and vapour pressure deficit ($D$). Numbers indicate day number as shown in Figure 2.4.

Figure 2.6: Mean deviation between observations and model estimates of transpiration in the afternoon, between 0.6 and 0.8 day.
To find differences of model behaviour in relation to input variables, the correlation between radiation and $D$ is again used. All half-hourly simulated transpiration values between day of year 91 and 365 are used to make contour lines of the differences of modelled transpiration plotted against radiation and $D$ (Figure 2.7). Contour lines are made by interpolation. The shaded parts are the 15 W m$^{-2}$ similarity intervals between the models. As the confidence interval of the eddy correlation measurements is even larger, it is clear that we will never find differences between LC and SBL (figure 2.7A). It means that $D$, which is included in SBL and not in the LC model, does not directly influence transpiration. The largest deviations occur with the Assim model at $D$ between 10 and 25 mbar and radiation between 100 - 400 W m$^{-2}$ (figure 2.7B and 2.7C). Figure 2.7C shows a larger deviation at radiation of 500 W m$^{-2}$ and $D$ of 15 mbar than shown in Figure 2.7C. These periods correspond to days with soil water stress and differences of LAI effect.

Figure 2.7: Differences between the models in W m$^{-2}$ against global radiation ($R_g$) and vapour pressure deficit ($D$). Shaded part is the 15 W m$^{-2}$ reliability range of eddy correlation measurements. (A) the difference of LC and SBL; (B) the difference between Assim and LC; (C) the difference between Assim and SBL; (D) the measurement combinations used for this analyses.
between the model results.

It should be possible to improve some model responses on the basis of the discrepancies found in the sub data sets. We realise, however, that these model responses of the system do not necessarily give the behaviour of the true mechanisms. This is certainly the case if models are calibrated on these system responses as shown in this analysis. This together with the relatively large error of the eddy correlation measurements makes it impossible to rule as invalid any of the different processes included in the three model types.

2.4 CONCLUSIONS

Forest transpiration can be modelled successfully from different perspectives because of the high correlation with radiation and the fact that we calibrate mean responses of coupled input variables. It means that all models confirm the observations, even a linear regression model with only radiation. As long as we calibrate transpiration models, focusing on similarities does not provide information about the validity of the models. To evaluate model concepts, we need to focus on discrepancies and selected periods of specific combinations of environmental conditions by either selection of periods of uncoupled input variables or selection of differences of model behaviour in relation to the input variables.

The diurnal hysteresis of vapour pressure deficit \(D\) causes large differences in the afternoon. Although differences in model responses can be observed and explained in terms of the model concepts, a rejection of one of the model concepts is impossible because the model results depend on calibration procedures. Consequently, all three model concepts may still describe the true mechanisms.

Acknowledgement

The authors thank Fred Bosveld from the Royal Meteorological Institute of the Netherlands for providing the meteorological data of 1995.
REFERENCES


3. MODELLING GAS EXCHANGE OF A DOUGLAS FIR STAND*

ABSTRACT

Modelling tree growth and water use is nowadays a major challenge, which indicates that the complex interrelation between water and CO₂ uptake at the canopy level must be known. The mechanistic physiological link between water vapour and CO₂ at the leaf scale is relatively well understood. In this study, photosynthesis measurements with gas exchange chambers are used to calibrate the combined Farquhar/Ball model. The calibrated leaf model is scaled up to the canopy level by the three-dimensional light interception model STANDFLUX in order to estimate CO₂ photosynthesis, transpiration and water use efficiency. Simulations with seasonal trends in LAI and model parameters, derived from the leaf measurements, are performed. Modelled canopy transpiration, calibrated on photosynthesis measurements, is independently validated on sapflow measurements. Simulated transpiration is in close agreement with measured transpiration (slope=1.016), while daily total deviations occur (R² = 0.60) which could not be explained by one of the simulations. To obtain an optimal fit, Ball's model parameter GI:AC is calibrated on measured daily sapflow, which results in a more constant WTU during the year. Correlations between GI:AC, temperature and soil water content are observed. To obtain better model estimates, alternative stomatal models should be used although it must be seen that the multiple effects on GI:AC are clearly identifiable.

3.1 INTRODUCTION

A major challenge in the context of global change is to understand the effects of increasing CO₂ and temperature on the carbon balance of forest ecosystems. In order to evaluate a variety of climate change scenarios, models that estimate forest gas exchange must be developed which correctly describe the basic processes of photosynthetic CO₂ uptake and CO₂ losses in respiration. In order to best validate these process descriptions, such models can only be tested at present under current natural conditions, except in very few cases where forests are exposed to free air carbon dioxide enrichment (FACE.

* submitted in a revised form to Journal of Hydrology by: S.C. Dekker, W. Bouten, F.M. Falge, J.D. Tenhunen and E.G. Steingröver
experiments). Even in these cases, exposures of forests to date have only been short-term and for few species. Thus, while the prediction of forest response under elevated CO₂ remains an even greater problem, forest gas exchange models that are tested against long-term records of net ecosystem CO₂ exchange (NEE) provide improved tools for the study of carbon sequestering and release from forests.

At the present time, canopy level measurements of gas exchange are being performed with eddy covariance techniques at many sites (Baldocchi et al. 1996). Annual NEE is very small compared to the large annual amounts of photosynthesis, which are offset by large respiratory fluxes (sum of soil, woody maintenance, and woody growth respiration). Further, large inter-annual variations in NEE occur because of climate influences on phenology, frost damage above- and belowground, degree of water stress, etc. Thus, an additional challenge in modelling the CO₂ exchange of forests is to improve our understanding and model performance with respect to the relative importance of time dependent and stress phenomena.

To obtain canopy fluxes, both aggregated (big-leaf) and distributed (multiple layer and three-dimensional) modelling approaches have been used (Jarvis and McNaughton, 1986; Raupach and Finnigan, 1988; Jarvis, 1995; Falge et al., 1997). Aggregated big-leaf models describe leaf processes in an abstract way, are relatively easily parameterised to measured canopy flux data, but must be, nevertheless, sensitive to the non-linearity in leaf response to light, at least as it is expressed at the canopy level. Distributed models clearly represent species differences at the leaf level and are able to scale up these differences to canopy level, dependent on their ability to correctly describe canopy structure and estimate light interception. Neither approach has yet been adequately tested with respect to efficiency in describing time and space dependent variation in ecosystem properties, i.e., to describe heterogeneity in ecosystem carbon balances due to landscape level influences on site properties or to time dependent changes in canopy structure and physiology.

Processes at the leaf scale are in general well-described for most important tree species. Photosynthesis is measured with chambers and is often modelled according to Farquhar et al. (1980), including a CO₂-assimilation-correlated stomatal component sensu Ball et al. (1987; see also Harley and Tenhunen, 1991; Wullschleger, 1993; Gunderson and Wullschleger, 1994). Via the Ball et al. formulation, stomatal conductance and water use are also obtained. Model parameters are normally derived from light manipulation experiments at differing temperatures or by observing time courses of gas exchange under natural habitat conditions (cf. Falge et al. 1996). The purpose of the current study was to
examine and model gas exchange of a stand of Douglas fir growing in the Netherlands. Model parameters at the leaf level were derived from branch chamber measurements under ambient conditions (Steingröver and Jans, 1995) with an inverse modelling approach. The calibrated leaf photosynthesis model was then tested with respect to measurements made at different positions in the canopy. In a third step, canopy fluxes of CO₂ and H₂O are obtained by up-scaling the leaf model with the three-dimensional forest canopy model STANDFLUX (Falge et al., 1997), which integrates leaf response with respect to canopy structure, light interception, and microclimate. Modelled canopy transpiration is independently validated based on measurements of sapflow. Finally, the residual remaining differences between modelled and measured transpiration are discussed in relation to the water use efficiency (WUE) and the physiological link between transpiration and photosynthesis.

3.2 MATERIALS AND METHODS

Research site

The research site Speuld is located in a 2.5 ha *Pseudotsuga menziesii* forest in the central Netherlands, near Garderen. The Douglas Fir forest is dense with 780 trees ha⁻¹ without understorey and planted in 1962. Average tree height between 1990 and 1992 is 21.6 m, lowest living whorl 10.4 m, mean diameter at breast height is 0.249 m and the single sided leaf area ranging from 7.8 m² m⁻² in spring to 10.5 m² m⁻² in summer, the ratio between surface and projected leaf area is 2.57 and stem area index ranging from 1.16 m² m⁻² to 1.54 m² m⁻². The soil is a well-drained Typic Dystrochrept (Soil survey staff, USDA, 1975) on heterogeneous sandy loam, which was transported and plowed by ice, and loamy sand textured river deposits. The water table is at a depth of 40 meter throughout the year. The 30-year-average rainfall is 834 mm y⁻¹ and is evenly distributed over the year, mean potential evapotranspiration is about 712 mm y⁻¹. Yearly transpiration reduction by water stress is low, although short periods with considerable drought stress occur (Tiktak and Bouten, 1994).

Measurements

In 1992, photosynthesis measurements were performed at the leaf level and during 1989 hydrological and meteorological measurements were carried out at the stand scale. Aboveground biomass measurements are made between 1990 and 1992 (Jans et al., 1994)
at five different heights in the canopy. Data that we used are given as average values in Table 3.1. From March to December 1992, as many as eight photosynthesis chambers were in use simultaneously.

Table 3.1: Aboveground biomass adapted from Jans et al., 1994.

<table>
<thead>
<tr>
<th>Tree height</th>
<th>layer</th>
<th>measurement period</th>
<th>no. of trees</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lowest living whorl</td>
<td>10.4 m</td>
<td>1990-1993</td>
<td>272</td>
</tr>
<tr>
<td>DBH</td>
<td>0.249 m</td>
<td>1990-1993</td>
<td>272</td>
</tr>
<tr>
<td>Crown levels</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.4-14.9 m</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.9-17.1 m</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17.1-19.4 m</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19.4-21.6 m</td>
<td>5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>No. of chambers:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>5</td>
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<tr>
<td>11</td>
<td>5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Needle surface area (m$^2$)*</td>
<td>37.8 m$^2$</td>
<td>2</td>
<td>1990-1991</td>
</tr>
<tr>
<td></td>
<td>42.2 m$^2$</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>24.5 m$^2$</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10.3 m$^2$</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>Branch surface area (m$^2$)*</td>
<td>5.1 m$^2$</td>
<td>2</td>
<td>1990-1992</td>
</tr>
<tr>
<td></td>
<td>5.2 m$^2$</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.8 m$^2$</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.9 m$^2$</td>
<td>5</td>
<td></td>
</tr>
</tbody>
</table>

* Branch and Needle surface area per tree are calculated by multiplying number of needles or branches, length and diameter.

The chambers were used to examine different needle classes, response at different heights, and response with respect to different trees. The temperature, vapour pressure deficit ($D$) and CO$_2$ concentration of the air entering each chamber were the same as in the surroundings (Posma et al., 1994). A PAR sensor was situated outside each photosynthesis chamber. The differences of CO$_2$ concentration of the air, which enters and leaves the chambers was measured continuously with an infrared gas analyser and stored as a 10 minute average value. Needle transpiration was calculated from the difference of partial $D$ between incoming and outgoing flow. These measurements do have a low quality because of instrumental problems.
During 1989, meteorological measurements were performed by the Royal Meteorological Institute of the Netherlands (KNMI) on a 36 m high guyed mast. Short wave incoming radiation was measured with a CM11 Kipp solarimeter. Temperature and humidity were measured with ventilated and shielded dry bulb and wet bulb sensors at 18 m above the forest floor. Wind speed was measured with a three cup-anemometer at 18 m above the forest floor. Eddy covariance of water vapour flux was measured 30 m above the forest floor with a response Ly-α hygrometer (Bosveld et al., 1992).

Sapflow velocities were measured by means of heat pulse velocity (HPV; Marshal, 1985). Hourly measurements were made with seven sensors from day 147 to 310, 1989. For each sensor, the HPV is linearly related to the xylem sapflow velocity. Absolute values should be treated with care because of effects of installation, light exposure, or non-uniformity of the trunk. Due to instrument limitations, velocities below 1.1 cm hour\(^{-1}\) could not be registered. So instead of direct averaging the HPV, all measurements of each sensor were first scaled by fitting sinusoid waves through the measurements and then averaged. These mean values were converted to sapflux densities by using absolute transpiration values from eddy correlation and soil water balance measurements (Bouten, 1992). During 1989, soil water was measured weekly by Time Domain Reflectometry (TDR) and with the neutron scattering method. A calibrated soil water balance model was used to interpolate these measurements (Tiktak and Bouten, 1994).

Leaf gas exchange model

The leaf photosynthesis model is based on Rubisco kinetics as proposed by Farquhar et al. (Farquhar et al., 1980) and as applied by Harley and Tenhunen (1991). Net CO\(_2\) exchange (\(NP\)) is reduced by CO\(_2\) evolution of dark respiration (\(R_d\)). It is assumed that \(R_d\) decreases from 100 to 50 % as PAR increases from 0 to 25 \(\mu\text{mol m}^{-2} \text{s}^{-1}\) (see Falge et al., 1996).

Stomatal conductance of water vapour, \(g_s\), is described as an empirical function (Ball et al., 1987), which depends on net photosynthesis:

\[
g_s = g_{\text{min}} + GFEIC \frac{1000 \left(NP + 0.5 \ R_d\right)}{C_i} b_r
\]  

(3.1)

where \(g_{\text{min}}\) is the conductance when the stomata are closed, \(b_r\) (-) is the relative humidity, \(C_i\) is the CO\(_2\) partial pressure at the leaf surface and \(GFEIC\) (-) is a constant which reflects sensitivity of stomata to changes in \(NP\), \(C_i\) and \(b_r\). \(C_i\) is calculated from ambient CO\(_2\) with
a boundary layer resistance dependent on wind speed. Equation 3.1 describes the dependency of \( g_s \) on \( NP \), but \( g_s \) also limits \( NP \). The gradient between ambient CO\(_2\) pressure \( (C_{a}) \) and internal CO\(_2\) pressure \( (C_{i}) \) depends on \( NP \) and \( g_s \):

\[
C_i = C_{a} - \frac{1.56 \cdot NP \cdot 1000}{g_s}
\]

(3.2)

where 1.56 reflects the ratio of the diffusion coefficients between CO\(_2\) and water vapour. With an iterative scheme, equations 3.1 and 3.2 were solved until a minimum difference of \( g_s \) of 1 mmol m\(^{-2}\)s\(^{-1}\) and \( C_i \) of 0.05 ppm were reached.

Ball's model parameter \( GH\cdot AC\cdot (-) \) was obtained directly by plotting Equation 3.1 over diurnal courses based on cuvette measurements. We only selected observations with a \( C_i/C_{a} \) ratio between 0.65 and 0.85 (Baldocchi, 1994). Minimal stomatal conductance \( (g_{\text{min}}) \) is 3.0 mmol m\(^{-2}\) s\(^{-1}\) and was derived from eddy correlation measurements (Bosveld et al., 1992).

**Optimising leaf response parameters at ambient conditions**

Leaf CO\(_2\) gas exchange was fitted by calibrating three model parameters, the activation energy of \( R_d \) and the scaling constants of the maximum carboxylation velocity \( (V\cdot C_{\text{max}}) \) and the potential rate of RuBP regeneration \( (P_{mol}) \) (Harley and Tenhunen, 1991; Falge et al., 1996). Other model parameters were fixed and found by Harley and Tenhunen (1991) as shown in Table 3.2. The temperature dependence of \( R_d \) is described by an exponential temperature function (Harley and Tenhunen, 1991):

\[
R_d = e^{(f \cdot E_a / R \cdot T_a)}
\]

(3.3)

where \( f (-) \) is a scaling constant and \( E_a \) (J mol\(^{-1}\)) is activation energy, \( R \) (J mol\(^{-1}\) K\(^{-1}\)) is the gas constant and \( T_k \) (K) is air temperature. During the growing season, higher dark respiration can be related to higher metabolic activity. Seasonal fluctuations were adequately described by fixing the scaling constant and varying the activation energy (Falge et al., 1996). Because \( NP \) equals \( R_d \) during night we fitted \( R_d \) to the night-time measurements in ten days periods by varying the activation energy.
Table 3.2: Constants and activation energies to determine temperature and light dependent values of leaf gas exchange. Bold values were analysed during this study. Other values are from Harley and Tenhunen (1991). All values relate to rates on a projected leaf area basis.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Period</th>
<th>Values</th>
<th>Units</th>
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<tbody>
<tr>
<td>Dark Respiration</td>
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<td></td>
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</tr>
<tr>
<td>$R_d$</td>
<td>Day number of the year</td>
<td>180-250</td>
<td>61000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>59000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>59800</td>
</tr>
<tr>
<td></td>
<td>average</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>fixed</td>
<td></td>
<td>25</td>
</tr>
<tr>
<td>Electron transport capacity</td>
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<td></td>
</tr>
<tr>
<td>$c(P_{\text{ad}})$</td>
<td>180-250</td>
<td>15.6</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>15.7</td>
<td>-</td>
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<tr>
<td></td>
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<td>15.7</td>
<td>-</td>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$H_e(P_{\text{ad}})$</td>
<td></td>
<td>44700</td>
</tr>
<tr>
<td></td>
<td>$\Delta H_e(P_{\text{ad}})$</td>
<td></td>
<td>2000000</td>
</tr>
<tr>
<td></td>
<td>$\Delta S(P_{\text{ad}})$</td>
<td></td>
<td>643</td>
</tr>
<tr>
<td>Carboxylase capacity</td>
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<tr>
<td>$qV_{\text{max}}$</td>
<td>average</td>
<td></td>
<td>36.0</td>
</tr>
<tr>
<td></td>
<td>minimum</td>
<td></td>
<td>35.0</td>
</tr>
<tr>
<td></td>
<td>$\Delta H_c(V_{\text{max}})$</td>
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<td>$\Delta H_c(V_{\text{max}})$</td>
<td></td>
<td>2000000</td>
</tr>
<tr>
<td></td>
<td>$\Delta S(V_{\text{max}})$</td>
<td></td>
<td>656</td>
</tr>
<tr>
<td>Carboxylase kinetics</td>
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<td></td>
</tr>
<tr>
<td>$f(K_c)$</td>
<td></td>
<td>31.95</td>
<td>-</td>
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<tr>
<td></td>
<td>$V_{\text{ad}}(K_c)$</td>
<td></td>
<td>65000</td>
</tr>
<tr>
<td></td>
<td>$f(K_o)$</td>
<td>19.61</td>
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</tr>
<tr>
<td></td>
<td>$V_{\text{ad}}(K_o)$</td>
<td></td>
<td>36000</td>
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<tr>
<td></td>
<td>$f(\tau)$</td>
<td>-3.9489</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>$E_{\text{ad}}(\tau)$</td>
<td></td>
<td>-28990</td>
</tr>
<tr>
<td>Light use efficiency</td>
<td></td>
<td>0.08*</td>
<td>mol CO$_2$/mol photonen</td>
</tr>
<tr>
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<td>mmol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$GF_{\text{ad}}$</td>
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<td>8.0</td>
<td></td>
</tr>
</tbody>
</table>

*Average measurement by (Steingröver and Jans, 1995)

$I_{\text{Cmax}}$ can be obtained from the initial slope of the dependency of net photosynthesis on $C_l$. $P_{\text{mi}}$ at saturated light and CO$_2$ pressure can be obtained from the slope of the dependency on temperature (Harley and Tenhunen, 1991). $P_{\text{mi}}$ can be described by:

\[
P_{\text{mi}} = \frac{V_{\text{ad}}(C_{\text{p}}) - \Delta H_e(P_{\text{mi}})}{RT_k} \cdot \frac{1}{1 + e^{\frac{-\Delta V_{p_c} - \Delta H_e(P_{\text{mi}})}{R T_f}}} \tag{3.4}
\]

and $I_{\text{Cmax}}$ can be described by:
where \( \epsilon (\cdot) \) are scaling constants, \( \Delta H_d \) (J mol\(^{-1}\)) are energies, \( \Delta S \) (J K\(^{-1}\) mol\(^{-1}\)) are entropy terms and \( \Delta H_d \) (J mol\(^{-1}\)) are deactivation energies.

\( P_{nl} \) and \( \Gamma \gamma_{max} \) were estimated with an inverse modelling approach rather than via experimental measurements with saturated light and saturated CO\(_2\). By using the simplex algorithm (Press et al., 1988), the scaling constants of \( \Gamma \gamma_{max} \) and \( P_{nl} \) were optimised simultaneously assuming 0.5R\(_d\) during day. For every 10 day period and for every chamber we calculated these model parameters. With the obtained model parameters, the minimum of Rubisco limited rate of carboxylation \( \text{II}^+ \) and the RuBP limited rate of carboxylation limited by light \( \text{II}^+ \) are used to calculate net photosynthesis.

STANDFLUX

The model STANDFLUX (Falge et al., 1997) integrates the three-dimensional aspects of canopy structure and light interception, one-dimensional vertical stand microclimate and the physiologically based leaf gas exchange model as mentioned above. Trees are divided in concentric cylinders and horizontal layers around the trunk assuming homogeneous leaf density. Only one tree class with average LAI is used to model the homogeneous Douglas fir stand. With the detailed biomass measurements of needle and branch surface area (Table 3.1), the tree is constructed with four outer layers in the crown and one inner layer of the trunk. The meteorological driving variables of the model are temperature, \( D \), wind speed, ambient CO\(_2\) pressure and PAR. Ambient CO\(_2\) pressure was fixed to 350 ppm because the model is not sensitive to changes of CO\(_2\) in the range of measurements. PAR was not measured in 1989, so we assumed that the average proportion of PAR is 51% of global radiation (Britton and Dodd, 1976). For every matrix point, the model calculates the gas exchange and integrates it with LAI to tree scale fluxes. Stand transpiration is calculated with both season dependent and annual average LAI and gas exchange parameters. It was observed that shoots grow between day 130 and 180. Assuming that the same amount of one-year-old needles falls linearly during the year, the LAI curve is constructed as a piecemeal linear form between 7.8 and 10.5 m\(^2\) m\(^{-2}\).

An independent validation of the stand gas exchange model was based on daily total sapflow scaled to stand level. Because of the time lag of sapflow measurements, half-
hourly measurements were averaged to daily totals between 6 am to 6 am next day and only daily values were compared with model performance. Because of instrument limitations of the HPV method at small velocities, we focus our analysis on the period between day 147 and 265. Deviations between measured and modelled daily transpiration were analysed. An optimal fit of the model for each day can be obtained by optimising Ball’s empirical model parameter $GFAC$ to the sapflow measurements. Relating the optimised values of $GFAC$ to meteorological driving variables provides information about stand response, which is not captured by the model.

---

**Figure 3.1:** Variations of optimised $E_a$ (Figure 3.1A), $c(V_{C_{max}})$ (Figure 3.1B) and $c(P_{ml})$ (Figure 3.1C) parameter of the 6 photosynthesis chambers located at different layers in the canopy.
3.3 RESULTS

Inverse modelling of leaf model response parameters

Figure 3.1A shows the seasonal and spatial trend of the optimised response parameter of $R_d$. Higher activation energy means a lower $R_d$. Dark respiration was maximal in late spring and decreased during summer as has been found with other species (cf. Falge et al., 1996).

This maximal dark respiration during spring can be related to higher metabolic activity during the development of new shoots. Significant differences between shade crown (chamber 13, layer 4) and what we originally considered the sun crown (chamber 9,11,14, layer 5) and spatial trends between the layers were not observed. During summer (day 180-270) an increase of $E_a$ was found, with an average of 61000 J mol\(^{-1}\). During winter an average of 59000 J mol\(^{-1}\) and a yearly average of 59800 J mol\(^{-1}\) were estimated. By using equation 3.3, at 20 °C $R_d$ equals 1.55 $\mu$mol m\(^{-2}\) s\(^{-1}\) on the basis of projected leaf area and 0.60 $\mu$mol m\(^{-2}\) s\(^{-1}\) on the basis of total leaf surface area. With this analysis, a separation between twig and needle respiration is not possible, but we assume that the twig contribution to respiration was small for the branch ends used. The results of the simultaneous fitting of the scaling parameters of $c(I\'_{\text{max}})$ and $c(P_{\text{ml}})$ are shown in Figure 3.1B and 3.1C. Yearly average values were $c(I\'_{\text{max}}) = 36.0$ and $c(P_{\text{ml}}) = 15.7$. Using the same periods as mentioned above we found $c(I\'_{\text{max}}) = 36.6$ and $c(P_{\text{ml}}) = 15.6$ during summer and $c(I\'_{\text{max}}) = 35.7$ and $c(P_{\text{ml}}) = 15.7$ during winter. Differences in model parameters between age or needles located in the upper or lower levels of the crown were not observed and the seasonal variations are small in comparison with the noise. With these model parameters and with PAR = 2000 $\mu$mol m\(^{-2}\) s\(^{-1}\) and ambient CO\(_2\) concentration of 350 ppm, $I\'_r$ and $I\'_d$ of Douglas fir were calculated as shown in Figure 3.2. If we assumed an average minimum value of $c(I\'_{\text{min}}) = 35$, carboxylation was limited by Rubisco and with larger $c(I\'_{\text{max}})$ or with smaller amount of light, carboxylation was always limited by light.

Wullschleger (1993) found an average ratio of 1.64 between the light saturated rate of electron transport ($J_{\text{max}}$) and $I\'_{\text{max}}$, where $P_{\text{ml}}$ equals 0.25$/J_{\text{max}}$ (Harley and Tenhunen, 1991). Both rates were calculated using $c(I\'_{\text{max}}) = 35$ and $c(P_{\text{ml}}) = 15.7$. By using equation 3.4 and 3.5, at 20 °C it results in $I\'_{\text{max}} = 50$ $\mu$mol m\(^{-2}\) s\(^{-1}\) and $P_{\text{ml}} = 21$ $\mu$mol m\(^{-2}\) s\(^{-1}\) and results in the ratio $J_{\text{max}}/I\'_{\text{max}} = 1.68$. 

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Figure 3.2: Calculated temperature response of $WF_f$ and $WF_j$ with PAR = 2000 $\mu$mol and CO$_2$=350 ppm.

Comparing modelled and measured photosynthesis

Daily totals of measured and modelled net photosynthesis, for different canopy layers are shown in Figure 3.3. Input data are those recorded in and directly adjacent to the branch chambers. The highest explained variance between diurnal measured and modelled net photosynthesis was $R^2 = 0.87$ (chamber 11) and the lowest was $R^2 = 0.61$

Figure 3.3: Comparison of modelled and measured values of daily photosynthesis (dark respiration included) per unit canopy layer. Photosynthesis modelled with variable (closed dot) and constant (open dot) leaf model parameters. Lines are 1:1.
(chamber 14). Using constant model response parameters and assuming always a light dependency where \( \epsilon (V_{\text{max}}) = 36 \), a small decrease in model fit occurred \( (R^2 = 0.53 \) of chamber 14 and \( R^2 = 0.86 \) of chamber 11). It shows that the leaf model can adequately describe the measurements of different seasons and positions in the canopy. It also shows that layer 4 has lower fluxes than layer 3, because of the position of the chamber and shading effects. Because of the reasonable fits at all sampled positions in the canopy with \( \epsilon (V_{\text{max}}) = 36 \), we can see that most of the needles in crowns are light limited at all times, which should be obvious for such a dense forest. The measurements that are analysed do not allow us to make conclusions about CO₂ limitations.

![Graph](image)

**Figure 3.4:** The relationship of equation 1, where \( g_f \) is calculated from leaf transpiration measurements. \( GFAC (=8.0) \) is determined as the slope of the regression with \( g_{\text{min}} (= 3.0 \text{ mmol m}^{-2} \text{ s}^{-1}) \) fixed, \( R^2 = 0.70 \).

The model parameter \( GFAC \) was obtained directly by plotting the relationship of equation 3.1 as shown in Figure 3.4. Assuming ambient \( C_a \) equals \( C_i \) in chamber experiments a constant value of 8.0 provided the best fit to the data. Leaf transpiration data were evaluated as reliable only for relatively short periods with the particular gas exchange techniques that were applied. From this sample of data, we could not establish significant differences between branches occurring in different layers as were found by Sala and Tenhunen (1996) for sun and shade leaves of *Quercus ilex*.
Upscaling results

Without any calibration procedure, the parameterised leaf model was scaled up with STANDFLUX and was independently validated with sapflow measurements. Three model runs of a total year were calculated with STANDFLUX, as shown in Figure 3.5. Run 1 was performed with seasonal trends in LAI and model parameters, run 2 with seasonal trends of LAI and constant model parameters, and run 3 with constant LAI (8.9 m$^2$ m$^{-2}$) and seasonal changes in model parameters. Change of $E_d$ from 61000 to the average of 59800 changed $R_d$ from 0.62 to 1.0 μmol m$^{-2}$s$^{-1}$ at 15°C. Increase of $(NP + 0.5R_d)$ in equation 3.1 leads to an increase in $C_f$ and $g_f$ and resulted in an increase of transpiration of maximally 10%. In run 3, the maximum change of LAI from 10.5 to 8.9 (15% change) decreased transpiration only by 5% via altered radiation extinction.

![Graph](image)

**Figure 3.5:** The ten days averaged modelled transpiration of run 1 with seasonal trends of LAI and leaf model parameters, run 2 with seasonal trend of LAI and constant leaf model parameters, and run 3 with constant LAI and leaf model parameters. Right axis shows the differences between the runs.

Figure 3.6 shows the deviations between measured and modelled daily total transpiration ($R^2=0.60$). Tikta and Bouten (1994) have modelled the same site with a soil water based model. They found a total annual transpiration of 400 mm, which is in agreement with the 380 mm estimated by STANDFLUX. Daily deviations between
measured and modelled transpiration are larger than 10% so they could not be explained by choosing either average or variable parameter settings as described above.

Figure 3.7 shows the daily trend of $GFAC$, which was obtained by optimising $GFAC$ to fit the measured daily sapflow. In our analyses, $GFAC$ varied between 4.8 and 14.5. Change of $GFAC$ from 8 to 14.5 increased transpiration by 45% and net photosynthesis by only 3%, while a change from 8 to 4.8 decreased transpiration by 46% and net photosynthesis by 20%. Thus, photosynthesis is relatively insensitive to $GFAC$ and robust with $GFAC$ changes over a smaller range.

**Analysing the residual errors**

Direct relationships between daily optimal $GFAC$, temperature and soil water are shown in Figure 3.7 and a high correlation between optimal $GFAC$ and temperature is shown in Figure 3.8. Figure 3.7 shows that temperature changes are mirrored in the seasonal course of $GFAC$ and that high temperatures lead to more effective restriction of transpiration. Overall it seems that a single response through relative humidity as used in Ball’s empirical model is not consistent with stomatal responses to water vapour and temperature, which was also discussed by Aphalo and Jarvis (Aphalo and Jarvis, 1991; 1993). Tenhunen et al. (1990, 1994) showed that Ball’s model parameter $GFAC$ changes during periods with soil water stress. Tikta k and Bouten (1994) concluded that short periods with soil water stress occur during summer at the Speulder forest. Direct
Figure 3.7: Seasonal trend of optimised model parameter GFAC (dotted line), daily average temperature and daily modelled water content of the topsoil (0-50 cm).

Figure 3.8: Comparison of daily average temperature with GFAC. Explained variance $R^2=0.72$.

correlation between water content of the soil and the response of the stomata are apparently not observed because time lags between changes in soil water stress and operation of mechanisms that affect stomatal regulation (Figure 3.7). Using the optimised $GFAC$ also changes water use efficiency ($WUE$), shown in Figure 3.9. $WUE$ is defined as the ratio between modelled total daily net photosynthesis and modelled total daily tree transpiration. A potential indication of the validity of varying $GFAC$ is the more constant behaviour of $WUE$ throughout the year (Dewar, 1997).
3.4 DISCUSSION AND CONCLUSION

The inverse modelling approach to obtain gas exchange parameters at the leaf level gives a reasonable estimate of the $J_{\text{max}}/V_{\text{Cmax}}$ ratio of 1.68, which indicates a strong limitation of electron transport capacity on photosynthesis of needles throughout most of the crowns of Douglas Fir. Testing of the model at several levels within the crown suggests that the calibrated leaf model is valid at least within the range of the measurements. The results also indicate that Ball's model parameter $GFAC$ used together with the leaf model and stand light climate routines of STANDFLUX provide a good first approximation of stand level water use (slope of 1 in Figure 3.6). In other applications to date of the Farquhar model combined with the approach of Ball et al., $GFAC$ has been treated as unalterable under non-water-stressed conditions. As such, Sala and Tenhunen (1996) demonstrated the usefulness of $GFAC$ for describing seasonal drying of soil during the Mediterranean summer.

The current analysis considers $GFAC$ to be a more dynamic parameter than previously thought and examines variation in $GFAC$ in the context of leaf mesophyll characteristics, which are seen to vary only slightly and more slowly. The results obtained with the data set from Douglas Fir indicate that better correspondence between sapflow-based stand transpiration estimates and transpiration predicted by STANDFLUX is
obtained when \(GF\cdot AC\) is considered to be influenced directly by either soil water availability or canopy temperature. Simulations of soil moisture in the main root zone indicate that water availability could be reduced enough to account for much of the observed variability in \(GF\cdot AC\). Alternatively, the Ball et al. equation (equation 3.1) assumes that any temperature effects on stomatal conductance are described by temperature effects on \(\text{CO}_2\) gas exchange with a proportional adjustment in stomatal aperture. The present analysis in agreement with arguments of Aphanlo and Jarvis (1991, 1993) suggests that this may not be the case. It has long been known that there are interactive effects of temperature and humidity on stomatal conductance (Hall and Kaufmann 1975). A separate temperature effect on the sensitivity to humidity, which is independent of mesophyll function was demonstrated for epidermal strips with \(P. vulgar\) (Lösch 1977, see also Lösch and Tenhunen 1981).

Other observations in retrospect similarly raise a question about sensitivities of \(GF\cdot AC\) to environmental factors. Sala and Tenhunen (1996) described considerable variation in \(GF\cdot AC\) for leaf level experiments with \(Q. ilex\) during the winter and spring. Only during the drought period, e.g., when regulation via drought overrides other influences, was a tight coupling between predawn water potential and \(GF\cdot AC\) observed. During the spring with frequent rain at montane sites in the Vosges Mountains of France, \(GF\cdot AC\) determined for stands of \(P. abies\) also were quite variable in the range found here for Douglas Fir. It is reasonable that changing temperature as well as water availability at opposite ends of the water continuum could act to modify water distribution and flows, especially at stand level.

One possible conclusion from such observations is that an alternative stomatal model should be used that better captures the essence of stomatal response to these several atmospheric and soil variables. On the other hand, it must be seen whether the phenomena described are demonstrable in a manner consistent enough that multiple effects on \(GF\cdot AC\) are clearly identifiable. Additional factors such as emptying and refilling of trunk storage, direct influences of interception, dying and re-growth of fine roots, etc. also occur which affect forest stand function with complex time dynamics. The practical utility of different stomatal models will change depending on the data sets available for parameterisation and testing.

In general, the modelling effort permitted us to successfully relate ecophysiological studies of gas exchange, tree level measurements of water use, and changes in soil water storage dependent on stand level function. To contribute to questions of climate change,
NEE, and forest carbon sequestering, the current efforts must be extended to accomplish validation with respect to CO₂ fluxes measured via eddy covariance and to examine the specific effects of soil water extraction on soil CO₂ release. The results, however, of the current modelling effort are also important in the context of these other problems. Models are suggested as tools to aid in filling data gaps at long-term measurement sites and they provide also the basis for projecting our knowledge to other situations. While we have touched on questions that concern the relative importance of accurate parameterisation of leaves with particular existing models and the importance of considering new process linkages, we cannot yet say whether the daily optimisation of a parameter such as $G$:AC should be carried out in order to obtain the best annual carbon balance numbers. We can say that it is important to continue with field studies that combine both experimental work and modelling analyses and that the best formulation of stand level models is a theme that requires continued careful attention.

Acknowledgments
The authors thank Fred Bosveld from the Royal Meteorological Institute of the Netherlands for providing the meteorological data of 1989 and Wilma Jans from Alterra, Wageningen, for providing the biomass and physiological measurements.
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32-year old Douglas-fir stand in the Netherlands. 94/1:1-42, IBN-DLO, Wageningen, the Netherlands.


4. ON THE INFORMATION CONTENT OF FOREST TRANSPERSION MEASUREMENTS FOR IDENTIFYING CANOPY CONDUCTANCE MODEL PARAMETERS*

ABSTRACT

Generally, forest transpiration models contain model parameters that cannot be measured independently and therefore are tuned to fit the model results to measurements. Only unique parameter estimates with high accuracy can be used for extrapolation in time or space. However, parameter identification problems may occur as a result of the properties of the data set. The aim of this study is to select environmental conditions that yield a unique parameter set of a canopy conductance model. The Parameter Identification Method based on Localisation of Information (PIMIL) as used to calculate the information content of every individual artificial transpiration measurement. Independent criteria were assessed to localise the environmental conditions, which contain measurements with most information. These measurements do not overlap and the measurements that were not selected do not contain additional information that can be used to further maximise the parameter accuracy. Thereupon, the independent criteria were used to select eddy correlation measurements and parameters were identified with only these measurements. It is finally concluded that PIMIL identifies a unique parameter set with high accuracy, while conventional calibrations on sub-data sets give non-unique parameter estimates.

4.1 INTRODUCTION

Forest transpiration is often modelled in terms of a Single Big Leaf (SBL) based on the Penman-Monteith equation (Monteith, 1965). In a hydrological context, the most important characteristic of the SBL model is its stomatal resistance to transpiration. This resistance is controlled by a number of environmental variables, which can be incorporated in the SBL model by empirical response functions (Jarvis, 1976; Stewart, 1988) containing several model parameters. The best model-to-data fit in terms of Sum of Squared Errors (SSR) was found by calibrating these model parameters to latent heat fluxes (e.g. Dekker et al., 2000; Huntingford, 1995).

* submitted by S.C. Dekker, W. Bouten and F.C. Bosveld to Hydrological Processes
However, only unique parameter estimates with high accuracy can be used for extrapolation in time and space. Concern about parameter identification problems is justified, as shown in for instance soil-vegetation-atmosphere-transfer (SVAT) modelling (e.g. Beven and Binley, 1992; Franks et al., 1997). It is known that the identification of the parameters is dependent on the range and distribution of the data (e.g. Gupta and Sorooshian, 1985; Gupta et al., 1998; Kuczera, 1982; Musters and Bouten, 2000; Sorooshian et al., 1983; Yapo et al., 1998) and dependent on extreme values (Finsterle and Najita, 1998; Legates and McCabe, 1999). A unique parameter estimate with high accuracy is a prerequisite to understand the system, or to find transfer functions that link these unique parameter estimates to independently measured properties and to use the parameter for extrapolation in time and space.

A time series of environmental conditions that control forest transpiration contains many periods with coupled conditions and redundant information while other combinations of conditions may be hardly measured. Coupled boundary conditions, in other words correlated input variables, for describing two separate response functions result in correlated parameters of the response functions. Therefore, measurements with coupled conditions do not contribute to the identification of unique parameters.

The aim of this paper is to select the environmental conditions that yield unique parameter estimates with high accuracy. A forest transpiration SBL model with six parameters was subjected to a sensitivity analysis for a time series of half-hourly simulated transpiration values (artificial measurements). The Parameter Identification Method based on Localisation of Information (PIMLI; Vrugt et al., 2000) was used to calculate the information content of every individual artificial transpiration measurement. The information content of one measurement with respect to a specific parameter represents the standard deviation of the parameter estimate within a preset acceptance criterion. The environmental conditions that contain measurements with most information are localised in the total time series and selected in separate sub-data sets. A sub-data set is selected for the identification of each parameter and the accuracies of the parameter estimates are calculated by only the selected measurements. Thereupon, the total data set is analysed to test whether measurements are available in the data set that can contribute to further maximise the accuracy of the parameter estimates. At last, the accuracy of the parameter estimates is assessed on the basis of true eddy correlation measurements of forest transpiration by using the same selected conditions. These parameter estimates are compared with calibration results that use different randomly selected sub-data sets.
4.2 METHODS AND MATERIALS

SBL Model

It was assumed that the environmental factors that influence canopy conductance (\( g \)) are day number of the year (DOY) to describe changes of Leaf area Index (L), Vapour Pressure Deficit (D), solar radiation (R), air temperature (T) and water content (\( \theta \)):

\[
g = g_{c,ref} f_{L}(DOY) f_{D}(D) f_{R}(R) f_{g}(\theta) f_{T}(T)
\]

where the \( g_{c,ref} \) is a parameter, representing the canopy conductance at reference conditions and \( f \)'s are reduction functions representing the effect of measured environmental conditions (Appendix 4.1). Every reduction function contains one fit parameter. Functional shapes of the response functions are plotted in Figure 4.1 and realistic maximum parameter ranges of the six parameters are shown in Table 4.1. The calibrated soil water model SWIF (Tiktak and Bouten, 1994) was used to calculate the soil water content of the mineral soil.

<table>
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<th>Max</th>
<th>Ref. Value</th>
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</tr>
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<tr>
<td>( a_{T} ) (-)</td>
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<td>0.50</td>
<td>0</td>
</tr>
</tbody>
</table>

Parameter Identification Method based on Localisation of Information (PIMLI)

In general, model parameters are optimised with the total data set by minimising the squared residuals between model results and measurements. If each measurement has its own measurement error \( \varepsilon_{n} \), than the so-called chi-square (\( \chi^{2} \)) function (Press et al., 1988) can be used as objective function:
Figure 4.1: Response functions of Leaf area index (L), Vapour Pressure deficit (D), global radiation (Rg), Temperature (T) and soil water (θ). Solid lines are values of the Speulderbos and dotted lines are parameter ranges.

\[ \chi^2 = \sum_{i=1}^{N} \frac{(y_i - \hat{y}(x_i; a_1, \ldots, a_m))^2}{\varepsilon_i^2} \]  

(4.2)

where \( N \) is the number of measurements, \( y_i \) is the \( i \)th transpiration measurement, \( \hat{y} \) is the modelled transpiration, \( x_i \) the vector of environmental variables and \( a_1, \ldots, a_m \) the vector of model parameters. Although the total data set is used with the \( \chi^2 \) fitting, individual measurements contribute differently to the parameter estimate. Measurements with a low
\[ \varepsilon_i \text{ as well as a high model-sensitivity for a parameter } \frac{\partial f}{\partial (\alpha_1 \ldots \alpha_m)} \text{ contribute heavily to the parameter estimate. However, all information on the sensitivities of these measurements are lumped into one single number, the } \chi^2, \text{ and this number is minimised with the Simplex or the Levenberg-Marquardt method (Press et al., 1988), by optimising all parameters at the same time.} \]

The identification of parameters is dependent on the properties of the data. \textit{PIMIJP} was used to assess the criteria for selecting measurements with highest information content yielding unique parameters with high accuracy (Musters and Bouten, 2000; Vrugt et al., 2000). ‘Artificial measurements’ were simulated with a reference set of parameters to first avoid problems with systematic errors. The confidence interval (\( \alpha \)) of a measurement was used to discriminate between parameter sets, for which a simulation does or doesn’t fit a measurement.

\textit{PIMIJP} is an iterative procedure. Before the iteration starts, a large number of parameter sets is drawn from pre-set parameter ranges using the Latin-Hypercube method (McKay et al., 1979). As a first step of the iteration, the model is run for all these parameter sets. In the second step, at each measuring point, parameter sets are accepted if the difference between the model result (\( y \)) and the measurement is smaller than \( \alpha \). The information content (\( IC \)) of an individual measurement (\( i \)) with respect to a parameter (\( a \)) is defined as:

\[ IC_{i,a} = 1 - \frac{\sigma(a)_i}{\sigma(a)_0} \]  \hspace{1cm} (4.3)

where \( \sigma(a)_i \) is the standard deviation of accepted parameter values at an individual measurement and \( \sigma(a)_0 \) is the standard deviation of the pre-set parameter range at the start. The \( IC \) of a measurement varies with the parameter. A high \( IC_{i,a} \) stands for a measurement that yields a parameter estimate with high accuracy.

The third step of \textit{PIMIJP} is to find criteria that can be used to select environmental conditions that lead to a high \( IC_{i,a} \). In other words, we select boundary conditions where the model sensitivity to a parameter (\( \frac{\partial y}{\partial \alpha} \)) is high, while the model sensitivity to the other parameters (\( \frac{\partial y}{\partial (a_2 \ldots a_6)} \)) is low and the confidence interval of the measurement is small. Once a sub-data set of these specific conditions is localised for a parameter, the mean and standard deviation of accepted parameter values are calculated. Then, in the fourth step new parameter sets are drawn with a normal distribution with this mean and
standard deviation. Hereafter the iteration starts again. As soon as the selection criteria are known for all parameters, only these selected measurements are used and steps two and three are by-passed. The iteration is repeated until the standard deviation of the parameter estimate no longer decreases.

**A case study**

*PIMLI* is first run on a time series of artificial forest transpiration measurements, derived from a calibrated SBL model for a Douglas fir forest (Speuld) in the central Netherlands, near Garderen (Bosveld and Bouten, 1992). The model parameters used to simulate this artificial time series are shown in Table 4.1. Transpiration was simulated with half-hourly micro-meteorological conditions, measured at 36 m above the forest floor, of $R_n$, $R_a$, $D$, $T$ and $u$, in which $R_n$ is net radiation and $u$ is wind speed to calculate the aerodynamic resistance. Only periods with dry canopy and relevant footprint were selected. In total, 1633 half-hourly measurements are available in the period April to November 1995. Eddy correlation was measured with a fast response Ly-α hygrometer and a sonic anemometer-thermometer system (Bosveld et al., 1998). The standard deviation of a half-hourly eddy correlation measurement amounts 15 % of the flux (Bosveld and Bouten, 1992) with an additional offset of 5 W m$^{-2}$. The acceptance criterion ($\alpha$), used as a confidence interval in *PIMLI* to discriminate between fitting and non-fitting simulation runs was derived from errors of the eddy correlation measurements and ranges between 5 and 37 W m$^{-2}$.

For every sub-data set, 10 measurements were selected. After selection of the sub-data sets of artificial transpiration measurements, the sub-data sets of true measurements with the same environmental conditions were used for parameter identification. A comparison is made with the conventional calibration with simplex with the normalised root mean squared error (NRMSE) as objective function. With the Jackknife method (Efron, 1981), 100 calibrations were performed on 100 different sub-data sets containing 300 random sampled measurements. The initial parameter values are randomly drawn from the pre-set parameter ranges of Table 4.1.
4.3 RESULTS AND DISCUSSION

Parameter Identification Method based on Localisation of Information (PIMLI)

The SBL model was run 1000 times with different parameter sets sampled within the parameter ranges shown in Table 4.1. The minimum number of accepted parameter sets was 169 for one of the 1633 measurements. Any combination of parameters was already accepted for 689 measurements. This means that these measurements have no information for identifying the parameters due to their limited reliability. For every parameter and for every measurement the $IC_i(a)$ was calculated and plotted against $DOY$, shown in Figure 4.2. A maximum $IC_i(g_{i,ref})$ of 0.71 was found meaning that the original $g_{i,ref}$ parameter range can be reduced with 71% on the basis of a particular measurement. The $IC_i$'s of the other parameters were much lower.

The next step in PIMLI was to localise environmental conditions that involve measurements with a high $IC_i(a)$. The measurements with high $IC_i(g_{i,ref})$ are found at

![Plot](image)

**Figure 4.2:** Plot of Information Content of every individual measurement of the 6 parameters ($IC_i(a)$) against Day number of the Year ($DOY$).
conditions with a $R_c > 700 \text{ Wm}^{-2}$ but without water stress and after the growing season ($DOY > 170$). Figure 4.3A shows the $IC(g_{cnf})$ of those measurements plotted against $D$. Then measurements with lowest $D$ were selected from Figure 4.3A and were used in the sub-data set for $g_{cnf}$. The mean value of $IC(g_{cnf})$ of all measurements equals 0.15, while the mean $IC_{min}(g_{cnf})$ of the selected subset 0.52, meaning a reduction of 52% of the initial standard deviation. The mean value of $g_{cnf}$ calculated from the subset was $13.9 \times 10^{-3} \text{ m s}^{-1}$ and the standard deviation $3.8 \times 10^{-3} \text{ m s}^{-1}$. A new parameter distribution of $g_{cnf}$ is calculated as a normal distribution with this mean and standard deviation.

In the second iteration, the model was simulated again 1000 times with this new $g_{cnf}$ parameter distribution. Again $IC(a_i)$ of all measurements were calculated. Due to the smaller $g_{cnf}$ parameter range $IC(a_i)$ increased to a maximum of 0.56, a maximum $IC_{min}(a_i)$ to 0.46 and $IC_{min}(a_0)$ to 0.49. The maximum of $IC_{max}(a_i)$ and $IC_{max}(a_1)$ were respectively 0.17 and 0.04. Therefore, measurements were selected during this second iteration to identify $a_i$, $a_R$, and $a_0$. The selection for $a_0$ was made by using only measurements with $R_c > 700 \text{ Wm}^{-2}$ without water stress and after the growing season, shown in Figure 4.3B. Then measurements with highest $D$ were selected and used in the subset. Mean $IC_{min}(a_0)$ was 0.54 with a mean $a_0$ of 0.13 mbar$^{-1}$ and standard deviation of 0.040 mbar$^{-1}$. The selection for $a_R$ was made by using only measurements with $D < 10 \text{ mbar}$, a simulated transpiration flux of more than $25 \text{ W m}^{-2}$ and again without water stress and after the growing season, shown in Figure 4.3C. Only measurements with a simulated transpiration flux of more than $40 \text{ Wm}^{-2}$ were selected because lower values have relatively larger acceptance criteria. The measurements with lowest $R_g$ were selected and used in the subset. Mean $IC_{min}(a_0)$ was 0.38 with a mean $a_0$ of 310 \text{ W m}^{-2} and a standard deviation of 80 \text{ W m}^{-2}. The last selection in this iteration was made for $a_0$ by using only measurements with $D < 10 \text{ mbar}$ and $R_c > 250 \text{ W m}^{-2}$, shown in Figure 4.3D. The measurements with lowest $a_0$ were selected and used in the $IC_{min}(a_0)$. Mean $IC_{min}(a_0)$ was 0.42 with a mean $a_0$ of 30 and a standard deviation of 10.

In the third iteration the three parameters ranges were reduced and the $IC_{max}(a_i)$ and $IC_{max}(a_1)$ were calculated. Maximum $IC_{max}(a_i)$ was 0.26 and maximum $IC_{max}(a_1)$ was only 0.05. The selection for $a_i$ was made by using only measurements during the growing season (around $DOY \approx 130$) with $D < 10 \text{ mbar}$, shown in Figure 4.3E. The measurements with highest $R_g$ are selected from this figure and used in the subset. Mean $IC_{min}(a_i)$ was 0.25 with a mean $a_i$ of 0.29 and a standard deviation of 0.13.
Figure 4.3: The Information Content of every measurement ($IC$) of every parameter on the $y$-axis against different daily environmental conditions ($x$-axis). Only measurements after selection are plotted. The 10 best measurements are plotted as black dots.

In the fourth iteration, with five reduced parameter ranges, the $IC_{\text{at}}$ was calculated. The maximum $IC_{\text{at}}$ was 0.10. The selection of measurements for $\text{at}$ was made by using measurements with low $T$ and with a simulated transpiration flux of more than 40 W m$^{-2}$, because measurements with lower values have relatively larger acceptance criteria (Figure 4.3F).

In summary, the selection of the six parameters is based on measurements with a high signal to noise ratio, a high sensitivity to the selected parameter ($\partial y/\partial a$) and a low
sensitivity to the other five parameters. Due to the low sensitivity to the other parameters, the selected measurements are the most uncoupled situations available in the total data set. The selected sets of measurements do not overlap.

Parameters were finally identified with these six sub-data sets. All parameter ranges were reduced simultaneously if an $IC_{\text{subtot}}$ of more than 5% was calculated. Figure 4.4 shows the $IC_{\text{subtot}}$ of the six parameters against the number of iterations. After ten iterations, the $IC_{\text{subtot}}$ were at their maximum. Again fastest identification was obtained with $g_{\text{ref}}$ and slowest identification with $dT$. Final feasible parameter variances are shown in Table 4.2.

$PIMLI$ was only performed on the stomatal conductance parameters and not on the aerodynamic conductance parameter. The sensitivity of the roughness length, that calculates the aerodynamic conductance, is very low for the prediction of transpiration. Therefore, this parameter was not taken into account.

| Table 4.2: Initial standard deviation of parameters at the start of the iterations and after ten iterations. Last column are final mean values. |
|-----------------|-----------------|-----------------|
| Start $\sigma$ | End $\sigma$ | Mean |
| $g_{\text{ref}}$ (m s$^{-1}$) | $7.1 \times 10^{-3}$ | $1.1 \times 10^{-3}$ | $13.8 \times 10^{-3}$ |
| $a_T$ (mbar)$^{-1}$ | 0.086 | 0.011 | 0.120 |
| $a_{\text{rg}}$ (W m$^{-2}$) | 130 | 33.2 | 280 |
| $a_0$ (s$^{-1}$) | 17.3 | 2.82 | 29.0 |
| $a_1$ (s$^{-1}$) | 0.173 | 0.056 | 0.303 |
| $a_T$ (s$^{-1}$) | 0.29 | 0.14 | 0.02 |

Information content of not selected measurements

The total data set was analysed to test whether other measurements can contribute to further maximise the accuracy of the parameter estimates. In total 1000 parameter sets were drawn within the final parameter ranges obtained by $PIMLI$ and were run on the total data set. A decrease of the standard deviations of every parameter for every measurement could not be found, meaning that other measurements do not contain more information to identify the parameters.
Figure 4.4: Increase of the Information Content of the sub-data set ($IC_{subset}$) of the six parameters against number of iteration. $IC_{subset}$ is constant after 10 iterations.

Hypothetically, the accuracy of the parameter estimates could be maximised further by extrapolating the trends of Figure 4.3 to a higher $IC$. Extrapolation of the $g_{ref}$ trend (Figure 4.3A) to a smaller $D$ in combination with high $R_g$ would give a higher accuracy. However, these conditions are very rare and only occur just after fog or rain. A contribution of evaporation to the measured vapour flux then cannot be excluded. Extrapolation of the $a_D$ trend (Figure 4.3B) would not lead to a higher $IC$, while a higher accuracy for $a_Rg$ (Figure 4.3C) would not be found because low values of $R_g$ correspond to low flux values with relatively high uncertainty. The poor identifications of $a_\theta$ (Figure 4.3D) and $a_T$ are a result of the limited number of measurements with respectively low water content and high radiation around DOY 130. Finally, $a_T$ would only be better identified from measurements with low $T$ and high $R_g$, which do not occur in the considered forest. As a result, we agree with Gupta et al. (1998) who pointed out that parameter identification problems will not simply disappear with the availability of more measurements.

Accuracy of parameter estimates from eddy correlation measurements

PLMLI was run on simulated artificial data to show that the original parameter values are retrieved from selected subsets. The 60 selected measurements were also used to
assess the parameter values from true eddy correlation measurements. Results of the mean estimates and standard deviation are shown in Table 4.3. Because true measurements can suffer from systematic errors, a parameter set is accepted if the simulation fits 7 of the 10 measurements within the confidence interval, based on the standard deviation of the eddy correlation measurement. With the PIMLI parameter set, a NRMSE of 0.3665 was calculated for the total data set. Calibration of all parameters with the Simplex algorithm by using all measurements results in a NRMSE of 0.3645. The parameter values are those of the reference set (Table 4.1, column 3). If the total data set is used, the model can compensate systematic errors due to a wrong parameterisation. The parameter set obtained from the total data set fits within the PIMLI parameter ranges, although a relative large difference in \( a_t \) is observed. This large difference can be caused due to a wrong parameterisation caused by the limited number of data to identify \( a_t \).

Table 4.3: Final mean values and standard deviations of parameter estimates from eddy correlation measurements using PIMLI and the conventional simplex calibration.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>PIMLI Mean</th>
<th>PIMLI ( \sigma )</th>
<th>Conventional calibration Mean</th>
<th>Conventional calibration ( \sigma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g ) (m s(^{-1}))</td>
<td>13.6 ( 10^3 )</td>
<td>1.6 ( 10^3 )</td>
<td>13.2 ( 10^3 )</td>
<td>2.3 ( 10^3 )</td>
</tr>
<tr>
<td>( a_1 ) (mbar(^{-1}))</td>
<td>0.125</td>
<td>0.018</td>
<td>0.123</td>
<td>0.027</td>
</tr>
<tr>
<td>( a_2 ) (W m(^{-2}))</td>
<td>292</td>
<td>45.9</td>
<td>284</td>
<td>66.0</td>
</tr>
<tr>
<td>( a_9 ) (-)</td>
<td>28.3</td>
<td>4.7</td>
<td>31.8</td>
<td>4.9</td>
</tr>
<tr>
<td>( a_t ) (-)</td>
<td>0.356</td>
<td>0.061</td>
<td>0.309</td>
<td>0.125</td>
</tr>
<tr>
<td>( a_T ) (-)</td>
<td>0.0</td>
<td>0.3</td>
<td>0.389</td>
<td>0.7625</td>
</tr>
</tbody>
</table>

The results of the conventional simplex calibration with the Jackknife method, by minimising the NRMSE, on 100 sub-data sets containing 300 random sampled measurements are shown in Table 4.3. The fit-error was calculated by running the parameter set on the total data set and the accuracy was calculated by the standard deviation of the calibrated parameter values. The uncertainty of the parameter sets obtained with the conventional method is not taken into account, but is in the same order of magnitude as found with PIMLI. The accuracy of the parameter estimates is smaller and the fit error is larger than calculated with PIMLI. This large variety in parameter estimates is caused due to the properties and distribution of the data used for calibration,
and due to non-unique solutions. Using 100 sub-data sets containing 60 random sampled measurements leads to a 10 times larger standard deviations of the parameter ranges as found with PLMIJ.

As a result, PLMIJ gives one unique parameter set, with a certain accuracy, while the results of the conventional simplex calibration leads to 100 'best' parameter sets. To improve the understanding of the system, we want in further applications to link independently measured system properties to parameter values. For those links, it is a prerequisite to have unique parameter estimates.

**4.3 CONCLUSIONS**

Optimal environmental conditions with 'artificial' measurements that yield unique parameter estimates with high accuracy of a Single Big Leaf model were selected with the Parameter Identification Method based on Localisation of Information (PLMIJ). It was shown that every measurement has a different information content with respect to each of the model parameters. For every parameter a separate sub-data set was selected involving 10 measurements with the highest information content. These sets of measurements are independent and do not overlap. It was shown that the remaining measurements do not contain more information for identifying the parameters. A higher accuracy of the parameter estimates can only be reached with extreme situations with measurements with lower $D$ and high $R_s$, measurements with lower soil water content or with more measurements with high $R_s$ during the growing season. Consequently, identification problems will not simply disappear with the availability of more measurements. Parameter estimates based on PLMIJ analyses of true Eddy-correlation measurements are compared with conventional calibrations using different sub-data sets. It is finally concluded that PLMIJ identifies unique parameters with high accuracy, while the normal calibrations give a larger variation in parameter values.
APPENDIX 4.1: Response functions for stomatal conductance functions

A piece-wise linear form for the growth curve \( f_i \) was assumed, that starts at DOY 130 and ends at DOY 180:

\[
\begin{align*}
    f_i'(DOY) &= 1 - a_{i1}(DOY + 185)/315 & 0 \leq DOY \leq 130 \\
    f_i'(DOY) &= 1 - a_{i1}(180 - DOY)/50 & 130 \leq DOY \leq 180 \\
    f_i'(DOY) &= 1 - a_{i1}(DOY - 180)/315 & 180 \leq DOY \leq 365
\end{align*}
\]

(4.11)

where \( a_i \) is the free parameter to be optimised.

The response function for \( D (f_D) \) is:

\[
f_D(D) = \frac{1}{1 + a_D(D - D_r)}
\]

(4.12)

where \( a_D \) (mbar\(^{-1}\)) is the free parameter and \( D_r \) (mbar) a reference \( D \), here chosen at 4.6 mbar at which \( f_D \) becomes 1. For \( D < 1.5 \) mbar the response function was set to \( f_D(D = 1.5 \) mbar).

The light response function \( (f_R) \) is described with:

\[
f_R(R) = \frac{R_g(1000 - a_Rg)}{R_g(1000 - 2a_Rg) + a_Rg 1000}
\]

(4.13)

where \( a_Rg \) (Wm\(^{-2}\)) is the free parameter and 1000 is the maximum radiation (W m\(^{-2}\)).

The response function for \( T (f_T) \) is:

\[
f_T(T) = 1 - a_T + a_T(\frac{40 - T}{40 - T_{opt}})^{2-\pi/20}(\frac{T}{T_{opt}})^{1-20}
\]

\[0 \leq T \leq 40^\circ\]

(4.14)

where \( a_T \) is the free parameter and \( T_{opt} \) is the optimum temperature set to 25\(^\circ\)C.

The soil water content \( (f_b) \) is described with:

\[
\begin{align*}
    f_b(\theta) &= 1 & \theta \geq 0.072 \\
    f_b(\theta) &= 1 - a_b(0.072 - \theta) & \theta < 0.072
\end{align*}
\]

(4.15)

where \( a_b \) (-) is the free parameter and 0.072 represents the so called reduction point, e.g.
the starting level at which soil water stress occurs.

REFERENCES


Tiktak, A. and Bouten, W., 1994. Soil water dynamics and long-term water balances of a Douglas fir


5. IDENTIFICATION OF RAINFALL INTERCEPTION MODEL PARAMETERS FROM MEASUREMENTS OF THROUGHFALL AND FOREST CANOPY STORAGE*

ABSTRACT

This study aims at identifying the parameters of a rainfall interception model from throughfall and canopy storage measurements using PIAIIJ (Parameter Identification Method based on the Localisation of Information). It is shown that every rainfall event and both measurement types contain different information with respect to the model parameters. The uniqueness of model parameters turned out to be much better when identified from storage measurements compared to throughfall measurements. Independent throughfall and canopy storage measurements were both better predicted with parameters calibrated on storage measurements. From throughfall measurements, exclusively the interception fraction could be identified with comparable accuracy as with canopy storage measurements.

5.1 INTRODUCTION

Interception and evaporation of rainfall are important hydrological processes in forest ecosystems. In the past, several physically based (Gash, 1979; Rutter et al., 1971) and stochastic models (Calder, 1986) were developed to simulate throughfall, evaporation and canopy storage. New model extensions, based on these models, were suggested by many authors (Calder, 1996; Gash et al., 1995; Valente et al., 1997).

If only long-term values of interception losses, measured over a range of storm sizes and durations, are available only very simple models can be constructed with a minimum of parameters (Calder and Hall, 1997). It is evident that a too complex model generates problems for the identification of unique parameters with high accuracy. It is also known that the identification of model parameters is far more dependent on the information content of the data than the amount of data (Gupta and Sorooshian, 1985; Gupta et al., 1998; Kuczera, 1982; Sorooshian et al., 1983; Yapo et al., 1998). A unique parameter set with high accuracy is a prerequisite to understand the system, or to find transfer functions

* submitted to Water Resources Research by S.C. Dekker and W. Bouten
that link these unique parameters to independently measured properties and to use the parameters for extrapolation in time and space. Recently, a new Parameter Identification Method based on the Localisation of Information (PIMI) (Musters and Bouten, 2000; Vrugt al., 2000) was developed to assess the information content of measurements. The idea of this method is that each measurement in a time series contains a different amount of information with respect to a specific model parameter. Only measurements with high information content are used to identify that parameter.

In most studies, model parameters of a rainfall interception model were identified by using only throughfall measurement (Aboal et al., 1999; Jetten, 1996; Loustau et al., 1992). However, other measurement types can also be used to identify these parameters. For instance, Bouten et al. (1991) have used storage canopy measurements to identify the model parameters of a four-layer rainfall interception model and recently, Gash et al. (1999) have measured evaporation from wet canopies with measurements using the combined eddy correlation/energy balance method.

Throughfall, canopy storage and evaporation processes are all dependent on each other. If rainfall interception model parameters are identified from a time series in which all these three processes occur at the same time, then a dependency between the parameters can be found. In this study, the uniqueness and accuracy of the rainfall interception model parameters are assessed by using the information content of throughfall and canopy storage measurements. Therefore, a simple four-parameter model is used. PIMI is applied to assess the criteria for selecting measurements with highest information content yielding unique parameter with high accuracy. Artificial simulated measurements were used to first avoid problems with systematic errors. As soon the selection criteria are known for all parameters, true measurements were used to identify the parameters.

5.2 MATERIALS AND MEASUREMENTS

Research site

The research site, Speuld, is located in a 2.5 ha Douglas fir forest stand, in the central Netherlands, near Garderen. The stand is dense with 780 firs ha⁻¹ without understorey and planted in 1962. Average tree height between is 18 m and the single sided leaf area in summer ranges from 9.0 m² m⁻² to 12.0 m² m⁻² (Jans et al., 1994). The 30-year average rainfall is 834 mm y⁻¹ and is evenly distributed over the year.
Measurements

Gross rainfall was measured every 2.5 minutes just above the forest with two funnels with a resolution of 0.02 mm rainfall, and additionally with one funnel in a large clearing 0.8 km away with a resolution of 0.05 mm of rainfall. Half-hourly measurements of meteorological driving variables were measured by the Royal Meteorological Institute of the Netherlands (KNMI) (Bosveld et al., 1998) on a 36 meter high guyed mast to calculate the potential evaporation ($E_o$) (Monteith, 1965). Stemflow was never observed.

Throughfall was measured every 2.5 minutes with 11 automatic funnels (480 cm$^2$) from July to September and with 18 automatic funnels from October to December. The coefficient of variation (CV) of the throughfall measurements is large due to spatial variability between the funnels and decreases with the amount of throughfall (Figure 5.1). But even with mean weekly values, up to 70 mm throughfall, a minimum CV of 20% was found. The measurement resolution of one funnel was 0.02 mm. Smaller values of throughfall, plotted in Figure 5.1, were calculated by averaging the funnels.

Water storage was measured using a microwave transmitter and receiver (Bouten and Bosveld, 1991; Bouten et al., 1991) mounted in a hoist attached to towers standing 15 m apart. Every half-hour six complete vertical scans were carried out during which 20 measurements per second were performed. From April to December 1989, the system was

![Figure 5.1: The coefficient of variation (CV) of the mean automatic throughfall measurements, averaged over 0.25 hour, 1 hour, 3 hour, 1 day and 7 day.](image)

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operational for about 88% of the total time. Estimated measurement error on average half-hourly measurements was 0.04 mm (Bouten et al., 1996).

Model

Bouten et al. (1996) have modelled the canopy water storage by using a numerical multi-layer interception model based on the Rutter Model (Rutter et al., 1971). In this study, for simplicity, a single-layer model was used. The water balance is calculated according to:

\[
\frac{\Delta V}{\Delta t} = I - D - E;
\]  

(5.1)

where \( V \) (mm) is the water storage in the canopy, \( t \) (d) is time, \( D \) (mm d\(^{-1}\)) is drainage rate and \( E \) (mm d\(^{-1}\)) is the evaporation rate. The water interception rate, \( I \) (mm d\(^{-1}\)), is calculated with:

\[ I = a \ P \]  

(5.2)

where \( a \) is the interception efficiency parameter and \( P \) (mm d\(^{-1}\)) is the gross rainfall. It is assumed that drainage only occurs if \( V \) is larger than the storage capacity \( c \) (mm) and for simplicity a linear threshold model was used:

\[ D = b \ ( S - c ) \]  

(5.3)

in which \( b \) (d\(^{-1}\)) is an empirical drainage parameter. Evaporation rate is calculated with

\[ E_E = d \ ( E_0 \ \frac{V}{c} ) \]  

(5.4)

in which \( d \) is an empirical evaporation efficiency and \( E_0 \) is determined by (Monteith, 1965):

\[ E_0 = \frac{R_n + \rho C_p D(z_e + z_w)}{\lambda (s + \gamma)} \]  

(5.5)

where \( s \) the slope of the saturated water vapour curve, \( R_n \) the net radiation, \( \rho \) the density of air, \( C_p \) the specific heat capacity of air, \( D \) the vapour pressure deficit, \( \gamma \) the
psychrometer constant, \( g \); the aerodynamic resistance, \( g \); the excess resistance and \( \lambda \) is the latent heat of vaporisation.

The model contains four parameters that must be identified. Bouten et al. (1996) found a yearly trend of the optimised \( \epsilon \) model parameter, which reflects the biomass dynamics.

**Parameter Identification Method based on Localisation of Information (PIMLI)**

The identification of parameters is dependent on the properties of the data, meaning that parameter identification problems will not simply disappear with the availability of more measurements. PIMLI was used to establish the criteria for selecting measurements with highest information content yielding unique parameters with high accuracy (Musters and Bouten, 2000; Vrugt et al., 2000). ‘Artificial measurements’ were simulated with a reference set of parameters, deduced from Bouten et al. (1996), to first avoid problems with systematic errors. In the identification procedure, PIMLI uses the confidence interval \( (\alpha) \) of a measurement was used to discriminate between parameter sets, for which a simulation does or does not fit a measurement.

**PIMLI** is an iterative procedure. Before the iteration starts, a large number of parameter sets is drawn from pre-set parameter ranges using the Latin-Hypercube method (McKay et al., 1979). As a first step of the iteration, the model is run for all these parameter sets. In the second step, at each measuring point, parameter sets are accepted if the difference between the model result \( (y) \) and the measurement is smaller that \( \alpha \). The information content \( (IC) \) of an individual measurement \( (\beta) \) with respect to a parameter \( (\beta) \) is defined as:

\[
IC_{\beta}(\beta) = 1 - \frac{\sigma_{\beta}(\beta)}{\sigma(\beta)_b}
\]

(5.6)

where \( \sigma(\beta)_b \) is the standard deviation of accepted parameter values at an individual measurement and \( \sigma(\beta)_b \) is the standard deviation of the pre-set parameter range at the start. The \( IC \) of a measurement varies with the parameter. A high \( IC_{\beta}(\beta) \) stands for a measurement that yields a parameter estimate with high accuracy.

The third step of PIMLI is to find criteria that can be used to select conditions that lead to a high \( IC_{\beta}(\beta) \). In other words, we select conditions where the model sensitivity to a parameter \( (\partial y/\partial \beta) \) is high while the model sensitivity to the other parameters
(\frac{\partial v}{\partial (P_2, \ldots, P_4)}) is low and the confidence interval of the measurement is small. Once a subset with these specific conditions is localised for a specific parameter, the mean and standard deviation of accepted parameter values are calculated. Then, in the fourth step, new parameter sets are drawn with a normal distribution with this mean and standard deviation. Hereafter the iteration starts again. As soon as the selection criteria are known for all parameters, true measurements instead of 'artificial measurements' are used and steps two and three are by-passed. The iteration is repeated until the standard deviation of the parameter estimate no longer decreases.

Parameter Identification with throughfall and canopy storage measurements

As can be expected from equation 5.1-5.4, the throughfall, canopy storage and evaporation processes and parameters can be separated in time. The \( a \)-parameter can be derived from rainfall and throughfall or storage measurements and is independent of other parameters if storage has not yet reached its saturation point (no drainage) and if \( E_0 \) is negligible. As the measurement errors decrease with increasing precipitation, this means that the \( a \)-parameter is best identified from measurements with low evaporation during night-time and just before saturation. However, the maximum accumulated precipitation until the storage reaches saturation, is dependent on the lowest possible value of the \( c \)-parameter and the maximum value of the \( a \)-parameter \((P < \epsilon_{\min} / a_{\max})\). This means that only measurements at the start of the event can be used for the identification of the \( a \)-parameter as long as the values of these two parameters are uncertain.

Equation 5.1 and 5.3 show that canopy water storage measurements reflect the \( c \)-parameter and are independent to drainage or evaporation in periods after heavy rainfall \((P > \epsilon_{\max} / a_{\min})\) has ceased and when \( E_0 \) is negligible. The difference between accumulated precipitation and throughfall at that point determine the \( c \)-parameter. The uncertainty of the parameter value is dependent on the \( a \)-parameters, the uncertainty of the throughfall measurement and the uncertainty of the evaporation. As the uncertainty of throughfall measurements increases with higher precipitation amounts, events that are just large enough to saturate the canopy with minimal drainage are optimal for identification of the \( c \)-parameter.

Drainage is only active if canopy storage is above saturation. Equation 5.3 shows that \( S \) and \( c \) must be known to be able to identify the \( b \)-parameter. With throughfall measurements only, \( S \) is not known and therefore \( b \) can only be identified if storage measurements are available. The \( b \)-parameter is best identified at low \( E_0 \) and high rainfall. [End of text]
intensities.

By the end of a rain event the difference between precipitation and throughfall equals the sum of the storage capacity and the cumulative evaporated amount. The $d$-parameter also determines the slope $\partial S/\partial t$ in a drying time series. It can best be identified during conditions without rain starting from the point that $I_n$ increases to a high $I_{in}$.

At first, PIMLI is applied on rain events with simulated throughfall and storage, calculated with the reference parameter set of Table 5.1. In this first step, the above hypotheses are tested, selection criteria are assessed and PIMLI is used to find out if the reference parameter set is retrieved. To calculate the $IC(p)$, 1000 parameter sets were drawn within the parameter ranges of Table 5.1 (last 2 columns). The confidence interval for the simulations was based on the function from Figure 5.1 for throughfall measurements and 0.04 mm for storage measurements (Bouten et al., 1996).

**Table 5.1**: Model parameters calculated by Bouten et al. (1996) for total year and for Day Number of the Year (DOY) 258, 211. Last two columns are minimum and maximum values of parameters.

<table>
<thead>
<tr>
<th></th>
<th>average</th>
<th>DOY258</th>
<th>DOY211</th>
<th>min</th>
<th>max</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.83</td>
<td>0.83</td>
<td>0.83</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>b (d)</td>
<td>135</td>
<td>135</td>
<td>135</td>
<td>1</td>
<td>1000</td>
</tr>
<tr>
<td>c (mm)</td>
<td>2.07-2.58</td>
<td>2.13</td>
<td>2.50</td>
<td>0.5</td>
<td>5</td>
</tr>
<tr>
<td>d</td>
<td>0.79</td>
<td>0.79</td>
<td>0.79</td>
<td>0.1</td>
<td>2.0</td>
</tr>
</tbody>
</table>

After the selection criteria are assessed and tested for all parameters, true measurements of throughfall and canopy storage are used to identify the model parameters and to calculate their accuracy.

Finally, the accuracies of model predictions ($\sigma_{\text{model}}$) are evaluated on the basis of time series of measurements that were not used for the calibration. Model accuracies for both throughfall and canopy storage are calculated by drawing parameter sets within the parameter ranges obtained by both throughfall and canopy storage calibration.

### 5.3 RESULTS

**Accuracy of the interception (a) and storage capacity (c) parameter estimates**

The rain event during night at day number of the year (DOY) 257 has the best characteristics to identify the parameters $a$ and $c$. Figure 5.2A shows the cumulative
precipitation and the cumulative potential evaporation for this period. Accumulated throughfall and storage, simulated with the parameter set of Table 5.1 are shown in Figure 5.2B. For this reference simulation, the storage reached saturation ($Y = e$) at a cumulative precipitation of 2.56 mm ($\bar{c} / a$).

The first PIMLI iteration starts with the parameter ranges of Table 5.1. The $IC(a)$ and $IC(c)$ of throughfall measurements was calculated and plotted in Figure 5.2C (thick lines). The $IC(a)$ increases to a maximum of 0.85, with a mean value of the $a$-parameter ($\mu_a$) of 0.83 and standard deviation ($\sigma_a$) of 0.0402. In the same iteration, the minimum value of the $c$-parameter range increases from 0.5 to 1.45 mm. As a result, the canopy storage reaches saturation at a cumulative precipitation of at least 1.7 mm ($c_{\min} / a_{\min}$). At this point the $IC(a)$ equals 0.82, with $\mu_a=0.83$ and $\sigma_a=0.0456$. In the second iteration of PIMLI, $IC(a)$ and $IC(c)$ were calculated again and plotted in Figure 5.2C (thin lines). The $a$-parameter is best identified at a cumulative precipitation of 2.08 mm ($c_{\min} / a_{\min}$), denoted as a dot in Figure 5.2C. The $c$-parameter is best identified after rain at the end of the period, also denoted as a dot in Figure 5.2C. Final parameter estimates and accuracies are shown in Table 5.2. By using these artificial measurements, the original reference parameter values were retrieved.

True measured throughfall is shown in Figure 5.2D. From the simulations that fit within the $\alpha$ of the two selected cumulative points, mean and standard deviations of the $a$ and $c$-parameter were calculated (Table 5.2). Standard deviations of the model results and the measurement accuracy are plotted in Figure 5.2D. Parameter ranges are slightly larger than obtained with the sensitivity analysis as the $CI'$ is higher at low cumulative throughfall amounts than used with the analysis of artificial measurements.

Table 5.2: Mean parameter estimates ($\mu$) and accuracy ($\sigma$) using artificial (artf) and true measurements (meas) for DOY 258 for both throughfall and canopy storage calibration.

<table>
<thead>
<tr>
<th></th>
<th>$\mu_{artf}$</th>
<th>$\sigma_{artf}$</th>
<th>$\mu_{meas}$</th>
<th>$\sigma_{meas}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Throughfall</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a$</td>
<td>0.83</td>
<td>0.035</td>
<td>0.78</td>
<td>0.08</td>
</tr>
<tr>
<td>c (mm)</td>
<td>2.15</td>
<td>0.35</td>
<td>2.01</td>
<td>0.55</td>
</tr>
<tr>
<td><strong>Canopy Storage</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a$</td>
<td>0.823</td>
<td>0.027</td>
<td>0.83</td>
<td>0.046</td>
</tr>
<tr>
<td>c (mm)</td>
<td>2.18</td>
<td>0.036</td>
<td>2.15</td>
<td>0.040</td>
</tr>
</tbody>
</table>
With the same rain event, the $a$ and $c$ parameters were also identified from storage measurements. The $IC(a)$ and $IC(c)$ of the first PI MIL iteration are plotted in Figure 5.2E. The $IC(a)$ was calculated from the storage increase determined from the start of the rainfall event. The confidence interval of 0.04 mm was doubled because two measurements were now used. At a cumulative precipitation of 0.5 mm ($c_{min} / a_{max}$), the $IC(a)$ was 0.85, with a $\mu_a = 0.825$ and $\sigma_a = 0.037$. In the second iteration the maximum $IC(c)$ equalled 0.97 with $\mu_c = 2.15$ and $\sigma_c = 0.04$.

The best identification of the $a$-parameter is reached at a cumulative precipitation of 2.38 mm ($c_{min} / a_{max}$). All measurements between a cumulative precipitation of 0.5 and 2.38
mm were used to identify $a$. The best identification of $c$ is achieved with measurements without precipitation and with a low $E_0$ of 4 mm d$^{-1}$. After DOY 258.4 the $IC(c)$ decreases due to the increase of $E_0$. Selected measurements are plotted in Figure 5.2E and results are shown in Table 5.2. Again the original reference parameter values were retrieved.

For these two selected periods, the parameter estimates and accuracies were again calculated with the true measurements (Table 5.2). Standard deviation of the model results are plotted in Figure 5.2F.

**Accuracy of the drainage (b) and evaporation efficiency (d) parameter estimates**

The drainage parameter ($b$) and evaporation efficiency parameter ($d$) were identified with the rain event at DOY 211. Cumulative precipitation and potential evaporation are shown in Figure 5.3A. Reference simulations of cumulative throughfall and canopy storage, again simulated with the reference parameters of Table 5.1, are shown in Figure 5.3B. In the first PIMLI iteration, only information on the $a$ and the $c$-parameters was found from throughfall measurements (Figure 5.3C). However, due to higher drainage amounts, the $IC(c)$ was now much lower.

In the second iteration, the $IC(b)$ and $IC(d)$ remained zero, even with the $a$ and $c$ accuracy obtained from the first analyses. As expected from equation 5.3, $b$ cannot be identified if $S$ is unknown. At the end of the rain event, total simulated reference evaporation was 2.96 mm while the measurement error of throughfall was 6.7 mm. On half-hourly basis, maximum $E_0$ during rain was only 10 mm d$^{-1}$ while it can reach 80 mm d$^{-1}$. Using equation 5.4 and assuming an $S/c$ of 1.0 and 0.1<$d$<2, the evaporation was between 0.02 and 0.41 mm for a half-hourly measurement and was lower than the measurement error. Figure 5.3D shows the measured cumulative throughfall and model results. It is shown that the confidence interval for the measurements is even larger than the model uncertainties, meaning that the initial parameter ranges of $b$ and $d$ were chosen too small.

From canopy water storage measurements, however, far more information was found. In the first PIMLI iteration, information on the $a$-parameter was found again during the wetting stage of the canopy. Dots are plotted at the position with cumulative precipitation between 0.5 and 2.4 mm, shown in Figure 5.3E. In the second iteration, the $IC(c)$ was again at its maximum after rain and with a low $E_0$ of 4 mm d$^{-1}$ (around DOY 212.2). Measurements that satisfy the criteria are plotted as dots in Figure 5.3E and results are shown in Table 5.3.
Figure 5.3: Rain event at DOY 211: For explanations see text. Figure (B), throughfall is divided by 5. Lines in (C) are first iteration. In (D) and (F), dots are measurements, line is model and dotted lines are σ of model results.

In the third PI MILJ iteration, information was found for b and d, shown in Figure 5.3E. The IC(b) was at its maximum at periods with a saturated canopy and with precipitation rates of more than 50 mm d⁻¹ for a half-hourly measurement. Measurements are plotted as dots in Figure 5.3E. The IC(d) is at its maximum during the drying cycle of the canopy storage and is calculated by ΔS, starting from the point that E₀ is larger than 4 mm d⁻¹. Half way the drying cycle, at the maximum first derivative, the information is at its maximum. Final parameter estimates and accuracy are shown in Table 5.3. Again, the reference parameter values were retrieved.
Table 5.3: Mean parameter estimates (μ) and accuracy (σ) using artificial (art) and true measurements (meas) for DOY 211 for both throughfall and canopy storage calibration.

<table>
<thead>
<tr>
<th></th>
<th>μ_{art}</th>
<th>σ_{art}</th>
<th>μ_{meas}</th>
<th>σ_{meas}</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Throughfall</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>b  (d⁻¹)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>c  (mm)</td>
<td>2.75</td>
<td>0.96</td>
<td>2.60</td>
<td>1.05</td>
</tr>
<tr>
<td>d</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td><strong>Canopy Storage</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>0.823</td>
<td>0.027</td>
<td>0.83</td>
<td>0.046</td>
</tr>
<tr>
<td>b  (d⁻¹)</td>
<td>135</td>
<td>15</td>
<td>170</td>
<td>52</td>
</tr>
<tr>
<td>c  (mm)</td>
<td>2.50</td>
<td>0.041</td>
<td>2.70</td>
<td>0.062</td>
</tr>
<tr>
<td>d</td>
<td>0.79</td>
<td>0.025</td>
<td>0.96</td>
<td>0.15</td>
</tr>
</tbody>
</table>

True canopy storage measurements are plotted in Figure 5.4F. With the same selection criteria, the parameter ranges were calculated from true measurements. Results are shown in Table 5.3 and in Figure 5.4F. The measurements during the wetting stage and the steady state period, dealing with the $a$ and $c$-parameters, fit all within the accuracy range. However, during the first drainage peak, the model can only fit the measurements with $\mu_\delta = 900$ d⁻¹ and $\sigma_\delta = 130$ d⁻¹, while the other two peaks can only be described with $\mu_\delta = 170$ d⁻¹ and $\sigma_\delta = 52$ d⁻¹. It is also shown that the simulated storage is lower than the measurements at the end of the drying cycle. However, to fit this part, $\mu_d = 0.6$ must be used while then large deviations were found halfway the drying period.

**Model evaluation**

The parameter sets $p_{\text{through}}$, obtained from throughfall measurements, and $p_{\text{stor}}$, obtained from storage measurements, are both evaluated on a time series of measurements containing 389 half-hourly measurements between DOY 238 and 285. A linear decreasing trend of the $c$-parameter between the calibrated values at DOY 211 and 258 was used (Bouten et al., 1996). Accumulated throughfall is predicted with both parameter sets. Small differences in model performance were found, resulting for $p_{\text{through}}$ in $R^2 = 0.664$ and for $p_{\text{stor}}$ in $R^2 = 0.684$. The model error ($\sigma_{\text{model}}$), calculated as the mean $\sigma$ at the end of the period was 10.6 mm with $p_{\text{through}}$ and 4.2 mm with $p_{\text{stor}}$, while the
measurement error ($\sigma_{\text{meas}}$) was 10.3 mm. This means that the model with $p_{\text{stor}}$ can estimate throughfall more accurately than as it was measured. However, due to the dominating $\sigma_{\text{meas}}$, the model performances were almost equal. Canopy water storage was also predicted for the same period. Large differences in model performance were found, resulting for $p_{\text{through}}$ in $R^2 = 0.825$ and for $p_{\text{stor}}$ in $R^2 = 0.912$. The $\sigma_{\text{model}}$ for $p_{\text{through}}$ is 0.42 mm and for $p_{\text{stor}}$ is 0.12 mm.

5.4 DISCUSSION

As shown in the above analysis, parameters can be estimated more accurately with storage measurements. From canopy storage measurements, Bouten et al. (1996) found a yearly trend of the calibrated $c$-parameter following the biomass dynamics. With throughfall measurements, however, this trend can never be established. In the total data set of 158 days, only six suitable rain events with a cumulative precipitation between 2.5 and 4.0 mm were found. The $\mu$, of these events ranges from 1.55 to 2.75 mm with a mean $\sigma$, of 0.65, while a yearly trend was not found.

In summary, throughfall measurements have limited information. In fact, only the $a$-parameter range was identified with satisfying accuracy. As Calder and Hall (1997) pointed out, only a very simple model, in this case a one-parameter model, can be used if only throughfall measurements are available. Therefore, all model parameters of drainage and evaporation functions from studies with only throughfall measurements must be taken with care due to the problems of non-uniqueness of the parameters. It seems to be premature to compare parameter estimates of different species, that were obtained by throughfall measurements only (e.g. Hertwitz, 1985; Klaassen et al., 1998; Rutter et al., 1975; Valente et al., 1997) or to develop models with more parameters.

The throughfall measurements obtained with funnels have a too low accuracy to assess the four model parameters. Lundberg et al. (1997) have therefore developed a new measurement approach, with weighing troughs, with an accuracy of 0.1 mm and a time resolution of 1 minute. Using the same analysis of artificial data, an equal result of the $a$-parameter ($\sigma_a = 0.035$) and a much better result of the $c$-parameter ($\sigma_c = 0.043$) are found for DOY 258. To identify evaporation, the end of the rain event of DOY 211 was used. Using the uncertainties in the other parameters, $d$ can be reduced to $\mu_d = 0.80$ and $\sigma_d = 0.053$. This uncertainty is still twice as high as found with storage measurements due to the correlation with the $b$ and $d$-parameters, while $b$ can still not be identified.
With PIMLI, the uniqueness and accuracy of the parameters was identified by analysing individual periods. As a result, specific positions, for instance the first drainage peak at DOY 211 and the evaporation period, can be marked and be used to improve the model. For the evaporation function it can mean that the linear decrease $S/c$ may not be correct. However, using a classical calibration, based on the best fit of the total data set, systematic model errors can be compensated by the calibration. Therefore, the discrepancies at individual points are much more difficult to interpret.

5.5 CONCLUSIONS

This study shows that every measurement of throughfall or canopy water storage has a different information content to identify each of the parameters of a rainfall interception model. From throughfall measurements, only the interception fraction could be identified with comparable accuracy as with canopy storage measurements. The best identifications of the interception fraction and the storage capacity parameter were achieved during nights with low evaporation and rather low rainfall amounts. The drainage parameter can never be identified, as storage is not measured directly while the evaporation parameters could not be identified in a unique way due to correlation between the parameters and high measurement errors. If only throughfall measurements are available, than it is concluded that unique parameters can only be achieved with a very simple model with only one parameter.

With canopy storage measurements, parameters were identified during the independent stages of the drying and wetting cycles. A much higher accuracy of all parameter estimates was thus obtained. It was further shown that the uncertainty in throughfall predictions simulated with the parameter set based on storage measurements was even lower than the standard deviation of the throughfall measurements. It is finally shown that by using PIMLI, specific situations can be selected to improve the model.
REFERENCES


6. ANALYSING FOREST TRANSPIRATION MODEL ERRORS WITH ARTIFICIAL NEURAL NETWORKS

ABSTRACT

A Single Big Leaf (SBL) forest transpiration model was calibrated on half-hourly eddy correlation measurements. The SBL model is based on the Penman-Monteith equation with a canopy conductance controlled by environmental variables. The model has eight calibration parameters, which determine the shape of the response functions. After calibration, residuals between measurements and model results exhibit complex patterns and contain random and systematic errors. Artificial Neural Networks (ANNs) were used to analyse these residuals for any systematic relationship with environmental variables that may improve the SBL model. Different sub-sets of data were used to calibrate and validate the ANNs. Both wind direction and wind speed turned out to improve the model results. ANNs were able to find the source area of the fluxes of the Douglas fir stand within a larger heterogeneous forest without using a priori knowledge of the forest structure. With ANNs, improvements were also found in the shape and parameterisation of the response functions. Systematic errors in the original SBL model, caused by interdependencies between environmental variables, were not found anymore with the new parameterisation. After the ANNs analyses, about 80% of the residuals can be attributed to random errors of eddy correlation measurements. It is finally concluded that ANNs are able to find systematic trends even in very noisy residuals if applied properly.

6.1 INTRODUCTION

Transpiration of water by vegetation is an important component of the energy exchange at the earth surface. Single-layer, multi-layer and three-dimensional models exist, simulating transpiration of the vegetation at local, regional, and global scale (Raupach and Finnigan, 1988). In such models it is common to describe the vegetation as if it were a Single Big Leaf (SBL) (for example SiB by Sellers et al., (1986) and BATS by Dickinson et al. (1986)). In these models the calculation of the transpiration flux is based on the Penman-Monteith equation (Monteith, 1965). In a hydrological context, the most important characteristic of the SBL is its stomatal resistance to transpiration. This

* Submitted to Journal of Hydrology by S.C. Dekker, W. Bouten and M.G. Schaap.
resistance is controlled by a number of environmental conditions, which can be incorporated in the SBL model with physically based or empirical response functions (Stewart, 1988). By optimising the parameters in the response functions, the SBL model can be made to fit observations of latent heat fluxes above vegetation (e.g. Dekker et al., 2000; Huntingford, 1995). However, residuals between measurements and model results still remain after calibration. These residuals are caused by random and systematic measurement errors and model inaccuracies, and may contain information that can be used to improve the SBL model.

Artificial Neural Networks (ANNs) can be used to analyse whether any patterns occur in the residuals between measured and modelled transpiration. ANNs are a very suitable tool for this purpose because they are able to find relationships in complex non-linear systems, without an a priori model concept (Hecht-Nielsen, 1991; Wijk and Bouten, 1999).

Recently, Huntingford and Cox (1997) used ANNs to detect how stomatal conductance responds to changes in the local environment and compared it with the Stewart stomatal conductance model. They concluded that the Stewart-Jarvis and ANN stomatal conductance model both perform well, although the models explain different parts of the variances. In the present study we want to test a method, which is less sensitive for the chosen data set by using different sub-sets of data to calibrate and validate the ANNs. Therefore we use a data set of a Douglas fir stand in the Netherlands, which was already used to model forest transpiration with an SBL model by Bosveld and Bouten (1992) and Dekker et al. (2000). We explore patterns in the residuals between observed time series of transpiration and those modelled by a calibrated SBL model for the Douglas fir stand. With ANNs, we distinguish between random errors on one hand and systematic errors or model errors on the other hand. Only systematic errors with an identifiable physical basis are used to further improve the existing SBL model. Model improvements may consist of incorporation of additional environmental variables that were not considered in the original model or may be an improved response to an environmental variable. When all relevant information is incorporated in the existing SBL model, we explore the mathematical forms of the response functions.

6.2 MATERIALS AND METHODS

Research Site

The research site, Speuld is located in a 2.5 ha Douglas fir stand, in a large forested
area, in the central Netherlands near Garderen. The Douglas Fir forest is dense with 780 trees ha\(^{-1}\) without understorey and planted in 1962. Average tree height in 1995 was 25 m, lowest living whorl 13 m, mean diameter at breast height is 0.25 m and the single sided leaf area, including stem area, ranging from 9.0 m\(^2\) m\(^{-2}\) to 12.0 m\(^2\) m\(^{-2}\) in summer (Jans et al., 1994). The forested area has different stands with dimensions of a few hectares. Most dominant species are Douglas fir, Beech, Scots Pine and Japanese Larch. The soil is a well-drained Typic Dystrochrept (Soil Survey Staff, USDA, 1975), with a forest floor of 5 cm on heterogeneous ice pushed sandy loam and loamy sand textured river deposits. The water table is at a depth of 40 meter throughout the year. The 30-year average rainfall is 834 mm y\(^{-1}\) and is evenly distributed over the year, mean potential evapotranspiration is about 712 mm y\(^{-1}\). Yearly transpiration reduction by water stress is low (about 5 %), although short periods with considerable drought stress do occur (Tiktak and Bouten, 1994).

Models

Forest transpiration was modelled with the Single Big Leaf model (SBL) based on the Penman- Monteith equation (Monteith, 1965):

\[
\lambda I = \frac{\alpha R_n + \rho C_p \Delta}{\varepsilon + \gamma (1 + g_u / g_s)}
\]  

(6.1)

where \(\lambda I\) is the latent heat flux, \(\alpha\) the slope of the saturated water vapour curve, \(R_n\) the net radiation, \(\rho\) the density of air, \(C_p\) the specific heat capacity of air, \(\Delta\) the vapour pressure deficit, \(\gamma\) the psychrometer constant, and \(g_u\) and \(g_s\) are the aerodynamic and surface conductance, respectively.

Aerodynamic conductance \((g_u)\) is calculated with (Monteith and Unsworth, 1990):

\[
g_u = \frac{\nu^2}{u'}
\]  

(6.2)

where \(\nu\) is the friction velocity derived from the wind profile equation under neutral conditions and \(u\) is the wind speed (m s\(^{-1}\)). Friction velocity is calculated with (Monteith and Unsworth, 1990):
\[ u_\kappa = \frac{k_\mu}{\ln\left(\frac{z-d}{z}\right)} \]  \hspace{1cm} (6.3)

where \( k \) is the von Kármán constant, \( z \) the measurement height (36 m), \( d \) the zero plane height taken as \( 2/3 \) of the tree height (17 m), and \( z_0 \) is the roughness length.

Surface conductance, \( g_s \), is composed of the stomatal conductance (\( g_t \)) and the remaining conductance when stomata are closed (\( g_\infty \)):

\[ g_s = g_t + g_\infty \]  \hspace{1cm} (6.4)

\( g_\infty \) is related to cuticular transport of water vapour.

For the 1989 data set, Bosveld and Bouten (1992) modelled stomatal conductance as a product of response functions of environmental variables. They found that \( g_t \) depends on leaf area index (\( I_\lambda \)), vapour pressure deficit (\( D \)), global radiation (\( R_t \)), air temperature (\( T \)) and volumetric soil water content (\( \Theta \)):

\[ g_s = g_{s, ref} f_1(DOY) f_D(D) f_{Rt}(R_t) f_{\Theta}(\Theta) f_T(T) \]  \hspace{1cm} (6.5)

where the \( g_{s, ref} \) is a parameter, representing the canopy conductance at reference conditions and \( f_i \) are reduction functions of the environmental conditions or time. The functional shapes of the response functions, used by Bosveld and Bouten (1992), are plotted in Figure 6.1.

A piece-wise linear form for the growth curve (\( f_{\lambda} \)) was assumed. It was observed (Tiktak et al., 1991) that shoot growth starts at DOY 130 and ends at DOY 180:

\[ f_{\lambda}(DOY) = \begin{cases} 1 - a_{1,\lambda} (DOY + 185) / 315 & 0 \leq DOY \leq 130 \\ 1 - a_{1,\lambda} (180 - DOY) / 50 & 130 \leq DOY \leq 180 \\ 1 - a_{1,\lambda} (DOY - 180) / 315 & 180 \leq DOY \leq 365 \end{cases} \]  \hspace{1cm} (6.6)

where \( a_{1,\lambda} \) is the free parameter to be optimised.

The response function for \( D \) (\( f_D \)) is:

\[ f_D(D) = \frac{1}{1 + a_D(D - D_r)} \]  \hspace{1cm} (6.7)
where \( a_f \) (mbar\(^{-1}\)) is the free parameter and \( D_r \) (mbar) a reference \( D \), here chosen at 4.6 mbar at which \( f_D \) becomes 1. For \( D < 1.5 \) mbar the response function was set to \( f_D \) (\( D = 1.5 \) mbar).

The light response function \( f_{RL} \) is described with:

\[
f_{RL}(R_L) = \frac{R_L \left(1000 - a_{RL}\right)}{R_L \left(1000 - 2a_{RL}\right) + a_{RL}1000}
\]  

de \( a_{RL} \) (Wm\(^{-2}\)) is the free parameter and 1000 is the maximum radiation (Wm\(^{-2}\)).

The response function for \( T_1(f_l) \) is:

\[
f_1(T) = 1 - a_T + \frac{\left(40 - T\right)^2 - T_{OPT}/20}{T_{OPT}/20}
\]

where \( a_T \) is the free parameter and \( T_{OPT} \) is the optimum temperature set to 25°C.

The soil water content \( f_{soil} \) is described with:

\[
f_{soil}(\theta) = \begin{cases} 1, & \theta \geq 0.072 \\ 1 - a_{soil}(0.072 - \theta), & \theta < 0.072 \end{cases}
\]

where \( a_{soil} \) (-) is the free parameter and 0.072 represents the so called reduction point, e.g. the starting level at which soil water stress occurs.

In summary, the SBL model has eight parameters. One parameter, \( \varphi_0 \), is used to calculate \( g_h, g_0 \) accounts for canopy conductance when the stomata are closed. \( g_h, g_0 \) is used to scale the five response functions, which together contain five parameters.

**Measurements and Data Processing**

Transpiration was calculated from measured half-hourly latent heat fluxes minus the forest floor evaporation. Only periods with a dry canopy were selected to avoid evaporation fluxes of intercepted rain. In total, 4048 half-hourly measurements remained in 1995. The latent heat flux was measured at 30 m above the forest floor with a fast response Ly-\( \alpha \) hygrometer and a sonic anemometer-thermometer system (Bosveld et al., 1998). With half hourly measurements, the random error amounts to 15 % of the flux (Bosveld and Bouten, 1992) with an additional offset of 5 W m\(^{-2}\). The forest floor evaporation was simulated with the model of Schaap and Bouten (1997), who used a
Penman-Monteith approach where surface resistance depends on the water content of the forest floor. For the same forest they measured and modelled a maximum forest floor evaporation of $25 \text{ W m}^{-2}$.

Half-hourly values of meteorological driving variables were measured by the Royal Meteorological Institute of the Netherlands (KNMI) on a 36 meter high guyed mast. Short wave incoming radiation was measured with a CM11 Kipp solarimeter. Ambient temperature and humidity were measured with ventilated and shielded dry bulb and wet bulb sensors at 18 m above the forest floor. Wind speed was measured with a three-cup anemometer at 36 m above the forest floor. The soil water model SWIF (Tiktak and Bouten, 1992; Tiktak and Bouten, 1994), calibrated on soil water content measurements of the same forest, was used to simulate daily water contents of the forest floor and mineral soil. To obtain representative water contents of the root zone, the simulated vertical water content profile was weighted with the root density.

**Analysis with Artificial Neural Networks**

The type of Artificial Neural Networks (ANNs) applied is a feed-forward back propagation (Haykin, 1994; Hecht-Nielsen, 1991) with three layers, an input, a hidden and an output layer. The number of input and output nodes corresponds to the number of input and output variables, while the number of hidden nodes depends on the complexity of the relationships between input and output variables. At each neuron, the input values are biased and weighted by model parameters. A sigmoid transfer function for the hidden layer and a linear transfer function for the output layer provide the non-linear capabilities of the ANN. A properly calibrated neural network is able to approximate any continuous (non-linear) function (Haykin, 1994; Hecht-Nielsen, 1991), therefore neural networks are well suited to explore the residuals between model predictions and observations. The neural network parameters were optimised with the Levenberg-Marquardt algorithm (Marquardt, 1963; Demuth and Beale, 1994), which minimises the root mean squared errors (RMSE) between measurements and model results.

When calibrating ANNs one has to cope with the flexible structure, local minima, overtraining and the high sensitivity to sets of calibration and test data (Morshed and Kaluarachchi, 1998). Problems with local minima were solved by initialising the model 20 times with different initial parameter values. Sensitivity analyses proved that 20 initialisations were enough. Problems with overtraining and high sensitivity to outliers were solved by using different sub-sets of data. The total data set was divided in
independent sets for calibration and validation. The calibration data sets were randomly drawn and contain 67% of the total data set. An ANN was calibrated on a calibration set and tested on the corresponding validation data set. In total 30 calibrations-validations were carried out. The best run of the 20 initialisations was selected. Mean and standard deviation were calculated from these best runs of the 30 sets.

**Approach and Presentation of Results**

This study follows two main steps. In the first step the parameters of the SBL model are calibrated on the eddy correlation data using the Simplex algorithm (Press et al., 1988). Subsequently, the residuals between the predicted and measured transpiration fluxes are analysed with ANNs to investigate if there are systematic deviations, which are correlated with the environmental variables. The ANN analyses of the residuals are carried out using Wind direction (WD), u, Rs, Rs, D, T, DOY and θ as input.

In the second step, the main goal is to establish improved response functions to predict optimal gc. To this end we use an iterative approach based on ANN analyses of the residuals between the SBL model and the observed transpiration. In the first iteration, only the gc,nc parameter of the SBL model is recalibrated on the data-set while all the reduction functions in equation 6.3 are set to 1.0 and go to 0.0. Because no reduction functions are present in this version of the SBL model, the residuals between model outcome (y1) and observations are large and are very likely correlated with one or more environmental variables. Five ANN analyses are carried out to establish the response of the residuals to variations of Rs, D, T, DOY and θ. The strongest response is selected and added to the predicted transpiration by the SBL model (y2) and the predicted offset is transposed to gc. Subsequently, gc can be found by inverting the Penman-Monteith equation with y1 as transpiration flux. To obtain the functional shape of the new response, this gc(y1) is divided by the gc(y2). After describing the response function in appropriate mathematical terms, it is incorporated in the SBL model of the first iteration. The SBL model is subsequently recalibrated for gc,nc,go and the parameter of the response function and once again the residuals are analysed with ANN after which a response function is established. This iterative improvement is carried out until no meaningful improvement of the SBL model is obtained.
6.3 RESULTS AND DISCUSSION

Systematic deviations of the residuals

Eight parameters of the SBL model were calibrated to fit the measurements (first column of Table 6.1. As found by Bosveld and Bouten (1992) for the 1989 data set, no temperature response could be identified and therefore $a_T$ was fixed to zero. The shapes of the four remaining response functions are plotted in Figure 6.1.

Table 6.1: Root Mean Squared Error (RMSE) and optimised free parameters of the canopy conductance model with different wind sectors.

<table>
<thead>
<tr>
<th>Wind Sector</th>
<th>0-360°</th>
<th>15-125°</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSF (W m⁻²)</td>
<td>26.41</td>
<td>21.85</td>
</tr>
<tr>
<td>$g_{r,m}$ (m s⁻¹)</td>
<td>18.1 $10^{-3}$</td>
<td>13.8 $10^{-3}$</td>
</tr>
<tr>
<td>$g_c$ (m s⁻¹)</td>
<td>0.50 $10^{-3}$</td>
<td>0.55 $10^{-3}$</td>
</tr>
<tr>
<td>$a_D$ (mbar⁻¹)</td>
<td>0.172</td>
<td>0.129</td>
</tr>
<tr>
<td>$a_t$ (-)</td>
<td>0.385</td>
<td>0.320</td>
</tr>
<tr>
<td>$a_g$ (W m⁻²)</td>
<td>260</td>
<td>283</td>
</tr>
<tr>
<td>$a_T$ (-)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$a_H$ (-)</td>
<td>22.4</td>
<td>30.0</td>
</tr>
</tbody>
</table>

Improvements in model fit of the eight ANN analyses are shown in Table 6.2 as percentages of the original model fit. The ANNs with $WF$D as input showed the strongest improvement. This response together with the $u$ response is further evaluated. Figure 6.2A and 6.2B show residuals against $u$ and $WF$D. In these figures, a positive residual means that the SBL model underestimates the measurements. A clear systematic trend is not visible because of large random errors. Figure 6.2C and 6.2D show the trend found by the ANNs. Dashed lines are the standard deviations, calculated from the best 30 ANNs, representing the reliability of the trend. Responses that vary with wind speed and direction reflect the variations in forest structure and species. Bosveld (1997) determined different roughness lengths from wind profile relations for every 30° wind sector for the 1989 data set. He found deviant values in the sectors 210-330°, which he attributed to
Figure 6.2: Response functions to growth or Leaf Area Index $f_L$(DOY), Vapour Pressure Deficit $f_D(D)$, Global radiation $f_Rg(R_g)$, Temperature $f_T(T)$ and soil water content $f_w(\theta)$. Lines are calibrated values. Temperature response ($f_T$) was not found and $a_T$ was fixed to zero.

Table 6.2: Root Mean Squared Error (RMSE) of the SBL model with different wind sectors, and improvements of fits by ANN in % of the original RMSE.

<table>
<thead>
<tr>
<th>Wind Sector</th>
<th>0-360°</th>
<th>15-125°</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE_SBL</td>
<td>26.41</td>
<td>21.85</td>
</tr>
<tr>
<td>ANN_u</td>
<td>0.8</td>
<td>0.5</td>
</tr>
<tr>
<td>ANN_WD</td>
<td>1.8</td>
<td>0.2</td>
</tr>
<tr>
<td>ANN_\theta</td>
<td>1.1</td>
<td>1.2</td>
</tr>
<tr>
<td>ANN_D</td>
<td>0.3</td>
<td>1.0</td>
</tr>
<tr>
<td>ANN_Rg</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>ANN_T</td>
<td>0.3</td>
<td>0.2</td>
</tr>
<tr>
<td>ANN_DOY</td>
<td>0.2</td>
<td>0.1</td>
</tr>
</tbody>
</table>
Figure 6.3: Residuals between model results and measured transpiration against wind speed (u) and wind direction (A and B). Systematic residuals against u and wind direction found by the ANNs (C and D). Dashed lines are standard deviations of the 30 best runs. A positive fit means that the original model underestimates the measurements. The scale of the A and B figures are 10 times larger.

other tree species. Although roughness lengths changed between 1989 and 1995, Figure 6.2D shows a constant residual in the wind sector 15-185° and tends to confirm a homogeneous forest structure in that direction. With the data of this sector only, the ANN analysis was repeated again with u and WD as input at the same time. Still an improvement of 1.6% was found. The response found by the ANN (Figure 6.3) corresponds with the characteristics of the forest stand. The sectors above 125° are dominated by Scots Pine. The sector 50-125° has the largest fetch of the Douglas fir although Figure 6.3 shows that the conditions are not constant. Bouten et. al (1992) found wetter soil conditions for this wind sector at about 150 meter distance from the meteorological tower. The underestimation by the model between 50-125° and high u can possibly be caused by these wetter conditions. As a result of this analysis, it is shown that variations in forest structure can be derived from transpiration observations.
Figure 6.3: Systematic errors found by the ANN with wind direction and wind speed \((u)\) as input using the data with wind direction between 15-185°. A positive value means that the SBL model underestimates the measurements.

To reduce the effect of forest structure heterogeneity and with a focus on the source area of Douglas fir only we used data from the 15-125° wind sector for further analyses resulting in a reduced data set of 1633 measurements. The SBL model was calibrated again (Table 6.1, column 2) and the ANN analyses were repeated (Table 6.2, column 2). Only a small improvement in \(WD\) remained, indicating that the forest structure is sufficiently homogeneous in the selected wind sector. The ANN response to \(\theta\) and \(D\), which show the largest improvements, are plotted in Figure 6.4. The trend in Figure 6.4A shows that the model underestimates the transpiration at water contents between 0.067-0.088 m³ m⁻³. This model underestimation cannot be caused by soil water stress reduction, because the initial soil water stress reduction point was set to 0.072 m³ m⁻³. Therefore, this systematic error must be caused by the interplay of environmental variables that lead to the evolution of \(\theta\). This interplay is caused by coupled environmental conditions, which are present in these kinds of monitoring data sets, as pointed out by Huntingford and Cox (1997) and Dekker et al. (2000).

The relationship of the SBL model residuals and \(D\) shows a shift at 17 mbar (Figure 6.5B). However, ANNs responses were not conclusive at higher water vapour deficits as reflected by wide uncertainty ranges. A further reduction of the data set was therefore not considered.
Figure 6.4: Systematic trends of residuals against water content ($\theta$) and vapour pressure deficit ($D$) found by ANN on the reduced data set. Dashed lines are standard deviations of the 30 best runs. A positive value means that the original model underestimates the measurements. Dots are mean daily values.

Optimisation of canopy conductance responses

In this step, improved response functions were established with an iterative approach to predict optimal $g_0$. In the first iteration, only the free parameter $g_{\text{inf}}$ was recalibrated on the reduced data set of Douglas fir (Table 6.3, first column). The $R_g$ response caused the strongest reduction in the RMSE indicating that it is the most important controlling factor in stomatal behaviour. The residual fit found by the ANN is plotted in Figure 6.5A, dashed lines are again the standard deviations, calculated from the best 30 ANNs, representing the reliability of the trend. Figure 6.5B (left y-axis) shows the response function of the conductance, which is calculated for 30 classes of $R_g$. The $R_g$ response function shows a linear trend between 0 to 600 W m$^{-2}$ with a slightly decreasing response at values above 600 W m$^{-2}$. This decreasing response is caused by the interference of $D$. A high $D$, which is correlated to a high $R_g$, causes a lower response. As this response is not used yet we neglected the decrease in the $R_g$ response. As $R_g$ response, we used a piecewise linear function, with a maximum at $R_g \geq 600$ W m$^{-2}$ ($a_{R_g,\text{max}}$). Minimum $R_g$ response was found at 0.5. To conform to commonly used response functions we rescaled the light response between zero and one (right axis in Figure 6.5B) while the remaining conductance during night-time is optimised with $g_0$. Jarvis (1976) and Stewart (1988) both used a non-linear light response curve as shown in Figure 6.1C, which was suggested by plant physiological studies carried out under controlled conditions. Our analysis, however, does not support a non-linear light response curve for this forest.
Figure 6.5: (A) shows the ANN fit to $R_g$ during iteration 1. Dashed lines are standard deviation values of the 30 best runs. (B) shows the light response of the bulk stomatal conductance model by inverting the Penman-Monteith equation with uncertainties (left Y-axis). Solid line is the functional shape used as response function (right Y-axis). (C) and (D) functions with $D$ (Iteration 2). (E) and (F) functions with $\theta$ (Iteration 3). (G) and (H) functions with DOY (Iteration 4). Dots in (E) and (G) are daily mean values containing minimal 5 half-hourly measurements during daytime.
In the second iteration, the SBL model was optimised with $g_{net}, g_t$ and $d_{Ric,max}$. Results of calibration and the ANN analyses are shown in Table 6.3. Strongest residual fit was found with $D$ (Figure 6.5C). The high uncertainties at $D > 25$ mbar were caused by the limited number of measurement points (29). The response function (Figure 6.5D) shows a similar shape as the original one (Figure 6.1B). The high uncertainty in the first constant part is caused by low transpiration fluxes. The uncertainty at high $D$ seems small, 0.04 (Figure 6.5D, right axis), but the fluxes are high, resulting in a high uncertainty as shown in Figure 6.5C.

**Table 6.3: Results of ANN analyses of 5 iterations.** For each iteration, the calibrated parameter values and the Root Mean Squared Errors (RMSE) of the SBL model between modelled and measured transpiration is given. Five ANN analyses are carried out to establish the response of the residuals of this calibrated SBL model to variations of $R_s, D, T, DOY$ and $\Theta$. RMSE errors of these ANN fits are shown in last 5 lines. Bold value is strongest response and new mathematical function of this variable is incorporated in the SBL model. Then the iteration is repeated by recalibrating the parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Iteration1</th>
<th>Iteration2</th>
<th>Iteration3</th>
<th>Iteration4</th>
<th>Iteration5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{net}$</td>
<td>10.3 m s(^{-1})</td>
<td>3.8</td>
<td>3.5</td>
<td>13.2</td>
<td>13.4</td>
</tr>
<tr>
<td>$g_t$</td>
<td>10.3 m s(^{-1})</td>
<td>0.91</td>
<td>0.66</td>
<td>0.67</td>
<td>0.68</td>
</tr>
<tr>
<td>$a_{Ric,max}$</td>
<td>W m(^{-2})</td>
<td>390</td>
<td>578</td>
<td>595</td>
<td>592</td>
</tr>
<tr>
<td>$a_D$</td>
<td>mbar(^{-1})</td>
<td>-</td>
<td>-</td>
<td>0.181</td>
<td>0.159</td>
</tr>
<tr>
<td>$\lambda_{th}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.360</td>
<td>0.358</td>
</tr>
<tr>
<td>$a_t$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.353</td>
</tr>
<tr>
<td>RMSE(_{SBL})</td>
<td>W m(^{-2})</td>
<td>41.2</td>
<td>34.6</td>
<td>25.4</td>
<td>22.9</td>
</tr>
<tr>
<td>RMSE(_{R_s})</td>
<td>W m(^{-2})</td>
<td>35.3</td>
<td>33.2</td>
<td>25.3</td>
<td>22.8</td>
</tr>
<tr>
<td>RMSE(_{D})</td>
<td>W m(^{-2})</td>
<td>40.5</td>
<td>30.2</td>
<td>25.2</td>
<td>22.8</td>
</tr>
<tr>
<td>RMSE(_{\Theta})</td>
<td>W m(^{-2})</td>
<td>40.0</td>
<td>32.6</td>
<td>24.1</td>
<td>22.8</td>
</tr>
<tr>
<td>RMSE(_{DOY})</td>
<td>W m(^{-2})</td>
<td>41.0</td>
<td>33.4</td>
<td>25.3</td>
<td>22.5</td>
</tr>
<tr>
<td>RMSE(_{T})</td>
<td>W m(^{-2})</td>
<td>41.1</td>
<td>32.3</td>
<td>25.4</td>
<td>22.9</td>
</tr>
</tbody>
</table>

In the third iteration, the SBL model was optimised with $g_{net}, g_t, d_{Ric,max}$ and $a_D$. Results of calibration and ANN analyses are shown in Table 6.3. Strongest response was found with $\Theta$ (Figure 6.5E, 6.5F). Because $\Theta$ is constant during the day, only daily average values were plotted in Figure 6.5E. Although there is some scatter in the conductance plot, the
soil water stress response curve is almost identical to the original one and the reduction point was also found at 0.072 m³ m⁻³.

In the fourth iteration, the model was optimised with \( g_{e,n}, g_t, a_{R_{\text{max}}}, a_1 \) and \( a_0 \) (results shown in Table 6.3). Strongest ANN response was found with DOY (Figure 6.6G, 6.6H). From these growth curves, we assume that shoot growth starts at DOY 130 and ends around DOY 200. A linear decrease after DOY 200 as shown in Figure 6.1D was not found. A systematic trend before DOY 130 could not be found due to a lack of data. Therefore constant values are assumed before DOY 130 and after DOY 200, while the steepness of the change between DOY 130 and 200 was used as free parameter.

In the last iteration, the model was optimised with \( g_{e,n}, g_t, a_{R_{\text{max}}}, a_1, a_0 \) and \( a_1 \) (Table 6.3, column 5). No clear improvements could be found by including \( T \) in the canopy conductance model. In comparison with the first analyses, the irrational shape part of the \( \Theta \) curve (Figure 6.4A) and the shift at 17 mbar of the \( D \) curve (Figure 6.4B) from the first analysis were not found anymore. This justifies the conclusion that both systematic errors were caused by interdependencies among environmental variables, meaning that the iterative approach, presented in this study, leads to a set of stomatal conductance response functions without interdependencies.

The improvement in model fit, from 26.41 to 21.85 due to the reduction of the forest structure heterogeneity and from 21.85 to 20.82 W m⁻², due to the new parameterisation may seem small. However the random error of half-hourly eddy correlation measurement was estimated at a RMSE of 16.7 W m⁻² by Bosveld and Bouten (1992), 80% of the total error. As a result only an error of 4.1 W m⁻² remains to be explained.

This remaining error can be caused by measurement errors of the environmental conditions, model errors of soil evaporation and soil water or by the wetter soil conditions at larger distance, as shown in Figure 6.3.

Improvements of the SBL model with this data set are not foreseen. As pointed out before, high uncertainties in the ANN response was found at high \( D \) (Figure 6.5C) and in the ANN response before DOY 130 (Figure 6.5G). Both uncertainties were caused by a lack of data, meaning that these functions can be better estimated with more measurements during these specific conditions.
Artificial Neural Networks (ANN) show trends in residuals between results of a forest transpiration model (SBL) and eddy correlation measurements that were related to both wind speed and wind direction. They were able to localise the source area of the fluxes of the Douglas fir stand within a larger heterogeneous forest without using a priori knowledge of the forest structure. After restricting the data set to wind sections with homogeneous forest, the response functions of the canopy conductance model were also analysed with ANNs in an iterative approach. The analysis led to a piece-wise linear light response curve with saturation at 600 W m$^{-2}$ while only small changes for the other functions were found. Systematic errors in the original model were caused by interdependencies between environmental variables. These errors were not found anymore with the new parameterisations. The method presented here, that used different sub-sets of data to calibrate and validate the ANNs, is able to trace systematic trends even in very noisy residuals.

Acknowledgement
The authors thank Fred Bosveld from the Royal Meteorological Institute of the Netherlands for providing the meteorological data of 1995. We also thank Guda van der Lee for critical comments on the text of an earlier draft.

REFERENCES

7. MODELLING AND MONITORING FOREST EVAPOTRANSPIRATION: SOME FINAL REMARKS

From a scientific point of view, models can be used to improve the insight in processes, to extrapolate in time and space or to determine variables, which cannot be directly measured. To achieve these goals, confidence must be gained in the model concepts and model parameters. A model concept or values of model parameters can only be evaluated by comparing model results with measurements. As a consequence, the system behaviour must always be linked to the model behaviour. As shown in Figure 1.1, this confidence can be reached by improving the understanding of the model concepts by a focus on cause-effect relationships and by improving the interpretation of model parameters in terms of system properties. In this thesis, several methodologies were developed and used to improve the understanding of forest evapotranspiration model concepts and the interpretation of the model parameters. In this chapter, some final remarks for future research are given.

7.1 MODEL PARAMETERS

Nowadays, most hydrological and ecological models have several fit-parameters that cannot be measured independently. These fit-parameters are identified with optimisation algorithms. Due to increased computer power and standardisation of software, these optimisation algorithms are commonly used. However, as pointed out in this thesis, a wrong parameterisation can compensate systematic model errors. Due to these wrong parameterisations, fitted model-parameters can become unrealistic and it is difficult to trace the true causes of misfits between model results and measurements. With the methods developed and used in this thesis, as the Parameter Identification Method based on Localisation of Information (PIMLI) and the analysis of residuals with Artificial Neural Networks (ANN), the insight in the model errors caused by wrong parameterisations and wrong concepts is improved.

One way to improve the understanding of parameters and therefore the understanding of the system, is to link the parameter values to independently measured system properties with transfer functions. These functions will help to improve the interpretation of the model parameters, but only if the parameter estimates are unique.
Another way to improve the understanding of the model parameters is to avoid calibration by using, or re-using, the so-called 'non-calibrated models'. In these models, parameters are directly assessed from the field, laboratory or from literature. With these models, the understanding of the parameters can be improved and the parameters are less dependent on the chosen model. Without fitting, the remaining residuals between measurement and model results are easier to interpret and the deviations between model results and observations become more realistic. However, we must realise that parameters from literature were often also derived from calibration.

The idea of the plant physiological model, as used in chapter 3, is that it is a more realistic model closer to the processes. Species dependent model parameters can be established and used without calibration for different situations at different sites. However, this type of model still contains several fit-parameters, which need to be calibrated and the stomatal conductance model is still empirical. Soil water stress, seasonal variations in LAI, fluctuations of nitrogen concentration in the leaf and adaptation due to global change causes all variations in the assimilation and transpiration rates at the leaf level. Direct cause-effect relationships of most of these processes are not known and the best until now is to use empirical relationships in the model concepts containing several fit-parameters, which need to be calibrated. Consequently, using the plant-physiological model does mean a use of a non-calibrated model. Future research should focus on linking the model parameters to system properties and including cause-effect relationships in the model concepts. For instance the seasonal variations of LAI should be linked to phenology (e.g. (Kramer et al., 1996)) and cause-effect relationships should be included in the model concepts between leaf nitrogen concentration and the photosynthetic coefficients (Kull and Jarvis, 1995).

### 7.2 MODEL CONCEPTS

Although the problems of parameter identification are impressive, little attention is often paid to it. The main cause is probably that most studies only focus on confirmation. In that case, problems with non-uniqueness of parameters are not an issue, because the model behaviour fits the system behaviour satisfactory. However, the insight in the processes is limited if interpretation of the parameters is missing. With confirmation, model results are compared to measurements by a subjective choice of the statistical measures, e.g. $R^2$, RMSE, $\chi^2$. These measures only highlight specific aspects in the time
series and models. As a result, confirmation gives little information on the behaviour of the system and may even give misleading information. The general approach to identify the parameters is to split the total data set in a calibration and confirmation data set. Due to this subjective splitting, the calibration data set can perform less than the confirmation data set. As shown in this thesis, every observation has its own information content with respect to a specific parameter. Therefore, the size of the data sets should not be the determining factor for constructing the calibration and confirmation data set, but it should contain an equal amount of information with respect to every parameter.

As shown in this thesis a focus on discrepancies gives more information, confidence and insight in the model concepts and parameters than a focus on confirmation. Model concepts were developed with different perceptions and therefore models perform differently during various conditions. With a focus on discrepancies, these different responses of models can be traced better. However, expected differences between models may disappear during calibration.

7.3 CONSEQUENCES FOR MEASUREMENT STRATEGIES

As stated clearly in this thesis, improvements in the understanding of the system in terms of concept and parameters can be achieved by the interaction between modelling and measuring.

As mentioned in chapter 1, there is no consensus about the model concepts of forest transpiration. In chapter 2 it was shown that several calibrated forest transpiration models could describe transpiration to an acceptable level. Main reasons that no consensus is established are that: (i) a linear regression with only global radiation gave good results; (ii) the standard deviation between model results and measurements is almost equal to the random error of the eddy-correlation measurements (chapter 2, 4 and 6); (iii) a mean response was easy to find due to the strong correlations between input variables, while short periods when these correlation were uncoupled are very rare and (iv) all models were calibrated and the values of these fit-parameters were not linked to system properties.

As a result, it means that further improvements in the understanding of cause-effect relationships of forest transpiration are not expected with the use of monitoring measurements as used in this thesis. As shown in chapter 4, more monitoring measurements will not increase the information content of the measurements. As long as
the accuracy of the eddy-correlation measurements is not increased, improvement in the understanding of the system is not expected.

In laboratory or manipulation experiments, experimental design increases the information of measurement. In this study, time series of monitoring measurements were used. These kinds of data have a limited amount of information to identify the parameters. By using $PIM_{ML}$, this information is increased by selecting specific measurements. With $PIM_{ML}$ the most relevant periods to identify the parameters, to confirm the model behaviour or to falsify the model concepts can be calculated. It means that $PIM_{ML}$ can be used as a method for experimental design. However, using experimental design in monitoring research has some disadvantages. In practice, it is usually easier to measure the total period instead of specific conditions because of problems by setting up the instrumental equipment. A second disadvantage is that an efficient experimental design is inextricably bound up with the chosen model meaning that much confidence is given in the model concept. As a result of such a measuring strategy, new insights in processes will be limited.

Consequently, to further improve the understanding of the system, future research should focus on increasing the information of measurements by direct measurements of transpiration. With manipulation experiments, correlation between environmental variables can be uncoupled and only one part of the process is than examined. Examples of manipulation experiments are for instance (i) the HELOX experiments of Mott and Parkhurst (1991) to find out if stomata response directly to a change in humidity or indirectly as a consequence of a change of transpiration, (ii) the experiment of Musters (1998), who manipulated the soil water dynamics with the help of a roof that intercepted precipitation, (iii) or the free air carbon dioxide enrichment (FACE) experiments (Herrick and Thomas, 1999).

For rainfall interception it was concluded that the throughfall measurements, measured with funnels as used in the Douglas fir stand, have limited information. This limited information was caused by the large measurement errors affected by the spatial variability between the funnels. To increase the information of throughfall measurements, spatially correct area measurements with plastic sheets (Calder and Rosier, 1976) or troughs (Lundberg et al., 1997) can be used. However, with these types of measurements, as shown in chapter 5, the drainage parameter can still not be identified and the uncertainties of the evaporation and storage capacity parameter are still high. To improve the understanding of the canopy storage dynamics and evaporation rates of the canopy,
more attention should be paid on direct measurements of canopy storage and evaporation rates.

In current Soil Vegetation Atmosphere Transfer (SVAT) model development, the complexity and number of parameters is increased by incorporating plant-physiological processes and heterogeneity in sub-grids. This increase in model parameters would not be a problem, if these kinds of models were non-calibrated ones. However, in general, the parameters cannot be measured independently at the scale of interest. As a result, the majority of the parameters should always be calibrated and problems as non-uniqueness will be found. To assess the maximum complexity of the model with respect to the information of the available measurements is a major problem in these kinds of models. A next step for future research will be to use the knowledge from this thesis in research in SVAT models at a larger scale.

REFERENCES

8. SAMENVATTING

HET MODELLEREN EN METEN VAN BOSEVAPOTRANSPIRATIE: GEDRAG, CONCEPTEN EN PARAMETERS

Modellen zijn binnen de hydrologie en ecologie noodzakelijk om processen beter te kunnen begrijpen en om het gedrag van het systeem te kunnen voorspellen gedurende veranderende omstandigheden. Een model is alleen waardevol als er vertrouwen is in de gebruikte modelconcepten en modelparameters. Door modelresultaten met metingen te vergelijken kunnen modelconcepten en schattingen van modelparameters worden getoetst. Dit soort toetsen wordt vaak validatie genoemd. Binnen de literatuur wordt vaak gezegd dat een model gevalideerd is zonder dat er wordt verwezen naar de gebruikte criteria.

Vanuit een wetenschappelijk oogpunt kunnen modellen gebruikt worden om het inzicht in de processen te vergroten, om te extrapoleren in tijd en ruimte of om variabelen die niet op een directe manier te meten zijn te berekenen. Om deze doelen te bereiken wordt het gedrag van het model vergeleken met het gedrag van het systeem oftewel de metingen. Het begrip van de processen wordt vergroot door identificatie van variabelen en processen die niet of niet optimaal in het modelconcept aanwezig waren. Voordat modelparameters geïnterpreteerd en gekoppeld kunnen worden aan systeemeigenschappen moeten eerst de unieke kenmerken van deze modelparameters vastgesteld worden. Dit proefschrift behandelt modelconcepten en parameters diebosevapotranspiratie van een Douglassparrenbos beschrijven.

De evapotranspiratie van vegetatie is een zeer belangrijke onderdeel van de energie- en wateruitwisseling aan het aardoppervlak. De belangrijkste uitdagingen binnen dit soort bodem-vegetatie-atmosfeer (SVAT) onderzoek zijn (1) gedetailleerd plotschaal onderzoek en (2) onderzoek naar het opschalen van deze SVAT processen in tijd en ruimte. Deze studie richt zich op het gedetailleerde plotschaal onderzoek voor zowel bostranspiratie als verdamping. Binnen het onderzoek is getracht verschillende modelconcepten te bevestigen en te falsifiëren. Tevens is aandacht besteed aan het lokaliseren van informatie uit metingen om zodoende betere parameterschatingen te maken en modelconcepten te verbeteren. Alle metingen binnen dit proefschrift zijn gedaan in het Douglassparrenbos, op een zure zandige bodem, te Speuld in Nederland.
Bostranspiratie: concepten en parameters

In hoofdstuk 2 zijn drie verschillende bostranspiratiemodellen met elkaar vergeleken. Het eerste model is gebaseerd op de warmtebalans van de naalden. Afkoeling van de naalden vindt plaats door lucht en verdamping, terwijl tegelijkertijd de naalden worden opgewarmd door straling.

Het tweede model is een CO₂ assimilatie model. Als de huidmondjes open zijn, zal uitwisseling plaats vinden tussen CO₂ en H₂O. Dit proces speelt zich af op naaldniveau. Omdat de assimilatie wordt berekend door een niet-lineaire functie met straling, wordt de straling in het kronendak beschreven door een drie-dimensionaal lichtinterceptie model om transpiratie van de gehele bosopstand te kunnen simuleren.

Het derde model is het zogenaamde ‘Single Big Leaf’ (SBL) model, dat gebaseerd is op zowel de energiebalans als op de waterbalans, waarbij de huidmondjesweerstand uit de Penman-Monteith vergelijking beschreven wordt als een responsfunctie van omgevingsvariabelen.

De modellen zijn niet allemaal even complex en hebben tussen de één en zes kalibratieparameters. De modelresultaten zijn vergeleken met dampflux-eddy-correlatiemetingen op halfuur basis. Alle drie de modelconcepten gaven ongeveer even goede prestaties (R² = 0.777-0.834) en werden alle drie bevestigd door de metingen. Dit betekent dus dat geen van de drie modelconcepten op basis van de metingen kon worden verworpen. Meer informatie over de verschillen tussen de drie modelconcepten werd gevonden door te kijken naar de afwijkingen tussen metingen en modelresultaten. De grootste afwijkingen werden gevonden door de responsen van het dampdruktekort en de ‘Leaf Area Index’ (LAI) anders te formuleren.

In hoofdstuk 3 is de uitwisseling tussen CO₂ en H₂O gemodelleerd op de schaal van een naald. De parameters van het plantfysiologische Farquhar/Ball CO₂ assimilatie model zijn geïdentificeerd met CO₂ flux metingen van zes takkamers. De hoogste correlatiecoëfficiënt tussen dagelijks gemeten en gecombineerde fotosynthese was $R^2 = 0.87$ en de laagste was $R^2 = 0.61$. De takkamers waren geplaatst in verschillende bomen en op verschillende hoogten in het kronendak. Hierna is het model STANDFLUX gebruikt om transpiratie, CO₂ assimilatie en de efficiëntie van het watergebruik in de gehele bosopstand te simuleren. Dit model integreert de drie-dimensionale aspecten van de structuur en de lichtinterceptie van het kronendak met een één-dimensionaal verticaal

**Informatieinhoud van metingen**

Tegenwoordig bevatten modellen veel parameters waarvan de waarde vaak wordt geschat door het fitten van de modelresultaten door metingen. Door de eigenschappen van de metingen en door de correlatie tussen parameters kunnen deze fitresultaten niet-unieke waarden van parameters als uitkomst hebben. Een unieke parameterset is een allereerste vereiste om de parameterwaarden te begrijpen en om deze waarden te gebruiken voor extrapolatie in tijd en ruimte. Om unieke parameterwaarden met hoge nauwkeurigheid te kunnen schatten is de Parameter Identificatie Methode gebaseerd op het Lokaliseren van Informatie (PLMLI) ontwikkeld. PLMLI selecteert metingen die een hoge gevoeligheid hebben voor één parameter, terwijl deze metingen weinig gevoelig zijn voor de andere parameters en het feit dat het betrouwbaarheidsinterval van de meting laag is.

Binnen een hydrologische context is het meest belangrijke onderdeel van het bostranspiratie SBL model het huidmondjesmodel. De huidmondjesweerstand is beschreven als een product van responsfuncties van dampdruktekort, globale straling, temperatuur, bodemwater en LAI. Kalibratieparameters en mathematische formuleringen maken een belangrijk deel uit van deze responsfuncties. In hoofdstuk 2 is een goede fit gevonden tussen de modelresultaten en de eddy-correlatie metingen. Tijdreeksen van omgevingsvariabelen die bostranspiratie berekenen, bevatten vele perioden met gekoppelde variabelen en overtollige informatie, terwijl deze variabelen onder andere omstandigheden nauwelijks gemeten zijn.

In hoofdstuk 4 is met PLMLI de informatieinhoud van elke meting voor elke modelparameater berekend. Metingen van transpiratie met hoge informatieinhoud zijn geselecteerd door middel van onafhankelijke metingen. Met deze onafhankelijke criteria
zijn tijdsperioden geselecteerd die maximale informatie bevatten voor de identificatie van de modelparameter. De metingen die niet zijn geselecteerd, bevatten geen extra informatie die nodig is om een betere parameter schatting te krijgen. Uit dit onderzoek blijkt dat problemen met de parameteridentificatie niet worden opgelost met meer metingen. De parameterwaarden en de fitfout met PLMIJ zijn vergeleken met een conventionele simplex parameteridentificatiemethode die gebruik maakt van de Jackknife methodiek. In totaal zijn 100 subdatasets van 300 metingen, die willekeurig zijn geselecteerd uit de totale dataset, gebruikt om de parameters te identificeren. De eigenschappen van de subdatasets en de niet-unique eigenschappen van de parameters veroorzaakten na berekening met de conventionele methode verschillende parametersets. PLMIJ daarentegen identificeert unique parameterwaarden met hoge nauwkeurigheid door gebruik te maken van beperkt aantal kalibratiedata.

In hoofdstuk 5 zijn modelparameters van een interceptiemodel geïdentificeerd door zowel metingen van doorval als metingen van waterbeging in het kronendak te gebruiken. Doorval, waterbeging en verdamping zijn alle drie afhankelijk van elkaar. Als parameters geïdentificeerd worden uit metingen waarbij deze drie processen een rol spelen dan zal een afhankelijkheid tussen de parameters gevonden worden. Metingen zijn met PLMIJ geselecteerd op momenten waarbij deze processen zo onafhankelijk mogelijk van elkaar zijn. Hierna is de uniekheid en nauwkeurigheid van de parameterschattingen berekend. Met metingen van doorval kon alleen de interceptiefractie goed geïdentificeerd worden. Deze fractie is gedurende de periode waarbij de waterbeging niet verzadigd is en de verdamping kan worden verwaarloosd, onafhankelijk van de andere parameters. De nauwkeurigheid van de schatting van de capaciteitsparameter bleef laag ($\sigma_1 = 0.55 \text{ mm}$). De beste identificatie van de capaciteitsparameter werd gevonden tijdens een regenbui die net groot genoeg was om de capaciteit te verzadigen, maar waarbij verdamping te verwaarlozen was. Volgens de formulering van het model kan de drainageparameter alleen vastgesteld worden als zowel de capaciteit als de berging bekend zijn. De verdampingsparameter kan aan het einde van een regenbui met doorvalmetingen worden geschat. Omdat de potentiële verdamping gedurende een regenbui zeer laag is en de onzekerheid van de capaciteitsschatting moet worden meegenomen, kan deze parameter moeilijk worden geïdentificeerd.

Veel nauwkeuriger parameterschattingen zijn gevonden met bergingsmetingen, met een $\sigma_2$ van 0.04 mm. Gedurende verschillende onafhankelijke perioden van vernatting en
verdroging van het kronendak, konden alle parameters geïdentificeerd worden. Met de verkregen parameterwaarden is doorval onafhankelijk gevalideerd. Het bleek dat de modelonzekerheid in de doorvalschatting lager was dan de onzekerheid van de werkelijk gemeten doorval.

Omdat PIMLI elke meting apart analyseert, is het makkelijker perioden aan te wijzen gedurende welke het modelconcept niet voldoet. Met een identificatie van de parameters volgens een conventionele methode, waarbij de totale dataset wordt gebruikt, zullen individuele afwijkingen verborgen blijven omdat er gezocht word naar een gemiddelde fit.

Residu analyse

Nadat parameters geïdentificeerd zijn, met PIMLI of via een conventionele methode, zullen altijd verschillen tussen modelresultaat en meting blijven bestaan. Deze verschillen worden veroorzaakt door willekeurige en systematische meetfouten en modelonzekerheden. Onzekerheden in het model kunnen ontstaan door zowel systematische fouten in de parameterschatting als door een fout in het modelconcept. In hoofdstuk 6 werden artificiële neurale netwerken (ANNs) gebruikt om systematische patronen in de verschillen te onderzoeken die voorkwamen in het SBL model. De invoerknooppunten van de ANNs waren de omgevingsvariabelen en het uitvoerknooppunt waren de verschillen. Alleen systematische trends die fysisch te interpreteren zijn, zijn gebruikt om het modelconcept of de parameterschattingen te verbeteren. Grote verbeteringen in fit werden gevonden door windrichting en windsnelheid te gebruiken als invoer voor het ANN. Het was mogelijk om, zonder kennis van bosstructuur en fluxprofielmetingen, informatie te vinden over de exacte footprint van het Douglasbos. Door het model alleen maar op deze windsector te kalibreren, nam de RMSE af van 26.41 naar 21.85 W m⁻². Met de ANNs zijn ook verbeteringen in de vorm en parameterisering van de responsfuncties gevonden. De verschillen die overblijven hebben na deze verbeteringen geen systematische afwijkingen meer en kunnen bijna geheel verklaard worden door de willekeurige meetfout van de eddy-correlatiemetingen.
8. SUMMARY

MODELLING AND MONITORING FOREST EVAPOTRANSPIRATION: BEHAVIOUR, CONCEPTS AND PARAMETERS

Mathematical models are univocal descriptions of our concepts. They represent our perception of the true world. These models are most valuable if confidence is gained in the model concepts and the model parameters. By comparing model results to measurements, model concepts and values of model parameters can be tested. In general, this is called validation. Modellers, however, often claim that a model is validated without any reference to their criteria and neglecting the complex process of gaining confidence.

From a scientific point of view, models can be used to improve the understanding of processes, to extrapolate in time and space or to determine variables, which cannot be measured directly. To achieve these goals, the model behaviour is compared with the system behaviour, e.g. the measurements. The understanding of the processes can be improved by identification of variables and processes that were not or not optimal included in the model concept. The uniqueness of the model parameters must first be determined before the parameter values can be interpreted and linked to system properties. This thesis deals with model concepts and model parameters that describe forest evapotranspiration of a Douglas fir ecosystem.

The energy and water exchange at the earth surface play an important role in climate and climate change research. The major issues in this so-called Soil Vegetation Atmosphere Transfer (SVAT) research are (1) detailed plot scale research and (2) research how to scale these SVAT processes up in time and space. This study deals with detailed plot scale research for both transpiration and evaporation. Attention is paid to confirmation and falsification of different model concepts and to the localisation of information in measurements to obtain better estimates of parameters and to improve the model concepts. All measurements used in this thesis are performed in the Douglas fir stand, on acid sandy soils, Speuld, the Netherlands.

Forest transpiration: Concepts and parameters

In chapter 2, three forest transpiration model concepts were evaluated. The first model is based on the leaf cooling and calculated transpiration on basis of the requirement of water for cooling the canopy. Trees are simultaneously warmed by incident solar radiation and cooled by ambient air and by transpiration.
The second model is based on the CO₂ assimilation. If stomata are open, gas exchange of CO₂ and H₂O takes place, which is described at the leaf level. Because CO₂ assimilation is determined by a non-linear function of radiation, the radiation regime in the canopy is modelled with a 3-dimensional light interception model to simulate transpiration at the stand level.

The third model is the so-called 'Single Big Leaf' (SBL) model based on the combined energy and water balance, where the bulk stomatal conductance of the Penman-Monteith equation was described as the products of response functions to several environmental conditions.

All models have different complexities and have different numbers of calibration parameters (ranging from 1 to 6). Model results were compared with half-hourly vapour flux eddy-correlation measurements. The performances of these models showed to be equally good, with $R^2 = 0.777$ to $R^2 = 0.834$, meaning that all concepts were confirmed by the measurements. As a result, a model concept could not be rejected. However, significant discrepancies become apparent when differences between model responses were examined. Main differences between the models were caused by another formulation of vapour pressure deficit and leaf area index (LAI).

In chapter 3 the exchange of CO₂ and H₂O was modelled. In this study CO₂ flux measurements, obtained by 6 gas exchange chambers, were used to identify the parameters of the combined Farquahar/Ball model applied at the leaf level. The highest correlation coefficients between diurnal measured and modelled net photosynthesis was $R^2 = 0.87$ and the lowest $R^2 = 0.61$. These chambers were placed in different trees and at different heights within the canopy. Thereupon, the model STANDFLUX was used to estimate transpiration, CO₂ assimilation and water use efficiency for the total stand. This model integrates the three-dimensional aspects of canopy structure and light interception, one-dimensional vertical stand microclimate and the Farquahar/Ball model. With detailed biomass measurements of needle and branch surface area, the trees were reconstructed and used as input for the STANDFLUX model. Daily deviations between simulated transpiration and measured sapflow were found. To obtain an optimal fit, Ball's model parameter $GFAC$ was calibrated. This, however, hardly influenced the assimilation. Clear correlations between $GFAC$, temperature and soil water content were observed, meaning that alternative stomatal models should be used to obtain better model predictions.
Information content of measurements

Nowadays models often contain many parameters of which parameter values are mostly estimated by fitting the model results to measurements. Non-unique parameter values can be found due to the properties of the measurements and the correlation between parameters. A unique parameter set with high accuracy is a prerequisite to understand the values and to use the parameters for extrapolation in time and space. The Parameter Identification Method based on the Localisation of Information (PLMIJ) was developed to assess unique parameter values with high accuracy. PLMIJ selects measurements where the model sensitivity to one parameter is high while the model sensitivity to the other parameters is low and the confidence interval of the measurement is small.

In a hydrological context, the most important characteristic of the SBL model is the stomatal conductance model. The stomatal conductance is described as a product of response functions to vapour pressure deficit, global radiation, temperature, soil water content and LAI. The model contains many calibration parameters and mathematical formulations of the response functions. In chapter 2, a good fit was found between the SBL model results and the eddy-correlation measurements. Time series of environmental conditions describing forest transpiration contain many periods with coupled conditions and redundant information while other conditions were almost not measured.

In chapter 4, the information content of every measurement for every parameter is calculated with PLMIJ. Measurements with high information content were selected by using independent measurements of environmental conditions. With these independent criteria, periods were selected that have maximum information to identify the parameters. Measurements that were not selected do not add more information to maximise the parameter accuracy further. It is concluded that identification problems will not disappear with the availability of more measurements. The parameter estimates and the fit error obtained by PLMIJ are compared with a conventional simplex parameter identification method using the Jack-knife method. In total 100 sub-data sets were drawn from the total data set containing 60 measurements and were used to identify the parameters. With the conventional method, different parameter sets were found due to the properties of the sub-data sets and due to the non-uniqueness. With PLMIJ, a better fit with smaller parameter accuracies was found. As a result, PLMIJ identifies unique parameter values with high accuracy by using a limited amount of calibration data.
In chapter 5 the model parameters of a rainfall interception model were identified from throughfall and canopy storage measurements. Throughfall, canopy storage and evaporation processes are all dependent of each other. If parameters are identified from a time series in which all these three processes occur at the same time, than a dependency between the parameters is found. *PIMLI* is used to assess the criteria for selecting measurements at periods in which the parameters and processes are independent. With only these measurements, the uniqueness and accuracy of the parameter estimates were calculated. With throughfall measurements, only the interception fraction could be identified with satisfying accuracy. This fraction is independent to other parameters and processes if storage has not yet reached its saturation point and if evaporation is negligible. The accuracy of the estimated storage capacity parameter remained low (σ = 0.55 mm). Best identification was achieved with rain events that are just large enough to saturate the canopy and where evaporation is negligible. The drainage parameter could not be identified from throughfall measurements. The model formulations show that this parameter can only be identified if both the storage capacity and the storage are known. The evaporation amount of the canopy is estimated at the end of a rain event. However, the potential evaporation during rain is very low and the identification of the evaporation parameter is dependent on the uncertainty of the storage capacity parameter. It was found that this parameter could also not be identified.

A much higher accuracy of all parameter estimates was obtained with canopy storage measurements. The accuracy of storage capacity parameter was σ = 0.04 mm. Parameters were identified during the independent stages of the wetting and drying cycle. It is shown that the uncertainty in throughfall predictions simulated with these parameter estimates was even lower than the standard deviation of the throughfall measurements. With *PIMLI*, it is shown that specific conditions can be selected to improve the drainage and evaporation functions of the model. In contrast, a normal identification focuses on a mean fit for the total data set and therefore individual deviations are more difficult to find.

**Analyses of residuals**

After parameter identification, residuals between model results and measurements still remain. Random and systematic measurement errors and model inaccuracies cause these discrepancies. The model inaccuracies are systematic errors due to wrong parameter estimates or due to a wrong model concept. In chapter 6, artificial neural networks (*ANNs*) were used to analyse the residuals for any systematic relationship that may
improve the performance of the SBL model. Several environmental conditions were used as input of the ANNs to analyse the residuals. Only systematic errors with an identifiable physical basis were used to improve the model concept or the parameterisation. ANNs show trends in residuals that were related to both wind speed and wind direction. They were able to localise the source area of the fluxes of the Douglas fir stand within a larger heterogeneous forest without adding a priori knowledge of the forest. By calibrating the model only on this source area, the root mean squared error (RMSE) between the SBL model results and measurements decreased from 26.41 W m$^2$ to 21.85 W m$^2$. With ANNs, improvements were also found in the shape and parameterisation of the response functions. The remaining residuals do not contain any systematic deviation, which is related to the environmental conditions and can be attributed to the random measurement error of the eddy correlation.
Curriculum Vitae


Na deze studies heb ik mijn vervangende dienstplicht vervuld bij de vakgroep fysische geografie en bodemkunde aan de UvA. In mei 1996 trad ik als OIO in dienst bij dezelfde vakgroep om het onderzoek van dit proefschrift uit te voeren. Vanaf 1 september 2000 zal ik werkzaam zijn als docent-onderzoeker milieusysteemanalyse en -modellering bij de afdeling milieuwetenschappen van de Universiteit Utrecht.
STELLINGEN

1. Er zijn geen modeluitkomsten en observaties maar gesimuleerde en geobserveerde modelresultaten.

2. Door de langere meetijd met de gamma-ray methode van Calder en Wright (1986) zal met deze methode het drainageproces in het kronendak nooit te identificeren zijn.

3. De zonsverduistering van 1999 was een uitstekende gelegenheid om metingen te verrichten waarbij de correlatie tussen omgevingsvariabelen, zoals straling en VPD, doorbroken was.

4. Omdat meerdere modelconcepten dezelfde empirische data kunnen verklaren (Duhem, 1904 and Quine, 1951), zou elke modelleur open moeten staan om meerdere modelconcepten te gebruiken.

5. Zolang in termen van meerdere parameter sets gesproken wordt (GUM: methode, Beven and Binley, 1992), mogen de hieruit voortvloeiende parameterwaarden niet fysisch geïnterpreteerd worden.

6. Bij het vergelijken van modelresultaten met metingen moet meer aandacht besteed worden aan de range, verdeling en signaal-ruis verhouding van de data.

7. Het gebruik van verschillende statistische maten om de 'goodness of fit' aan te geven heeft geleid tot verdere verloedering van de term validate.

8. Gezien het feit dat uniek gedefinieerd is als: 'het niet bestaan van een 2e exemplaar', leidt tot de conclusie dat 'uniqueness of parameter values', waaruit identieke oplossingen immer de resultante zijn, voorbij gaat aan de normale betekenis van uniek.

9. De openeurstelling, 'De afwijking tussen modelresultaat en meting geeft meer informatie dan de overeenkomst', is bij veel wetenschappers niet doorgedrongen vanwege de dichtedeurpolitiek op onderzoeksinstutnuten.


Stellingen bij het proefschrift 'Modelling Forest evapotranspiration: behaviour, concepts and parameters' van Stefan Dekker.