# UNIVERSITÄT LEIPZIG

Fakultät für Physik und Geowissenschaften Institut für Geographie

## Modelling of plant-relevant processes of organic farming using the model CANDY including the plant module SIWAPFLAN at the example of Bad Lauchstädt

Wissenschaftliche Arbeit zur Erlangung des Grades eines Diplom - Geographen

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Leipzig, 04.07.2008

"Success consists of going from failure to failure without loss of enthusiasm." Winston Churchill

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#### LIST OF ABBREVIATIONS

a.s.l.	above sea level
BBCH	Biologische Bundesanstalt, Bundessortenamt , Chemical Industry
CANDY	Carbon and nitrogen dynamics
CERES	Crop estimation through resources and environmental synthesis
CO <sub>2</sub>	Carbon dioxide
DC	Decimal code
DSSAT	Decision support system for agrotechnology transfer
E	Evaporation
ELCROS	Elementary crop simulator
EPIC	Erosion Productivity Impact Calculator
e.g.	For example
Eq.	Equation
ETP	Potential evapotranspiration
FAO	Food and Agriculture Organization of the United Nations
I	Interception
I.e.	That is
IPi	Input parameter
ISIP	Informationssystem Integrierte Pflanzenproduktion
IA	Index of agreement
LAI	Leaf area index
Ν	Nitrogen
n	Number of samples
n. d.	No date
Ō	Mean average of the observed data values
Oi	Observed values
OPi	Output value
Р	Precipitation
Perc	Percolation
Pi	Simulated values
R²	Coefficient of determination
rel. E	Relative error
RMSE	Root mean square error
Ro	Surface runoff
ΔS	Change of soil shortage
SI	Sensitivity index

SIMLEP	Simulation model for leprosy transmission and control
SPASS	Soil-plant-atmosphere system and its simulation
SUCROS	Simple and universal crop growth simulator
т	Transpiration
%RMSE	Percent root mean square error

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## **1** INTRODUCTION

The processes of plant growth are one of the most important agroecosystem functions. All are essentially determined by fluctuations of the environmental factors under natural conditions. Changes in environmental conditions influence e.g. soil moisture availability and the plant root uptake of soil nutrients and water. It also affects the ontogenesis and depends on the growth stage of a plant which can result in large losses of plant biomass (VLEK et al. 2007). Knowing the interactions of all factors on a specific site facilitates statements of plant-relevant processes due to environmental factors.

With the help of agroecosystem models it has been attempted to cope with complex natural processes and interactions for more than four decades. Those models abstract and quantify the natural processes and factors of influence using mathematical equations which are subsequently used to reveal the interactions. Based on the quantification, the effects of environmental and agronomic management factors on plant growth processes can be determined and analysed.

CANDY (Carbon and Nitrogen dynamics) (FRANKO 1995a) represents one model in a pool of various agroecosystem models. Its modelling is based on the results of an intensive monitoring and the long term experiments in Bad Lauchstädt. Until now, the model CANDY includes plant dynamics as a simple empirical approach without considering environmental factors. To improve this lack, the plant module SIWAPFLAN (FRANKO et al. n. d.) was implemented in the model CANDY with the aim to model extensive plant processes. The generic module for different plants reacts on the base of environmental influences and simulates plant-relevant variables and processes on the same basis.

Thus, the present study is understood as applicability assessment and improvement of the plant module SIWAPFLAN to describe plant dynamics. The assessment and improvement of the module are based on plant variables which represent and quantify the plant growth processes in an agroecosystem. A detailed observation and measurement time series of crop variables (e.g. leaf area index) are required.

## 2 AIMS AND APPROACH

The main objective of the present study is to assess and to improve the applicability of the plant module SIWAPFLAN regarding the description of plant development and growth processes at the example of the location of Bad Lauchstädt. This aim requires the following approach:

- 1. Analysis of agroecosystem-relevant processes in relation with CANDY
- 2. Analysis of plant-relevant processes and implementation in SIWAPFLAN
- Assembling and extension of an adequate data set as a base of the SIWAP-FLAN module assessment
- 4. Calibration of the plant module SIWAPFLAN
- 5. Validation of the plant module SIWAPFLAN
- Assessment of the results regarding the applicability of the plant module SI-WAPFLAN

The basis of agroecosystem modelling is the understanding of natural processes. Therefore, the analysis of natural agroecosystem processes and the implementation in the agroecosystem model CANDY will come to the fore in the first part of the present study.

The description of plant growth processes in a simplified form of a model demands to manage its complexity and to focus on the important and relevant aspects. Therefore, the gained insights about the natural plant-relevant processes will serve for the analysis of the plant module SIWAPFLAN which is included in the model CANDY and represents plant-relevant processes.

The investigation area Bad Lauchstädt with the experimental field 'land use experiment' - management system organic farming - provides a data set with plant-relevant variables and characteristics, e.g. development stages, biomass growth and nutrient uptake. These variables were already quantified. For the present study, the provided plant variables required to perform the following calibration and validation of the plant module SIWAPFLAN will be assembled. This study is concentrated on the three investigated crops winter wheat, potato and maize which represent the existing diversity of cultivated crops on the location. The already existing data set of Bad Lauchstädt will be extended by an actual collection of data focussing on the field work of the year 2007. The leaf area index (LAI) is an important plant-relevant variable for plants, particularly with regard to the plant module SIWAPFLAN for the simulation of the assimilation. Due to this fact, own LAI measurements were obtained using the LAI-2000 Plant Canopy Analyzer. The choice of this method is motivated by positive experiences during a previous project and the availability of the device.

The calibration of the plant module SIWAPFLAN will be conducted with the plantrelevant variables, e.g. plant development stages and biomass growth, as these represent the plant growth processes or are the result of those. The simulation of plantrelevant variables will also be used to test the module and to determine plant-specific parameters. The LAI will be represented a focus of the module calibration. The calibration is regarded successful, if the difference between the observed and simulated values is in an acceptable range of less than  $\pm 20$  %.

The plant module SIWAPFLAN should be validated under environmental conditions, to assess its accuracy concerning the performance of major processes. The validation of the plant module will be conducted with the simulation of plant growth processes in another time period. This procedure will show whether the module is able to simulate the plant variables and therefore, the plant-relevant processes. The results will be orientated on the literature-usual deviation of 20 % between the simulated and observed values.

A general discussion contains an assessment of the applicability of the module regarding the description of plant growth and development processes at the location. The concluding reflection of the obtained results is included in the conclusion and outlook section and completed by recommendation for future work.

The present study is focussed on plants dynamics in an agroecosystem. Therefore, the terms plant and crop are used synonymously.

## **3** AGROECOSYSTEM, CROP GROWTH AND ITS MODELLING

Agroecosystems are defined as systems of mutually interacting organisms and their environment in relation to crop production. They have a central role in the whole terrestrial cycle of energy, water and matter. The analysis of processes and interactions in system soil - plant - atmosphere - management are prerequisites for modelling the influences of weather, site characteristics and management. On this account, different complex models exist depending on the aim, purpose, species of plant and site.

The agroecosystem model functions can range from a focus of soil water balance, Cdynamics, soil nutrient balance, management strategies as well as biomass production and yield of crop.

The modelling of agricultural systems and its processes have gone through 40 years, when system analysis and the development of modern computers formed a basis of new techniques to scientists. Since then, modelling went trough a number of developmental stages (SINCLAIR & SELIGMAN 1996). Before the 1970s, individual processes were developed, e.g. soil water movement (RICHARDS 1931) and infiltration. In soilplant interactions model theories were produced for evapotranspiration (PENMAN 1948, MONTEITH 1963 cited in LANGENSIEPEN 2006) and photosynthesis (SAEKI 1960 cited in HIROSE 2005). In the same period, DE WIT focussed on plant growth, whereas the ther authors concentrated on soil nutrients (AHUJA et al. 2002). In the early 1970s, multiple component models of agricultural systems were developed. E.g. DE WIT (cited in BOU-MAN et al. 1996) designed the first dynamic model ELCROS (Elementary crop simulator) based on processes of photosynthesis. Furthermore, the model includes the concept of production which is based on growth – limiting factors. PENNING DE VRIES (1974) and GOUDRIAAN et al. (1975) extended this approach as they implemented the plant microclimate. VAN KEULEN (1980) developed the CROP ARID model for agricultural crops under consideration of soil water and management conditions. During the 1970s, the SUCROS model (Simple and universal crop growth simulator) (VAN KEULEN et al. 1982 cited in BOUMAN et al. 1996) was published and became an important basis for several models. At the beginning of the 1980s RITCHIE et al. (1987 cited in ENGEL et al. 1993) developed CERES (Crop estimation through resources and environmental synthesis) enabling the user to model the influences of weather, plant varieties, soil water content and availability of nitrogen. The model CANDY was developed by FRANKO (1995a) for soil-based processes in agriculturally used landscapes. From that time on module simulation systems have been dominating crop modelling (LANGENSIEPEN 2004). In recent years, agroecosystem models have become increasingly important representing the main component of agriculture-related decision-support systems (JAME & CUTFORTH 1996). DSSAT (decision support system for agrotechnology transfer) is a package of agroecosystem models for 16 different crops worldwide and helps decision-makers to analyse complex alternative decisions by reducing time and human resources (JONES et al. 2003).

The principle of modelling and its application are based on the understanding of natural processes, which are involved in the growth of crops, and using this understanding to describe processes of an agroecosystem including crop growth processes. The following section gives a short overview about agroecosystem processes. On the one hand, important natural processes will be explained and, on the other hand, the abstracted implementation of those natural processes into the CANDY model will be described as it establishes the 'framework' for this study. A short reflection of the aspects about management will complete the description of the modelling with CANDY.

Subsequently, a more detailed explanation of the crop growth process will be given focussing on the current state of knowledge as this is the main core of the present study. Important natural processes will be described and followed by the abstracted implementation of those processes into different models. In section 3.3, the implemented crop growth processes of the module SIWAPFLAN will be delineated.

## 3.1 Agroecosystem processes and its modelling with CANDY

The model CANDY was developed to simulate carbon and nitrogen dynamics in the unsaturated zone of agricultural soils. The one-dimensional simulation system integrates different modules and a database system for model parameters, measurement values, initial values, meteorological data (driving forces) and management data. A more detailed explanation of the model CANDY is available in FRANKO et al. (1995b).

A main focus of CANDY is the description of the C-dynamics, sustainability of soil organic matter and sequestration of carbon including the plant as an important component. The plant delivers the base of soil organic matter and stores carbon in the form of photosynthesis.

The agroecosystem simulation with CANDY includes the following five modules:

- climate module,
- management module,
- soil module (soil water and soil temperature),
- module of organic matter turnover including soil nitrogen (C-N-dynamics),
- different plant and crop modules, one of them is SIWAPFLAN.

The climate and management module and its data provide the driving forces for the model CANDY and its modules. The main processes of the soil module (soil water dynamics) and module organic matter turnover including soil nitrogen (C-N dynamics) are the base of the simulation of plant dynamics and vice versa. Soil nitrogen and soil water dynamics will be explained subsequently as both represent the most important influencing factors concerning crops within CANDY.

## 3.1.1 Soil water dynamics

Soil water directly affects plant growth by controlling the plant water status and indirectly due to its influence on aeration, temperature, nutrient transport and uptake as well as transformation (HAMAN & IZUNO 2003). The soil water dynamics depend on the water supply of precipitation, water loss by evapotranspiration and water uptake by plants as well as seepage and percolation. For a site with crop canopy the following water balance equation is valid (HUPFER & KUTTLER 2006):

$$\Delta S = P - I - E - T - R_o - Perc$$
 Eq. 1

The change of soil moisture storage ( $\Delta$ S) is calculated by the amount of precipitation (P) minus the interception loss (I) and the evaporation (E), transpiration (T), surface runoff (R<sub>O</sub>), percolation of water (Perc) and capillary rise (if percolation < 0).

The soil moisture storage refers to the amount of water held in the soil at any particular time. The amount of moisture in the soil depends on soil properties and varies for each

soil horizon. Thus, CANDY considers the following soil parameters in homogenous soil layers of 10 cm thickness for the simulation:

- soil horizon depth (dm),
- particle density (g cm<sup>-3</sup>),
- bulk density (g cm<sup>-3</sup>),
- permanent wilting point (VOL %),
- field capacity (VOL %),
- clay content < 2 µm (M %),</li>
- fine silt content 2-6.3 µm (M %),
- saturated conductivity (mm d<sup>-1</sup>).

Precipitation is the main driving variable for the soil water dynamic and especially for the infiltration into the soil, which is illustrated for a site in Figure 1. The hydrological processes of CANDY are based on the capacity concept after GLUGLA (1969 cited in DREYHAUPT 2001) which considers the drainage of water through gravitation forces.



Figure 1: Schematic of the soil water dynamics of a site (changed after FAO 1998)

Evapotranspiration represents the combined transfer of water into the air by transpiration, evaporation and interception. The actual evapotranspiration is the amount of water delivered to the air from these three processes and depends on moisture availability, temperature and humidity (FAO 1998).

Evaporation is a process whereby liquid water is converted to water vapour and removed from the evaporating soil surface whereas the plants are not involved. However, in spring, the evaporation is plant-relevant as the evaporation process decreases the soil water content in the topsoil. This effect is necessary for the sowing. The degree of shading of the crop determines the evaporation rate of the soil.

Transpiration represents a phase change when water is released into the air by plants. It is responsible for several processes: transport of minerals from the soil throughout the plant, plant cooling through evaporation, transport of sugars and plant chemicals and maintenance of turgor pressure. Thereby, the transpiration rate depends on the soil water content and on plant characteristics which are described by the LAI (EHLERS 1996).

The simulation of evaporation and transpiration in CANDY is driven by the potential evapotranspiration (ETP) determined by given meteorological conditions and with an unlimited supply of water. ETP constitutes the upper limit for the evaporation and transpiration process. Furthermore, the simulation of the transpiration is determined by the water uptake by roots. Due to the fact that the evaporation and transpiration are influenced by the crop canopy, both processes are calculated as a function of coverage in the model CANDY.

The interception describes the amount of precipitation that is directly lost by plants. The simulation of water interception in the crop canopy is realised by a simple capacity approach in CANDY. The interception capacity depends on the variables plant height and coverage (FRANKO et al. 1995a).

The surplus of precipitation, which cannot be added to the soil storage nor used for the actual plant transpiration, is involved in deep percolation, which represents the downwards transport of water from the root zone to the layer below the root zone. The capacity concept after GLUGLA in CANDY considers a possible downwards water flux if the soil moisture exceeds the layer specific field capacity. The capillary rise, which is the upwards transport into the rooted zone, is unconsidered in the soil module of CANDY. The capacity concept has the advantage of smaller requirements but it is a simple abstraction of water flux (KLÖCKING & SCHAAF 1993).

## 3.1.2 Soil nitrogen dynamics

The nitrogen cycle in soil includes different processes illustrated in Figure 2. In the soil, nitrogen is in a continuous state of flux. The basic assumption of CANDY formulates

that the micro organisms operate for processes of nitrogen transformation in soil and the turnover of carbon provides the energy of micro organism activity (FRANKO 1995a). The nitrogen turnover in CANDY is linked with the carbon turnover according to the specific C/N ratio and is calculated as first-order reaction kinetics. In addition, the plant available nitrogen is determined by the decomposition of organic soil matter. CANDY describes the processes of formation, decomposition and transformation of organic soil matter and dynamic of inorganic compound.



Figure 2: Schematic of the soil nitrogen dynamics (changed after WIEDERHOLT & JOHNSON 2005)

With the crop yield, a large amount of nitrogen is removed from the system. Surface runoff and soil erosion can cause losses of soil nitrogen. Other losses occur through volatilization of ammonia and leaching or denitrification of nitrate. On the contrary, four types of inputs can compensate nitrogen losses: mineral fertilisation, atmospheric deposition, organic amendment (manure) and nitrogen fixation by legumes. The latter one is the principal natural factor by which atmospheric nitrogen is added to the soil (Figure 2) (TRAUTMANN et al. n. d.). All components of the soil nitrogen dynamics are considered in the simulation of CANDY except the volatilization as it is assumed that the pool of ammonium is very small.

The input of mineral fertiliser directly provides the inorganic and plant available form of nitrogen. The manure contains organic nitrogen which is not directly available for plant uptake. Processes of mineralisation, nitrification and immobilisation are important for crop growth processes because it transforms the organic to inorganic nitrogen.

As plants and other organic residues decompose (soil organic matter), nitrogen is converted to ammonium by soil micro organisms which is the process of mineralisation. Plant roots absorb some of the ammonium ions. The simulated N mineralisation in CANDY follows the C mineralisation considering the specific C/N ratio.

The process of immobilisation is an uptake of ammonium by micro organism. This N is transformed from the mineral to the organic pool and is not available for plants. This part underlies the first-order reaction kinetic and also depends on the C/N ratio of soil organic matter in CANDY.

Bacteria transform the ammonium in the soil to nitrite and then to nitrate in a sequence of steps called nitrification. Nitrate is a negatively charged anion and therefore usually remains in the soil water rather than being adsorbed by soil particles. Plant roots take the nitrate ions up (SCHEFFER & SCHACHTSCHABEL 2002). In CANDY, the Michealis-Menten kinetics is used to describe this process.

Furthermore, in anaerobic condition, some bacteria meet their energy demand by reducing nitrate to dinitrogen gas or to nitrogen oxide ( $N_2O$ ). This biological process is called denitrification. It results in a loss of nitrogen from the soil and the return of nitrogen to the atmosphere (SCHEFFER & SCHACHTSCHABEL 2002). The process of denitrification is considered in CANDY with a reduction of soil temperature and moisture.

## 3.1.3 Plant dynamics

The modelling of plant dynamics varies in complexity, subject to the task and purpose of the model. With CANDY, the simulation of plant dynamics can be performed by selected provided plant modules according to the task and purpose of the simulation.

The selection of plant modules in CANDY is enabled by the hierarchical principle in the model structure. I.e. the plant dynamics is already represented by four crop variables independent of the internal complexity of the selected plant module. All mentioned modules of CANDY are linked with the selected plant module by four representative variables:

- crop height,
- root depth,

- coverage,
- N uptake.

In addition, the climate and management module provide the driving forces for CANDY. The link between the climate module and the plant module depends on the selected plant module. Figure 3 illustrates the general interaction and information exchange between the soil modules, the C-N dynamics module of CANDY and the plant dynamics.



Figure 3: Information exchange between the plant dynamics and the further modules of the model CANDY (own graphic)

The plant dynamics influence and depend on soil water dynamics. The plant capacity of precipitation interception, which is determined by crop variables coverage and crop height, minimises the infiltration into the soil. The coverage is also involved by the simulation of the actual evaporation and transpiration in the soil module. The crop variable root depth determines the water uptake which is also determined by the actual transpiration.

As shown in Figure 3, the second main interaction exists between the plant dynamics and the C-N dynamics. The soil organic matter is coupled with the biomass and its residues which remain in the system. The plant N uptake depends on the CANDY processes of mineralisation and nitrification which produce plant available nitrogen (soil nitrate and soil ammonium). Furthermore, the information about the mineral nitrogen input by atmospheric deposition, fertiliser and manure is exchanged to N uptake in the plant module. The turnover and transport processes of C-N dynamics in the soil are influenced by soil water and temperature dynamics (Figure 3).

The interactions and exchanges with the modules of CANDY, which are especially influenced by the module SIWAPFLAN, will be explained in section 3.3.

## 3.1.4 Management system

Processes of an agroecosystem are basically equal in the organic farming in comparison to conventional management. The difference between them is that organic farming excludes the application of mineral fertilisers and pesticides. The outcome of this is a feature for the crop growth processes of organic farming and its modelling. I.e. the natural nitrogen sources mainly consist of residues of N-fixing crops and organic amendment. This is the reason why crop growth processes without high N mineral input and pesticides underlie fewer control mechanisms and guarantors to obtain economic biomass production and yield. Hence, the biomass production and yield of organic farming are subject to fluctuations.

Regarding crop growth, especially in soil, equal main process dynamics occur independently to management systems. Therefore, the modelling of crop growth processes on organic farming with CANDY is considered possible. The conscious difference can be realised by parameter adaptation in the plant module.

## 3.2 Crop growth processes and its modelling

A crop growth model / module should consider the processes which are common to all plant types cultivated in an agroecosystem. The production of biomass, which results from all processes, is the most important fact for agriculture. It is basically the result of growth which can be described as an irreversible increase of volume and matter. The processes of growth are directly connected with development. Therefore, the increase in weight or in height is not possible without development. As a matter of fact, development is regarded as an irreversible process of change in the state of an organism and generally progresses to a more or less fixed and species-specific pattern (GOUDRIAAN & VAN LAAR 1994). Furthermore, both the development and biomass

growth are connected with the nitrogen uptake that is subducted from the agriculturally used system. This uptake is performed by roots which penetrate the soil.

In view of modelling in this study, the crop growth processes are assigned in three components: plant development, plant biomass growth and plant nitrogen uptake. I.e. the term 'crop growth processes' is used as a holistic description and identifies all plant processes of plant development, biomass growth and nitrogen uptake in this study.

## 3.2.1 Plant development

Plant development, usually called ontogenesis, is defined as a succession of stages whose number and characteristic depend on the used ontogenesis scale (WERNECKE & CLAUS 1996). In practice and in this study, the extended BBCH-scale is applied to estimate the development of investigated crops. The abbreviation BBCH derives from the <u>B</u>iologische Bundesanstalt (German Federal Biological Research Centre for Agriculture and Forestry), <u>B</u>undessortenamt (German Federal Office of Plant Varieties) and <u>Ch</u>emische Industrie (chemical industry). The entire developmental cycle of plants is subdivided into ten clearly recognizable and distinguishable longer-lasting developmental phases. These principal growth stages are described using numbers from 0 to 9 in ascending order (MEIER 2001) (Table 1).

Stage	Description
0	Germination
1	Leaf development
2	Tillering
3	Shoot development
4	Booting / Development of harvestable vegetative plant parts
5	Heading / Inflorescence emergence
6	Flowering
7	Development of fruit
8	Ripening of fruit
9	Senescence

 Table 1: Principal growth stages (changed after MEIER 2001: 2) The stages do not necessarily proceed in the strict sequence defined by the ascending order of the figures but can occasionally also proceed simultaneously

The 10 stages are not sufficient to define an exact plant development. Therefore, the secondary stages (00 to 99) can be used if points of time or steps in the plant development must be indicated precisely. This scale is a system for a uniform coding of

phenologically similar growth stages of all cultivated plant species. The decimal code (principal and secondary growth stages) are based on the cereal code developed by ZADOKS et al. (1974) in order to avoid major changes from this widely used phenological key (MEIER 2001).

Necessary agricultural procedures such as fertilisation, mechanical and chemical weed control and the time of plant protection procedures can be assigned to the development stage of the plant. Furthermore, delays of growth and damaging influences can be identified in time. In addition to that, the BBCH scale is suitable for comparison between results from preceding and following years. The code became generally accepted in international agriculture. It is standardised, internationally co-ordinated and thus a generally valid and world-wide code in research, consultation and practice accepted aid (MEIER 2001).

As previously described, the BBCH-scale allows the use of identical code numbers for similar ontogenesis stages. Figure 4 illustrates the theoretical explanations of the BBCH-scale for important development stages of winter wheat, potato and maize.



Figure 4: Schematic of important growth development stages of winter wheat, potato and maize (changed after LANDWIRTSCHAFTSKAMMER NORDRHEIN-WESTFALEN 2007)

Plant development in stages is a central component of crop growth models. This function acts as a time-related control variable for other processes which are initiated, stopped, accelerated or slowed down by ontogenesis. The exact simulation of development is necessary for partitioning and the course of biomass. In addition, the prediction of development stages is used for timing of fertilisation and plant protection (ROßBERG et al. 2005).

The basic approach for processes of development in crop growth models is the quantification of the influence of environmental factors on ontogenesis. These factors could be divided in two groups. The first group is more general and contains temperature and day length which are important for the whole growing season. The second group of factors is characterised by influence in defined development phases and / or a plantspecies dependent influence and includes the temperature effect (e.g. coldness, frost) and soil moisture. The effects of environmental factors can be mostly assigned to one major factor. However, in most cases a combination of different factors affect one process.

The temperature and its course is an essential factor for plant development (HEYLAND 1996). The close relation of temperature to development can be used for their calculation in stages. E.g. in the model SIMULAT, only the day mean temperatures are accumulated to temperature sums for every development stage. Subsequently, these values are used to predict crop development as a function of temperature (SCHRÖDER 1995). The influence of temperature could also be considered by comparing species-specific base temperature and the day mean temperature which results in growing degree days. This concept is realized in the model SPASS (Soil-plant-atmosphere system and its simulation) for potato (GAYLER et al. 2002). Also, the application of minimum and maximum day temperature is conducted to derive plant development. The heat units based on this concept are implemented in the model EPIC (Erosion Productivity Impact Calculator) (WILLIAM et al. 1993)

Furthermore, the photoperiod, also called day length, is determined for the rate of development because the duration of day length is positively related to the amount of daily radiation that is important for the assimilation. Three major groups of photoperiod types are categorized: short-day plants, long-day plants and day-neutral plants (SCHIL- LING 2000). E.g., temperate cereals are long-day plants and have a strong dependency on day length in the stages of heading (SCHRÖDER 1995).

The effect of coldness over a defined period (vernalisation) is necessary for winterform crops to return to vegetative growth in spring (HEYLAND 1996). The adaptation reaction of winter cereals is also influenced by day length which changes regularly and acts as signals or stimuli for the induction of metabolic changes (SCHILLING 2000). In the model SPASS (WANG 1997) the calculation of plant development is divided in development before and after emergence to consider the behaviour of vernalisation.

The influence of water content in the soil is important in the development process because seeds do not germinate if the soil is very dry. Also, high water content avoids the heating of soil and consequently delays the emergence of the crops (ROßBERG et al. 2005). This shows that moisture is a major external factor influencing the emergence. However, the length of the interval from sowing to emergence depends on soil moisture in combination with the temperature and air regimes within the soil (PETR 1991). WERNECKE & CLAUS (1996) developed the ontogenesis model ONTO which considers soil moisture for calculation of the ontogenetic progress. In the stages of ripeness, a consideration of the soil water should be used due to the fact that the harvest of crops depends on the moisture of the grain.

## 3.2.2 Plant biomass growth

All functions of plant and hence the biomass growth / production are more or less dependent on photosynthesis. The processes of the biomass growth, the development and the metabolism are involved in the photosynthetic apparatus which is the green biomass, mainly composed of leaves (SCHILLING 2000). The course of the light interception curve is characteristic and different for several types and species of plants. Therefore, in the photosynthetic-based models, the interception of light of the leaf area is calculated to simulate the production of photosynthesis. A common approach is the leaf light response curve for potential assimilation (MARCELIS et al. 1998). The model DAISY simulates photosynthesis by a single light response curve and light distribution of crop canopy in the form of Beer's Law (HANSEN 1993). In addition, leaf area development of the crop as a whole is simulated, rather than that of an individual leaf. This approach is called "big leaf". Based on big leaf, it is assumed that the process of potential assimilation of a crop stand is equal to a single leaf. Further approaches can be discerned. The EPIC model (WILLIAMS et al. 1993) considers the leaf area development as a function of development stages. The WOFOST model (DE KONING et al. 1995) multiplied the leaf weight by a specific leaf area. MARCELIS et al. (1998) discuss the leaf area or LAI as a given input. The model family AGROSIM (MIRSCHEL et al. 2002) uses the daily produced fresh matter as a reference value for the calculation of the LAI which is then used for the green biomass.

The examples show that the application of the green biomass is handled in a different way. The photosynthetic fixation of solar energy and carbon dioxide is determined by the leaves or leaf area in the form of the plant-specific maximum photosynthetic rate and thus results in a potential assimilation. Furthermore, the assimilation is depending on the mechanism of the CO<sub>2</sub>-fixation. Here, two kinds of plants must be distinguished. C4-plants (e.g. maize), naturally growing in warm and dry climate, have a higher profit of light energy. However, those plants need a higher ambient temperature to produce the higher assimilation. The other kind of plants is the C3-plants (e.g. wheat) which are adapted on a temperate climate (Figure 5) (HEYLAND 1996).

The effects of the environmental and management factors modify the potential assimilation in actual assimilation. This process has an optimum in a plant-specific temperature range (Figure 5). If the temperature falls below or rises above the optimum temperature, the assimilation is reduced and the growth activity declines (SCHILLING 2000).



Figure 5: Temperature dependency of assimilation activity (changed after EHLERS 1996)

Besides the assimilation, the respiration is important for maintenance of the produced biomass. Furthermore, the daily produced assimilates are partitioned between the different plant organs in a development-dependent way. Most models have an assimilation pool for the daily produced assimilates which are divided in parts for the biomass gain and the respiration (MARCELIS et al. 1998). The partitioning of the biomass gain between the considered crop components is ontogenesis-dependent. The considered components of the growth processes depend on the model purpose. Mostly, two parts (above-ground biomass and roots) or three parts (above-ground biomass, roots and shortage organs) are considered (KLÖCKING & SCHAAF 1993).

In addition, the daily assimilates are influenced by water availability (HEYLAND 1996). 90 % of the gas exchange happens through stomata. The process of gas exchange of the plant is assumed to be equal to the gas exchange of a single leaf. During day light the stomata of the leaves are open. Through them, CO<sub>2</sub> is assimilated and water vapour is emitted into the unsaturated ambient air. In an optimal case, the stomata are open during the whole time of the day light and so the maximum assimilation of CO<sub>2</sub> is possible. A lack of water results in partly or completely closed stomata. Consequently, the assimilation slows down or stops completely (EHLERS 1996). In this case, the water supply for the canopy gas exchange is restricted by the ratio of water uptake through roots and water loss by leaf transpiration. The stomatal and transpiration loss is influenced by temperature, humidity and movement of the air (PETR 1991).

The water supply for the canopy gas exchange in the model HERMES is indicated by the daily ratio of actual and potential transpiration (KERSEBAUM 2007). The degree of influence on assimilation is established by comparing calculated actual and potential transpiration. If the ratio of transpiration drops below a specific threshold, a stress situation for crops influences the assimilation.

An optimal plant water supply is connected with ontogenesis and has also a cropspecific aspect. The water deficit is one of the important factors which possibly reduce, e.g., the number and weight of caryopses (SCHILLING 2000).

For the utilisation of the absorbed radiant energy in photosynthesis, the plant does not only require adequate amount of water, but nitrogen as well. This element and its compounds are involved in the whole plant metabolism. Therefore, a non-optimal supply of nitrogen minimises the photosynthetic rate and so growth and biomass are also reduced (EHLERS 1996). The biomass production within the model DAISY is based on the concept of production levels (HEIDMANN et al. 2008). Level one, the potential production, represents the growth rate only depending on the radiation and temperature influence. At level two, the factor water limits the production of biomass from level one.

Further effects of biomass production have crop pests and diseases which exist in a great variety. Temperature is the most important factor for pests. Metabolism, rate of development, food intake and reproductive behaviour is regulated by the temperature course. Therefore, the size of pest population and the extent of damage are influenced by temperature in combination with further environmental conditions. The time of migration depends on pest-specific temperature thresholds. Furthermore, temperature is decisive for the infection process of fungal pathogens. The host crop can also be influenced by temperature with the change of their resistance. Moderate temperatures in the winter support the possibility of the survival of virus pathogens and influence their reproduction in the host plants (PETR 1991).

Daylight length and light intensity have similar influences on pests as well as on crops. Migration and reproduction of insects are influenced by the photoperiod. Light intensity often stimulates the activity start of insects and then the movement and sexual behaviour (PETR 1991).

A further major effect is humidity. A lot of diseases develop better in humidity years with high precipitation and throughout the growing season because the viability of pathogen spores is influenced by air humidity. The consideration of pests and diseases is not applied in most crop growth models (KLÖCKING & SCHAAF 1993) or the coupling with crop growth models is used because the pest populations' dynamic and the infection of diseases are often simulated in separate models. One example of a population model is SIMLEP (Simulation model for leprosy transmission and control) which serves for the prediction of the early development of potato beetles populations. The program ISIP (Informationssystem Integrierte Pflanzenproduktion) is an agriculture-related decision-support system in Germany which is developed to aggregate different monitoring programs and models for pest and disease. These facilities are provided and used for agriculturists and agricultural institutions (ISIP 2008).

## 3.2.3 Plant nitrogen uptake

The process of nitrogen uptake by plants is already mentioned above in the process of biomass production. This process should be described in detail. The rate of nitrogen uptake is highly variable during the growing season. It is influenced by factors such as plant development-dependency of nitrogen uptake and the N supply in the soil. In an optimal of soil nitrogen availability, the crop accumulates nitrogen in relation to growth rate and biomass accumulation. An important point is that the rate of nitrogen uptake is not only regulated by the soil availability but also by the biomass growth rate. Due to that, the increase of biomass causes the decrease of N uptake. It is assumed that a critical N concentration in plants is given which means a minimum of nitrogen by a maintained maximum of growth (GASTAL & LEMAIRE 2002). The critical N concentration declines during crop growth. The application of an ontogenesis-dependent critical N concentration variable is often used in crop growth models to calculate a lack of nitrogen.

The components of crop demand for N and the soil supply of N is simulated separately, whereas the lower one is used to determine the actual rate of uptake in the model CERES (JAME & CUTFORTH 1996). The actual concentration of N is compared to the defined critical concentration of nitrogen in the model and therefore, a lack could be detected and the growth will be reduced.

The plant reaction of nitrogen deficiency is ontogenesis-dependent. I.e. the leaf growth reaction to the lack of nitrogen is less sensitive. Nitrogen supply has a large effect on shoot growth and on N-shortage of caryopses (GASTAL & LEMAIRE 2002). The model N-SIM (ENGEL 1993) regulates the different influences of nitrogen lack with a nitrogen factor for each organ growth process.

Furthermore, the most important environmental factor, which affects nitrogen uptake, is the water regime of soil and plants. Water supplies nitrogen to plants and is involved in most soil and plant processes. The translocation of nitrogen occurs within the medium water (EHLERS 1996). In addition, the plant uptake of nitrogen is related to conditions of light. I.e. a high illumination of the above-ground biomass causes a high uptake and nitrogen can be utilised more efficiently in formation processes of protein and chlorophyll. A low photosynthesis affects a low uptake by plant. A reduction of photosynthesis corresponds to a low translocation of assimilation production into the roots. This results in a decrease of plant growth and also in a reduced nitrogen uptake. All this effects a secondary reduction of photosynthetic processes. Therefore, the amount of nitrogen uptake by plant is a major impact on overall crop growth rate (PETR 1991). Most of the crop growth models include the interconnection of nitrogen and biomass production.

The further effect of N supply for plants is related to rooting depth, root density and architecture. DE WILLINGEN & VAN NOORDWIJK (1995) discuss the modelling of nitrogen uptake by a root system with representative roots or non-regularly distributed roots. However, a part of crop growth models, e.g. WOFOST (EITZINGER et al. 2004) use only the initial and maximum root depth for the calculation of root extension. Furthermore, the growth of roots is influenced by soil temperature and moisture (PETR 1991). These relations are considered in the model TRITSIM (MIRSCHEL et al. 1993). Besides, the relation of the rooting depth, the rate at which roots of seedlings develop in certain depths, will be important (GASTAL & LEMAIRE 2002). In stages from sowing to heading, the temperature optimum for root growth ranges from 9 to  $16 \, \mathbb{C}$  (P ETR 1991).

The above mentioned main processes of crop growth are also considered in the plant module SIWAPFLAN which will be explained in the following section.

## 3.3 Crop growth processes of the plant module SIWAPFLAN

The plant module SIWAPFLAN was implemented in the model CANDY by FRANKO in cooperation with STENITZER and FEICHTINGER (FRANKO et al. n. d.) and includes the plant growth approach of the SIMWASER model. The deterministic model SIMWA-SER, which was developed by STENITZER (1988), focuses on the simulation of soil water balance in connection to plant growth (STENITZER et al. 2007).

The modelling approach of plant growth is described by STENITZER (1988) as follows: water flux and growth of plant are linked together by the physiological processes of transpiration and assimilation. The increase of plant biomass depends on the uptake of carbon dioxide via the stomata and the loss of water vapour from the inside of the plant into the unsaturated ambient air. As long as the water supply towards the stomata can meet the potential transpiration, potential assimilation and thus potential biomass pro-

duction is possible. Otherwise stomata will close and the formation of biomass will be reduced. All these processes depend on the plant development stages (STASTNA & STENITZER 2005).

The application of the model SIMWASER is mainly determined by aims and tasks on the soil water balance and soil structure at different locations (STENITZER & MURER 2003). Furthermore, the soil water balance of the model was calibrated and validated on lysimeter data (STENITZER & GASSNER 2004, STENITZER & HÖSCH 2007). The plant growth approach of the model SIMWASER is primarily validated with measured values of two sites in the "Vienna Southern Basin" (STENITZER 1988).

The plant module SIWAPFLAN contains the previously explained approach of STENITZER (1988) with the two sub modules 'Plant development' and 'Assimilation and biomass growth'. The sub module 'N uptake' (FRANKO & FEICHTINGER n. d.) completes the plant module which is illustrated in Figure 6. The main driving forces are the data of the CANDY climate module (temperature, global radiation, precipitation and day length). The sub modules simulate plant-relevant processes which are described in detail in the sections below.



Figure 6: Schematic of the plant module SIWAPFLAN (own graphic)

## 3.3.1 Sub module 'Plant development'

The photo thermal concept of NUTTONSON (1948 cited in WIELGOLASKI 1999) is the basis of the sub module 'plant development' of the module SIWAPFLAN. The approach uses a combination of temperature and day length which provides a simple method to calculate plant development stages from emergence to harvest in terms of photo thermal units (PTU). The duration of the individual development stages is defined by a cer-
tain sum of photo thermal units. The daily value of PTU is the difference between the mean air temperature and the base temperature ('BTEMP') multiplied by the day length (DAYLGT). 'BTEMP' describes a minimum value of temperature which has to be transgressed for plant development.

'BTEMP' minimum value of temperature for development - plant-specific parameter

The calculation of the actual development stage (DEVSTG) on each simulated day can be obtained by comparing the accumulated sum of the PTU with the sum of the photo thermal units that is necessary for the ripeness ('RIPING'). 'RIPING' is as well a plantspecific parameter (Figure 7).



Figure 7: Schematic of the sub module 'plant development' (the red line characterises the sub module, squares with a continuous line symbolise the driving forces, shapes with a dashed line are plant-specific parameters, diamond shapes show the internal quantity that could also be exported as an output result, e.g. development stages) (own graphic)

The calculation of development stages (DEVSTG) is based on the "scale of HANWAY" which classifies the development of crops in 10 stages. For the module output the development stages of HANWAY (1963) are converted in the scale of FEEKES (20 stages) and then in the scale of BBCH and decimal codes (DC) with 100 stages after MEIER (2001) and ZADOKS et al. (1974). In this study, both scales are equal and referred as BBCH / DC stages in the present study.

The classification of HANWAY (DEVSTG) is used for the internal computations and regulations of the plant module. Therefore, the internal DEVSTG is a central component of the module SIWAPFLAN and acts as a time-related control variable for other processes which are initiated, stopped, accelerated or slowed down by ontogenesis. I.e. the development stages (DEVSTG) are passed on to the sub modules 'Biomass

Eq. 2

growth' and 'N uptake'. The calculation of all the other processes of the whole module used the development stages. Therefore, the sub module 'Plant development' is superordinate which is illustrated by the place in the top of the triangle (Figure 6).

The simulation of plant-specific development of plant height (PH = output result) and root depth (RD = output result) are also realised by the current sum of photo thermal units and a given plant-specific maximum parameter of height or depth ('PHMAX'; 'RDMAX'). The calculation of the actual plant height and root depth on each simulated day can be obtained by comparing the accumulated sum of the photo thermal units with the sum of the photo thermal units that is necessary for the maximal height or depth. This is given by the plant-specific parameter 'ROOTING'.

$$PH = \min(PHMAX, \frac{PHMAX * SUMPTU}{ROOTING})$$
 Eq. 3

 $RD = min(RDMAX; \frac{RDMAX * SUMPTU}{ROOTING})$  Eq. 4

### 3.3.2 Sub module 'Biomass growth'

The main assumption of the sub module 'Biomass growth' is that all species of plant have a typical "light curve of assimilation" as reaction of environmental influences. Furthermore, the assimilation is calculated as a function of the typical "light curve of assimilation" of one single leaf. The maximum assimilation activity of the different species of a plant is within a certain range. However, in the sub module, the assimilation activity is implemented as a mean average value which is the parameter ('PHOTSR') of each plant species (Table 2).

Table 2: Rate of photosynthesis of diff	erent plant species (cha	anged after STENITZER 1988)
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	Group I	Group II	Group III
Rate of photo-	potato; barley, wheat;	tobacco; peanut; cotton;	maize; sugar cane; sor-
synthesis	oats; sugar beet; bean	soybean; rice; sunflower;	ghum
(kg CH <sub>2</sub> 0 ha <sup>-1</sup> h <sup>-1</sup> )	20-30	30-40	30-60

The following equation results from the met assumptions:

$$ASSIM(P) = (SLOPE * GLOB * PHOTR)/(SLOPE * GLOB + PHOTR)$$

ASSIM(P)	potential assimilation activity
GLOB	intensity of light on top of the leaf area (global radiation)
PHOTR	asymptotic limit of assimilation (PHOTR = 2.04 * PHOTSR-17)

Eq. 5

SLOPE slope of the light curve

'PHOTSR' maximum assimilation activity of a leaf (photosynthetic rate - plant-specific parameter)

The calculation of the potential assimilation on the other side is performed by an integration of the crop variable leaf area index after THORNLEY'S (1976 cited in STENITZER 1988) into the "crop stand light curve of the assimilation":

$$PSLOPE = APSLOPE * (1 - exp(-EXPAR * GRNLAI))$$
 Eq. 6

#### PASYMP = PHOTR \* GRNLAI

PSLOPE	slope of crop stand light curve of the assimilation
APSLOPE	slope of the light curve
PASYMP	asymptotic limit of "crop stand light curve of the assimilation"
EXPAR	reduction coefficient of the light ( $EXPAR = EXCOEF * 1.5$ )
'EXCOEF'	plant-specific parameter of coefficient of the light
GRNLAI	area index of green leaves

The individual rate of the potential assimilation results in:

$$ASSIM(P) = (PSLOPE * GLOB * PASYMP)/(PSLOPE * GLOB * PASYMP)$$
 Eq. 8

The potential amount of photosynthesis is decreased by 25 %. This is caused by the respiration of the new biomass of plant. Furthermore, the factor of temperature limits the assimilation for the simulated species of plant. It is a function of the mean air temperature and the typical "curve for the factor temperature" (Figure 8).



Figure 8: Curves of factor of temperature (changed after STENITZER 1988)

'T\_0', 'T\_1', 'T\_2' and 'T\_3' are plant parameters for temperature thresholds, which determine the specific temperature curve for each plant species (TFUNC) in the sub module. Between the parameters 'T\_1' and 'T\_2', the temperature optimum of the assimilation is described. Between the parameters 'T\_0' and 'T\_1' as well as 'T\_2' and

Eq. 7

'T\_3' the range outside the optimum is determined which results in reduction of assimilation.

In addition, the actual assimilation is calculated with the day length because the duration of day length is positively related to the amount of daily radiation. The growthlimiting factors of water and / or nitrogen deficiency are integrated in the term STRESS. An exchange from the soil module of CANDY to plant module is the ratio of the potential and actual transpiration which is decisive for the calculation of the water stress factor. In consideration of all factors the actual assimilation is calculated with the following equation:

ASSIM(A) = 0.75 * ASS	I(P) * TFUNC * DAYLGT * STRESS	Eq. 9
-----------------------	--------------------------------	-------

ASSIM(A)	actual assimilation
ASSIM(P)	potential assimilation
DAYLGT	day length (h)
TFUNC	function of temperature
STRESS	growth-limiting factors of water and / or nitrogen deficiency

The maximal actual assimilation can only take place under optimal conditions and thus the maximal biomass production can occur.

The proportioning of the new built assimilation products between roots, the rest of the plant as well as the area of the new grown leaves per weight-unit of leaf increase and the fraction of dead leaves on the total leaf area depends on the respective development stage.

E.g. at the beginning of development, a total of 40 % of the plant are roots. At the harvest, only 10 % of the plant are root mass. Corresponding to this fact the fraction of the roots is described as follows:

 $FRDMAT = \exp(0.26 - 0.52 * DEVSTG)$  Eq. 10

FRDMAT	fraction of root dry matter
DEVSTG	development stage

The sub module 'Biomass growth' assumes that growth of the root length ends with the development stage number five (flowering). The growth of the leaves happens only in the vegetative stages of the plant development. This fraction, which is not used for root growth, is used for the leave-growth and the other parts of the plant. In the development stage number two only the leaves grow, whereby from the development stage

number five on, no more leaf development exists. The proportioning of assimilation products between leaves and the rest of the plant is described as follows:

Eq. 11
f

FBULK gain fraction of the rest of the plant without leaves and roots

For the calculation of the daily gain of biomass, the actual assimilation is the source:

$\Delta GBULK = \Delta DMGAIN * FBULK$	Eq. 12
--	--------

$$\Delta DMGAIN = ASSIM(A)^* (1 - FRDMAT)$$
 Eq. 13

The gain of the leaf area index (TOTLAI) is calculated from the "rest" of the leaf growth and the mean weight of unit of leaf area which is a plant-specific parameter 'AREAWT':

$$TOTLAI = (\Delta DMGAIN - \Delta GBULK) * AREAWT Eq. 14$$

The fraction of the dead leaves (FDEADL) is described as:

$$FDEADL = \exp(-5 + 0.5 * DEVSTG)$$
Eq. 15

The calculation of green leaf area index:

$$GRNLAI = TOTLAI*(1 - FDEADL)$$
 Eq. 16

The fraction of respiration on 30 °C is defined as 0.01 (STENITZER 1988). Therefore, the amount of the respiration fraction is determined by the temperature increase or decrease (RESP):

TEMP mean air temperature ( $\mathfrak{C}$ )

The dry matter of biomass (DRYMAT) is calculated from the dry matter of the day step before, the fraction of gain and the fraction of respirated dry matter.

$$DRYMAT = DRYMAT + DMGAIN - DRYMAT * RESP$$
 Eq. 18

The crop yield is calculated from the weight of dry matter per area. The usable part (e.g.: grain from wheat) is calculated from the harvest index which depends on the specific characteristics of species and plant varieties.



All mentioned internal values and parameters of the plant module SIWAPFLAN are illustrated in Figure 9.

Figure 9: Schematic illustration of the sub module 'Biomass growth' (the red line characterises the sub module, squares with continuous line symbolise the driving forces, shapes with the dashed line are plant-specific parameters, diamond shapes show all the internal quantity, that could also export as an output result, e.g. dry matter) (own graphic)

## 3.3.3 Sub module 'N uptake'

The approach of the plant nitrogen uptake in the plant module SIWAPFLAN was developed by FEICHTINGER and extended by FRANKO et al. (n. d). The basic assumption is: the uptake depends on plant external factors such as availability of soil nitrogen and plant internal factors like ontogenesis. The root depth is essential, whereas the root density is not considered in the approach of plant nitrogen uptake.

The calculation of nitrogen uptake is realised by a control function. The optimum curve of nitrogen content is determined as a function of the development stages. The relative high concentration of N in plants at the beginning of the season and the lower concentration of N by the time of ripeness is regulated by parameters of plant-species. The calculation uses the following formula:

$$NC_{opt} = NC_{T1} + (NC_{T0} - NC_{T1}) / \exp(NC_{NF} * DEVSTG)$$
Eq. 19

Eq. 20

NC <sub>opt</sub>	optimum nitrogen content
NC <sub>T0</sub>	plant-specific parameter of nitrogen content on time T0
NC <sub>T1</sub>	plant-specific parameter of nitrogen content on time T1
NC <sub>NF</sub>	plant-specific parameter of curve form
The opposite	of the optimum nitrogen content is the actual nitrogen concentration:

NC <sub>act</sub>	actual nitrogen content
NUP <sub>acc</sub>	accumulated amount of N uptake

Nitrogen uptake is determined by transpiration of plants. Thus, the demand of nitrogen uptake results from transpiration. Furthermore, the supply of nitrogen gives feedback to transpiration which is realised by the ratio of actual and optimal nitrogen content.

$$NC_{rel} = NC_{act} / NC_{opt}$$
 Eq. 21

if 
$$|1 - NC_{rel}| \ge 0.125$$
, then  
if  $|NC_{rel} \ge 1.125|$ , then  $kf = (1.125 - NC_{rel})/0.125$   
if  $NC_{rel} \le 0.875$ , then  $kf = (0.875 - NC_{rel})/0.125$ 

The variable kf regulates the transpiration coefficient TRANSKO which is calculated with minimum and maximum plant-specific parameter of transpiration 'TKMIN', 'TKMAX' and kf:

$$TRANSKO = (\max(0,\min(TKMAX,\frac{(TKMAX + TKMIN)}{2} + kf\frac{(TKMAX - TKMIN)}{2})$$
Eq. 22

The calculation of the daily demand of nitrogen occurs in three steps. Besides the coefficient of transpiration, the actual evapotranspiration AET, which is an exchange from the soil module of CANDY, is considered.

$$N_{dem} = TRANSKO * AET$$
 Eq. 23

The second step of daily nitrogen demand is controlled by the simulated dry matter.

$$N_{dem} = \min(N_{dem}, DRYMAT * NC_{opt} * NC_{max} * NUP_{acc})$$
  

$$N_{dem} = \max(0, N_{dem})$$
Eq. 24

The last influence factor that is taken into account in the calculation of daily N demand of plant is the available soil nitrogen. The sum of the daily demand is accumulated in the amount of N uptake in the crop.

The effect from nitrogen deficiency of the assimilation is realised by a growth-limiting factor which is calculated with the following formula:

$$NSTRESS = \min(1, (\frac{(NC_{act} - NC_{kr})}{(NC_{opt} * 0.75 - NC_{kr})}))$$
Eq. 25  
NSTRESS = max(0, NSTRESS)  
NSTRESS growth-limiting factor through nitrogen deficiency {0

plant-specific parameter of critical nitrogen content

 $NC_{KR}$ 

In summary, the above mentioned plant module SIWAPFLAN and its sub modules simulate the following crop variables representing and / or being the results of the crop growth processes (Table 3).

Internal valuesRepresentative variablesDevelopment stages (DEVSTG)Crop height (PH)Leaf area index (TOTLAI)Coverage (CD)Biomass (DRYMAT)Root depth (RD)N uptake (N uptake)

Table 3: Simulated crop variables of the plant module SIWAPFLAN

Due to the hierarchical system of CANDY, the four representative variables are linked with further modules of CANDY. The three values are internal and influence the representative variables and interact among each other as well. E.g. the leaf area index determines the coverage. Furthermore, the leaf area index is linked to the biomass and vice versa. The biomass controls the N uptake. All values and variables are influenced by the inter value development stages.

All abbreviations, which are used to describe the simulation of the whole plant module SIWAPFLAN, are summarised in Appendix A.

## **4 DATA MATERIAL AND METHODOLOGY**

The following section includes the explanations and demonstration of the data requirement for the simulation application of SIWAPFLAN and CANDY. Afterwards, the investigation area will be introduced which was used to enlarge the already existing data set. The sampling of new data was important due to the importance of the LAI. On the one hand, the LAI represents an essential variable of plants. On the other hand, the simulation of assimilation in the sub module 'Biomass growth' bases on the LAI. The measurement methodology of the crop variable and subsequently, the realisation of LAI in the growing season 2007 will be described.

The assessment of the module SIWAPFLAN is the main objective of the present study. This will be realised in three phases: sensitivity analysis, calibration and validation. The already existing and extended data are the base for the calibration and validation. The methodological approaches of each phase will be briefly explained and afterwards applied on the plant module.

## 4.1 Data requirement of CANDY and SIWAPFLAN

The model CANDY within the plant module SIWAPFLAN requires a data set for operation. In addition, a data set will be assembled regarding the aim and task of the study. I.e. the realisation of calibration and validation of the module SIWAPFLAN demands an adequate data set to cope with the task. Both data requests can be covered with the available data set of the investigation area Bad Lauchstädt.

Data set of model operation encompasses a time period from 08<sup>th</sup> October 1996 to 31<sup>st</sup> August 2007 and falls into three parts: meteorological, soil and management data. The meteorological data in day steps are driving forces of the simulation and contain:

- mean air temperature at 2 m (℃),
- sum of precipitation (mm),
- sum of global radiation (J cm<sup>-2</sup>) or alternatively duration of sunshine (h).

Table 4 shows the applied soil physical parameters which are required for modelling.

Features of horizons							
No.	Depth (cm)	Soil texture	Content of organic carbon (%)	Bulk density (g/cm <sup>3</sup> )	Particle density (g/cm <sup>3</sup> )	Field capacity (vol%)	Wilting point (vol%)
1	0 - 30	silt loam	1.95	1.37	2.56	29.9	17.7
2	30 – 50	silt loam	1.00	1.38	2.60	28.9	19.9
3	50 – 130	silt loam	0.20	1.49	2.67	33.4	9.1
4	130 – 200	sandy loam	0.10	1.79	2.66	19.6	12.9

Table 4: General soil physical parameters for 'land-use experiment' (organic farming)

Mandatory data for management contain:

- crop species,
- date of sowing and harvest,
- date of soil tillage and depth,
- date of application for mineral fertilisation (type and quantity of N-Input),
- date of organic amendment (type and quantity of C-Input).

Appendix B includes whole management data which are applied for the simulation of all small plots from 1996 to 2007. The used meteorological data for the mentioned simulation period are listed on the Helmholtz Centre for Environmental Research - UFZ website (UFZ 2007).

As previously mentioned, the investigation area provides a data set of the management system organic farming from 1999 to 2007 with plant-relevant variables which contains three groups:

- plant development stages,
- plant biomass,
- plant nitrogen.

The check of the data show that this data base is congruent to the three main plantrelevant processes and is also conform to the structure of the plant module SIWAP-FLAN. Therefore, the data set will be used for the calibration (2004-2007) and for the validation (1999-2003). Detailed information about the three variable groups are listed in Table 5.

Data	Frequency	Methods	Modules
Development	Defined stages in each grow-	DC ( <u>D</u> ecimal <u>C</u> ode)	Plant
stages (BBCH/DC)	ing season (1999-2007)	BBCH ( <u>B</u> BA, <u>B</u> SA, <u>Ch</u> em.Ind.)	development
Biomass	Four times in each growing	Fresh matter analysis;	Biomass
(intermediate h.)	season (1999-2007)	Dry matter analysis	growth
Biomass	Once in each growing sea-	Fresh matter analysis;	Biomass
(main harvest)	son (1999-2007)	Dry matter analysis	growth
N content in crop	Four times in growing sea-	Method of nitrogen analysis	N uptake
(intermediate h.)	son 2007		
N uptake	Once in each growing sea-	Calculated size of biomass and	N uptake
(main harvest)	son (1999-2007)	N content	
N content in crop	Once in each growing sea-	Method of nitrogen analysis	N uptake
(main harvest)	son (1999-2007)		

A closer view on the module SIWAPFLAN shows that an improvement of the calibration procedure can be accomplished with the addition of further crop variables. The complex structure of sub module 'Biomass growth', which bases on the LAI, prompts the decision to investigate this crop variable on the location for the present study. Furthermore, the crop variables root depth and plant height should be measured and used for the calibration of the sub module 'Plant development'. Therefore, the existing data set is extended by the following crop variables (Table 6), with the focus on the LAI. The methodological base and the realisation of he LAI measurement will be carried out in section 4.3.

Table 6: Additional data set of crop variables (2007) for calibration of SIWAPFLAN

Data	Frequency	Methods	Modules
Plant height	Weekly during the growing	Own photo documentation,	Plant
	season 2007	metric measurement	development
Coverage	Weekly during the growing	Own photo documentation	Plant
	season 2007		development
Root depth	Every second week during	Own measurement	Plant
	the growing season 2007		development
Leaf area index	Weekly during the growing	Own measurement	Biomass
(LAI)	season 2007	LAI-2000 Plant Canopy Analyzer	growth

## 4.2 Investigation area

The investigated area 'land use experiment' is integrated in the Research Institution Bad Lauchstädt which is located at 51°24' N and 11°53' E at an elevation of 118 m a.s.l.. The institution is known for the Static Fertilisation Experiment that has been started in 1902 and is one of the most important 'long-term experiments' in the world (KÖRSCHENS & PFEFFERKORN 1998). With the foundation of the "UFZ-Centre for Environmental Research Leipzig-Halle", the experimental field was assigned to the Department of Soil Science and serves to study the interaction between soil, plant, atmosphere and water with regard to sustainable development (UFZ 2007). One part of the experimental field, called 'land use experiment', started in 1996 with the aim to collect primary data of soil and plant behaviour. The data are used for the validation of plant models. The 'land use experiment' contains the traditional crop rotation representing the Static Fertiliser Experiment rotation with winter wheat (*triticum aestivum L.*), sugar beets (*beta vulgaris L.*), spring barley (*hordeum vulgare L.*) and potato (*solanum tuberosum L.*). A treatment with and without mineral fertilisers is applied on the rotation. Besides the traditional management, some alternative agricultural systems were established characterising different types of land use: plots of black fallow, grassland and organic farming (FRANKO et al. 2007). The focus of the present study is the part of the organic farming.

The Centre for Environmental Research Leipzig-Halle collects data of biomass and crop development, nutrient uptake and important soil parameters such as temperature, soil moisture and water tension as well as the chemical composition of the soil water in different depths. Annually taken samples from the topsoil are analysed with regard to carbon, nitrogen and biological parameters (FRANKO et al. 2007).

A meteorological station, working on international standard, completes the background information and provides data on radiation, precipitation, wind (speed and direction), air humidity and air temperature on a 10-min time resolution. These data have been aggregated to hourly values and daily values. Measurements are taken at ground level and in different soil depths as shown in Table 7.

Elements of weather	Daily values
Air temperature (2 m above ground)	since 1956
Air moisture (2 m above ground)	since 1956
Precipitation (1 m above ground)	since 1956
Sunshine duration	since 1956
Soil temperature in depth of 5 cm, 10 cm, 20 cm, 50 cm and 100 cm	since 1992
Global radiation	since 1994
Wind speed	since 1994
Wind direction	since 1992
Air pressure	since 2000

 Table 7: Overview of measured meteorological data (PETERSOHN 2007)

### 4.2.1 Climate characteristic

The investigation area is located in the Saale region belonging to the climatic region of the Börde and Central Germany continental climate which is characterised by an average annual precipitation of 470-540 mm and an average annual air temperature of 8.5-9.0 °C. It is characterised by an average annual precipitation of 483.9 mm and an average annual temperature of 8.8 °C from the 111-year (1896-2007) average (Figure 10). Therefore, the research station of Bad Lauchstädt is characteristic for the region (PETERSOHN 2007).



Figure 10: Yearly dynamics of precipitation and air temperature in Bad Lauchstädt, mean temperature 8.8 °C, mean precipitation 483.9 m m (1896-2007) (own graphic)

### Climate characteristic during the year 2007

The year 2007 represents a year of dynamic temperature and precipitation at the location Bad Lauchstädt. With an annual temperature of 10.6  $\degree$  it was the second warmest year since the beginning of weather recordkeeping in 1896. The reason of this extreme is the mean air temperature in the first two quarters of the year. The temperature was 5.6  $\degree$  above the long-time average (Figure 11).

In comparison to the long-time average value the temperature was 1.8 °C warmer and there were 236 mm more precipitation than the average annual value. Consequently, the monthly precipitation sums of eight months were above the annual average. However, strong difference of the long-time average value arose in the months of April (8 %) and in May (330 %) (Figure 11). One example of this large deviation is one precipitation event in May with 74.4 mm representing the fourth highest intensity since 1896.



Figure 11: Course of precipitation and air temperature 2007 in Bad Lauchstädt in comparison to the long-time average value of temperature and precipitation (1896-2007) (own graphic)

In addition, the global radiation was exceeded by 65.5 kJ cm<sup>-2</sup>, being above the longtime average value throughout the year, and reached an extreme in April (160 %) (Figure 12). The months of July, August and September had a normal course of radiation and temperature (Figure 11). In summary, the year 2007 was warm, sunny and substantially too wet.



Figure 12: Course of global radiation 2007 in Bad Lauchstädt in comparison to the long-time average value of global radiation (1952-2007) (own graphic)

The weather course in reflection to the vegetation period 2007 is characterised by extremes. The sowings in April were problematic due to the long dryness and an intensive radiation (Figure 12). However, the period from May to September was characterised by above-average precipitation which was positive for the development of plants. Thus, after the beginning of the drought in April, the growing plants had no water stress in this period. Based on the high amount of precipitation and radiation, the mean value of actual evapotranspiration from January to June has been the highest since the existence of the field 'land use experiment'.

### 4.2.2 Soil characteristic

The research area is situated in the geomorpho-geological region called "Querfurter Platte". It belongs to the Chernozem area of Saxony-Anhalt which is part of a belt of loess sediment located in the south-east of the Harz Mountains. Loess, which was deposited in several meters thickness in parts of Central Europe during the last glacial period, is the parent material for soil formation and also contains carbonates.

Haplic Chernozem is dark brown to dark in colour caused by its content of high-quality humus (ca. 2 %) down to a depth of more than 40 cm. The soil consists of 70 % silt, 20 % clay and 10 % sand whereby the horizons contain medium to high saturated water conductivities and air capacities (ALTERMANN et al. 2005).

### 4.2.3 Management system - organic farming

The above mentioned experimental field 'land use experiment' consists of small plots which have an extent of 22 m in N-S-direction and a width of 10 m. In this study the investigation is only situated in the experimental area of organic framing (Figure 13).



Figure 13: Small plots of the management system - organic framing on the 'land use experiment' (changed after SCHMÖGNER 2006)

The small plots of this management system include lucerne (*medicago sativa L.*), winter wheat (*triticum aestivum L.*), winter barley (*hordeum vulgare L.*), potato (*solanum tuberosum L.*), spelt (*triticum spelta L.*), maize (*zea mays L.*) and spring wheat (*triticum aestivum L.*).

### 4.2.4 Sampling of crop data

As previously explained, a main task of the 'land use experiment' is the data sampling of crop growth. The plant development is determined by important plant-specific development stages (e.g.: sowing, emergence, flowering, ripening). In addition, soil tillage and specific events, e.g. weather events, are documented in the growing season.

Furthermore, to determine and sample the plant biomass, repeated harvests are conduct during growing season. On each of the four dates occurs a manual harvest (intermediate harvest) of plants from a sub-plot of about one m<sup>2</sup> size without disturbing the kernel plot. This 55 m<sup>2</sup> area is reserved for main harvest which only considers an inside part of the plot in order to avoid edge effects (SCHMÖGNER 2006). So, four intermediate harvests are carried out during defined development stages which are documented in Table 8.

Сгор	1 <sup>th</sup> Intermediate harvest	2 <sup>nd</sup> Intermediate harvest	3 <sup>rd</sup> Intermediate harvest	4 <sup>th</sup> Intermediate harvest
	Whole plant (above	-ground)		Main & by-product
Winter wheat	Beginning of tillering BBCH / DC 21	Booting: flag leaf sheath extending BBCH / DC 41	Full flowering BBCH / DC 65	Medium milk BBCH / DC 75
Potato	9 leaves of main stem unfolded (> 4 cm) BBCH / DC 15	First individual buds (1-2 mm) of first inflorescence visible (main stem) BBCH / DC 51	End of flowering in the first inflorescence BBCH / DC 69	90 % of berries in the first fructifi- cation have reached full size BBCH / DC 79
Maize	6 leaves unfolded	2 nodes detectable	Male: upper and lower parts of tassel in flower Female: stigmata fully emerged	Medium milk
	BBCH / DC 16	BBCH / DC 32	BBCH / DC 65	BBCH / DC 75

Plant biomass was analysed in the laboratory. The fresh material of above ground biomass was weighed. Afterwards, the dry matter was determined by drying the plant material by 65 °C until it reached a constant weight. Furthermore, the method of KJELDAHL (SCHLICHTING et al. 1995) was applied to analyse the total nitrogen content of plants. Both of these important quantities enable the calculation of N uptake.

$$N \text{ uptake} = \left(\frac{Plant \text{ biomass}(kg^* ha^{-1})}{N \text{ content}(\%)}\right) \div 100$$
Eq. 26

## 4.3 Leaf area index

The overview of processes of crop growth modelling and especially the plant module SIWAPFLAN shows that the LAI is applied as a major variable of most processoriented models that predict plant growth / biomass production (DE JESUS et al. 2001; SONNENTAG et al. 2007). Thus, the LAI represents the plant specific growth and involves the change of environmental circumstances under which plants grow.

LAI is the total one-sided area of leaf tissue per unit ground surface area (e.g. a LAI of 3.0 means that there are 3 m<sup>2</sup> of leaves distributed above 1 m<sup>2</sup> of ground) (WATSON 1947 cited in DE JESUS 2001). The value of LAI is a dimensionless quantity describing the plant canopy and representing a useful base for understanding water use, canopy light interception and plant growth, especially biomass production. It characterises the canopy atmosphere interface, where most of the energy flux exchanges occur. Also, any change of LAI in canopy (e.g. by drought, frost, hail, management practice) is accompanied by modifications in crop stand productivity (BRÉDA 2003).

Therefore, accurate measurements of LAI are essential to understand the interaction between canopy and environment for various aims, e.g. agroecosystem and crop growth modelling. To obtain those measurements, different destructive and non-destructive methods exist (JONCKHERRE et al. 2004; WILHELM et al. 2000; BRÉDA 2003). Destructive measurements are time consuming, labour intensive and not applicable in experimental field plots with different tasks.

A non-destructive, indirect, non-contact, optical and fast as well as common used method of LAI measurement offers the LAI-2000 Plant Canopy Analyzer. The device

measures canopy gap fraction (radiation transfer model) which is based on the radiation transmittance through the canopy. Results of the LAI-2000 were compared to values obtained from different methods and other investigations and furthermore validated with direct LAI measurements by destructive sampling. Based on these facts, the method has been widely used for ecophysiology of agricultural crops (BRÉDA 2003).

### 4.3.1 LAI-2000 Plant Canopy Analyzer

The device design and model theory were developed by WELLES & NORMAN (1991) and will be explained in the following sections. The LAI-2000 consists of an optical sensor and a data logger. The optical sensor contains a "fish-eye" lens with 148° field-of-view above and below the canopy which are used to determine canopy light interception at five zenith angles simultaneously (0-13°, 16-28°, 3 2-43°, 47-58°, 61-74°) (Figure 14).



Figure 14: Schematic of optical sensor, the fifth detector arranged in concentric rings (changed after LI-COR 2008) concentric rings: ring 1=0-13°, ring 2=16-28°, ring 3=32-43°, ring 4=47-58° and ring 5=61-74°)

The lenses project the image of its nearly hemispheric view onto five detectors arranged in five concentric rings. Only the radiation below 490 nm, representing the blue portion of the electromagnetic spectrum, can pass through the filter inside of the optical sensor. Leaves typically reflect the blue range and transmit relatively little radiation (JONCKHEERE et al. 2004). Measured data are automatically stored and calculated into the control logger.

### Model theory

The LAI-2000 Plant Canopy Analyzer and its principles of operation are based on the assumption that, to a certain probability, radiation is intercepted by foliage passing through plant canopy. The probability of interception is proportional to the path length,

foliage density and foliage orientation. Therefore, if the transmittance is known, it is possible to invert foliage information like the LAI (WELLES & NORMAN 1991). The detailed equations (1-8a) of LAI calculation are listed in Appendix C.

Some assumptions must be met for accurate estimation of foliage on which the calculation of the LAI is based (LI-COR 1992a):

- (1) The foliage is black. It is assumed that the readings do not include any radiation that has been reflected or transmitted by foliage.
- (2) The foliage is randomly distributed within certain foliage-containing envelopes. These envelopes might be parallel tubes (a row crop), a single ellipsoid (an isolated bush), an infinite box (turf grass) or an infinite box with holes (deciduous forest with gaps).
- (3) The foliage elements are small compared to the view area of each ring. An approximate guideline is this: the distance from the sensor to the nearest leaf over it should be at least four times the leaf width.
- (4) The foliage is azimuthally randomly oriented. That is, it does not matter how the foliage is inclined as long as all the leaves are not facing the same compass direction.

#### **Considerations of measurement**

Measurements of short canopies: the above canopy (A) and the below canopy (B) readings can be obtained using the same optical sensor. If needed, A-readings can be interspersed to allow changing sky conditions or changing directions of view. The optical sensor on the head of the instrument is about 2.5 cm in cross-section, so that any plant material higher than 2.5 cm can be detected (HICKS & LASCANO 1995).

When examining tall canopies, attention has to be paid to the fact that an above canopy (A) measurement is made in a sufficiently large clearing (radius greater than three times the canopy height), followed by the below canopy (B) readings and finally another above canopy reading in the clearing. For both reading types, the sensor is oriented skywards (LI-COR 1992b). One measurement point in the implemented campaign comprises several readings of transmittance: the first is made above canopy (A) followed by readings below canopy (B). A final above canopy reading (A) completes one measurement. The measurement of LAI took place on fixed measuring points along each transect. LAI in row crops (e.g. maize and potato) should be grouped in diagonal transects (LI-COR 1992a). A set of four below - canopy readings along a diagonal transect at 0, 25, 50, and 75 % of the distance across the row have been conducted (MALONE 2001).

The flexible and portable instrument can be used during both twilight hours and uniformly cloud weather or when the sensor and the canopy can be shaded to prevent detection of transmitted or reflected direct radiation. The LAI-2000 Plant Canopy Analyzer should not be used for LAI determinations in direct sunlight because leaf reflectance and transmittance of light will result in an underestimation of LAI. The method of shading the canopy is recommended so that the sensor is not exposed to the sun. Furthermore, the "fish-eye" lens of the optical sensor head should be kept clean and dry for comparable readings (WILHELM et al. 2000).

Advantages of the equipment are that it permits non-destructive and rapid in situ estimates of LAI. This allows day-to-day estimates of LAI throughout the growing season on the same plants without need of extensive field and / or labour-intensive leaf area harvesting and sampling.

Therefore, it is important to read the operators manual to identify and assess factors relative to the planned experiments. Only this permits to collect accurate data. The analyzer can provide estimations of LAI if recommended procedures are followed.

#### 4.3.2 Realisation of the LAI measurements with LAI-2000

The LAI measurement campaign was carried out at the part of organic farming of 'land use experiment' of the research station Bad Lauchstädt from May to August 2007. The implementation of LAI measurements on the small plots follows the principles mentioned above and considerations corresponding to the recommendations made by LI-COR (1992b). The weekly measurement campaign of the selective crops aims at a full-season experiment (Table 9). Only the measurements of winter wheat started at the earliest possible date (3<sup>rd</sup> May 2007) with the beginning of study and were taken weekly until harvest. The experimental setup is illustrated in Figure 15.

Wi	nter wh	eat		Potato	)		Maize	
3 <sup>rd</sup>	May	2007						
9 <sup>th</sup>	May	2007						
17 <sup>th</sup>	May	2007	17 <sup>th</sup>	May	2007	17 <sup>th</sup>	May	2007
23 <sup>rd</sup>	May	2007	23 <sup>rd</sup>	May	2007	23 <sup>rd</sup>	May	2007
30 <sup>th</sup>	May	2007	30 <sup>th</sup>	May	2007	30 <sup>th</sup>	May	2007
5 <sup>th</sup>	June	2007	5 <sup>th</sup>	June	2007	5 <sup>th</sup>	June	2007
12 <sup>th</sup>	June	2007	12 <sup>th</sup>	June	2007	12 <sup>th</sup>	June	2007
21 <sup>st</sup>	June	2007	21 <sup>st</sup>	June	2007	21 <sup>st</sup>	June	2007
28 <sup>th</sup>	June	2007	28 <sup>th</sup>	June	2007	28 <sup>th</sup>	June	2007
5 <sup>th</sup>	July	2007	5 <sup>th</sup>	July	2007	5 <sup>th</sup>	July	2007
12 <sup>th</sup>	July	2007	12 <sup>th</sup>	July	2007	12 <sup>th</sup>	July	2007
			18 <sup>th</sup>	July	2007	18 <sup>th</sup>	July	2007
			26 <sup>th</sup>	July	2007	26 <sup>th</sup>	July	2007
			31 <sup>st</sup>	July	2007	31 <sup>st</sup>	July	2007
			7 <sup>th</sup>	Aug.	2007	7 <sup>th</sup>	Aug.	2007
			12 <sup>th</sup>	Aug.	2007	12 <sup>th</sup>	Aug.	2007
						21 <sup>st</sup>	Aug.	2007

Table 9: Dates of the weekly LAI measurement for winter wheat, potato and maize

Repetitive weekly measurements with the LAI-2000 were conducted by marking the diagonal transect of 1.5 m segments with stakes. Thus, it could be taken at the same fixed measurement points in each recording session (Figure 15).



Figure 15: Experimental design of LAI measurements of the organic farming (own graphic)

Measurements were recorded during the morning hours (8.30-10.30 h) lasting approximately 30-60 minutes for a whole stand of winter wheat, potato and maize. To improve the mean average LAI value measurements were recorded on diagonal transects between the rows at even intervals regarding the method of MALONE (2001).

Also, the consideration of heterogeneous canopies was realised by the doubled number of taken measurement diagonals or transects (MALONE et al. 2002).

In order to obtain representative results at least eight replications are necessary (Figure 15) in order to be able to identify outliers. The first conducted measurement contained 16 replications. The statistical analysis showed that it was possible to reduce the sample number from 16 to 8 replications without increasing the measuring error substantially.

An umbrella was used during directly sunshine to shade an area around a fixed measurement point and the sensor. The shading method was only used, when the sky was generally clear or only partly clouded (HICKS & LASCANO 1995).

The previous documented experimental setup and the choice of crops demand some additional considerations. The manufacturer of the LAI-2000 recommends that its "fisheye" lens should be at least three times the crop height away from any edge for below-canopy readings so that objects outside the plot are not detected. E.g. the height of the maize amounts to 200 cm  $\pm$  30 on the small plots experiment. According to the recommendations, the measurements should be taken at a distance of 6 m from any edge. This condition was not met by the 10 m wide plots in this experiment (Table 10).

Сгор	Height (cm)	Distance (cm) from edge with 5 rings (3 times of height)	Distance (cm) from edge with 4 rings (1.6 times of height)	Distance (cm) from edge (possible position)
				300 (N-edge)
Maize	200 + 30	600	320	150 (E-edge)
	200 ± 00		020	150 (W-edge)
Winter				300 (N-edge)
wheat	<u> 90 ± 15</u>	210	126	150 (E-edge)
WIIcal	$00 \pm 10$	210	120	150 (W-edge)
				300 (N-edge)
Potatoes	70 . 10	240	110	150 (W-edge)
	70±10	240	112	150 (E-edge)

Table 10: Recommended and possible distance to the edges of small plots (the edges in S-direction are not listed, because enough distance is given)

HUNT et al. (1999) and WILHELM et al. (2000) describe similar problems. In order to obtain appropriate results regarding the LAI on small plots they neglected the outer-ring values in the LAI computation and reduced therefore the minimum plot size to 1.6 times the canopy height (LI-COR 1992a). The same application of this technique for all plots was accomplished during this study (Table 10) in order to avoid detecting objects or gaps outside small plots which would affect the LAI estimate (MALONE et al. 2002). Table 10 documents that the negligence of outer-ring number five does not conform to the recommendation of distance to the edges of small plots for maize. The reason is the maximum height.

GRANTZ & WILLIAMS (1993) concentrate the LAI research on vertical canopies and suggest comparative problems. By recalculation of the LAI estimation of the LAI-2000 on the basis of the data from three rings without the fourth and fifth ring, the relationship between the derived LAI values and destructively measured LAI increased. Therefore, the computation of the LAI values of maize was conducted without the outer-rings number four and five in the present study.

## 4.4 Model assessment

The application of simulation which describes plant-specific processes needs to be preceded by a thorough evaluation of the module that is used. The simulation with the plant module SIWAPFLAN will be assessed by using a procedure which includes a sensitivity analysis, a calibration and a validation phase. All three phases are a corollary because the gained insights of the passed phase are necessary for the following one. This section describes the important methodological principles and afterwards the used method of each assessment phase.

### 4.4.1 Sensitivity analysis

### **Methodological principles**

The purpose of sensitivity analysis is to study the behaviour of the model and should be an integral part of any solution methodology (PANNELL 1997). Sensitivity analysis is structured to determine the sensitivity of a model relative to changes. Usually, it helps evaluating the influence of the input parameters on the model results.

The definition and the application of the sensitivity analysis vary in literature. A review about different definitions of sensitivity analysis and applications offers the study of SALTELLI et al. (2000). Several examples use analysis of sensitivity in context of valida-

tion and optimisation of models. CROSETTO et al. (2000) formulate that the sensitivity can also be a tool for pre-calibration analysis.

A multiplicity of mathematical approaches and techniques to sensitivity analysis exist and range from simple to complex (e.g. linear regression or correlation analysis, measures of importance, sensitivity indices, etc.).

A common used mathematical approach to analyse the present model behaviour is represented by the sensitivity index (SI). This approach compares the change in one or more simulated outputs relative to the change in one or more parameters using numerical results (LOUKS & VAN BEEK 2005). PANNELL (1997) outlined a multiplicity of sensitivity indices in cases where only a single output variable is to be evaluated.

Another common used method of SI in literature is to change the value of one parameter in the model by percent. This form of sensitivity analysis calculates parametric sensitivity for a component of a more complex system by altering the input parameter at 10, 20 or 30 percent in each direction starting from a parameter reference value. One important check is whether the percentage change in the output is greater or lesser than that in the parameter value. Furthermore, the ratio of the change in the output to that in the parameter provides a simple measure of sensitivity. The values of the ratio indicate sensitivity and insensitivity respectively (ADDISCOTT 1993). The SI is calculated with the following equation (FÉLIX & XANTHOULIS 2005):

$$SI = \left(\frac{OP_{IP_{max}} - OP_{IP_{min}}}{OP_{IP_{mean}}}\right) \div \left(\frac{IP_{max} - IP_{min}}{IP_{mean}}\right)$$
Eq. 27

IP\_min / OPIPminminimum of input parameter / output value of IP\_minIP\_max / OPIPmaxmaximum of input parameter / output value of IP\_maxIP\_mean / OPIPmeanmean average value of input parameter / output value of IP\_mean

SI represents a relative size which calculates minimum and maximum input and output value with the help of the mean average value of both. The sensitivities of different parameters are compared with the index. Thus, the advantage of the SI for each input parameter is that all input parameters can be weighed by impact on the result. This shows promptly which parameters strongly affect the result and on which parameters priorities should be set (CULLMANN et al. 2006). With the computation of the SI only one parameter is changed in each case. The interdependent effects between the parameters can be seized (GIERTZ 2004). It is recognizable that the SI can be assumed

positive and negative. SI > 0 means that a change of input value results in a change of output value in the same direction. If SI < 0, then a change of the input parameter value effects a change in the output value in the opposite direction.

### **Applied method**

This study focuses on the parameter sensitivity of the plant module SIWAPFLAN. The aim of the analysis is to identify the most sensitive parameters of the sub modules. With the result of the sensitivity analysis, it should be decided which parameters are important for the adjustment in the following calibration procedure. Therefore, the SI of FÉLIX & XANTHOULIS (2005) (Eq. 28) is selected as SI realises the proposed requirements of the study's aim.

The sensitivity analysis is understood as a calculative preliminary study of the parameterisation and calibration only. Therefore, the initial parameterisation of the validation study of STENITZER (1988) is the basis of the analysis in order to avoid unrealistic parameter values. I.e. all module parameters of winter wheat are the reference values for the analysis. The plant module requires a multiplicity of input parameters so that the parameters are classified by the three sub modules (Table 11). This way a better overview is given for the sensitivity analysis.

The scenario is constructed for the analysis and contains seven growing seasons of winter wheat. The influence of several parameters will be analysed on the three model output results which are coverage, transpiration and N uptake. The calculation of SI starts from a given parameter reference value (Table 11). The parameter value was gradually changed ( $\pm$  10 %) using defined fixed levels. The range of the parameter value is determined with  $\pm$  30 %. The obtained outputs after each change are averaged over the seven years. All other values were maintained. In addition, the sensitivity analysis is realised in three parts corresponding to the sub modules. However, the same analysis was applied on all parameters.

The output result coverage is selected for the sensitivity analysis as it is directly depending on the LAI which is a basis of the sub module 'Biomass growth'. The modelling result transpiration has a similar meaning. Thus, the plant and its development are considered in the calculation of transpiration. On the one hand, the choice of the output result N uptake is explained to test the influence of the parameters determining the N uptake. On the other hand, all three sub modules are linked with each other and so the indirect influence of the N uptake is important. The sensitivity analysis with the three output results should offer a good insight for the following procedure of calibration and validation.

Parameter	Sub module	Value	Unit
'RIPING'	'Plant development'	18000	PTU
'BTEMP'	'Plant development'	4.8	C
'ROOTING'	'Plant development'	12000	PTU
'PHMAX'	'Plant development'	90	cm
'RDMAX'	'Plant development'	18	dm
Parameter	Sub module	Value	Unit
'AREAWT'	'Biomass growth'	0.004	ha kg⁻¹
'PHOTSR'	'Biomass growth'	12.5	kg CH <sub>2</sub> O ha <sup>-1</sup> h <sup>-1</sup>
'EXCOEF'	'Biomass growth'	0.3	-
'T_0'	'Biomass growth'	0	C
'T_1'	'Biomass growth'	10	C
'T_2'	'Biomass growth'	30	C
'T_3'	'Biomass growth'	40	C
Parameter	Sub module	Value	Unit
'TKMAX'	'N uptake'	1.78	-
'TKMIN'	'N uptake'	1	-
'NCT0'	'N uptake'	0.041	-
'NCT1'	'N uptake'	0.009	-
'NCNF'	'N uptake'	0.4	-
'NCKR'	'N uptake'	0.002	-

Table 11: Initial parameters of the sub modules 'Plant development',
'Biomass growth' and 'N uptake' for the sensitivity analysis

### 4.4.2 Parameterisation and calibration

#### **Methodological principles**

Parameterisation means finding values for parameters of general validity (ROTH et al. 1996). The process of determining the parameter values is called calibration. Model calibration is estimation and adjustment of model parameters which improve the agreement or a minimisation of the deviations between model output results and a measured data set (deviation in observed and simulated variable should be below 20 %). The aim of the calibration is to find an 'optimal' parameter combination. A calibration must be conducted for parameters that cannot be measured or for which no measured data are available or no literature information exist (RYKIEL 1996).

REFSGAARD & STORM (1996) state three generally used methods of the calibration:

- (1) Manual adaptation of parameters in trial and error procedure
- (2) Automatic calibration
- (3) Combination of manual and automatic calibration

A manual calibration in accordance with the trial and error procedure implies a manual parameter assessment through a number of simulation runs. This method is most frequently used representing the calibration that may be preferred to more complex models. A prerequisite of manual procedure is a graphical analysis of the simulation results (JANSSEN & HEUBERGER 1995).

The automatic calibration determines 'the optimal' parameters using procedures which combine many parameter combinations in order to minimise the differences between modelled and measured results. The procedures of autocalibration involve computation of prediction errors using an equation (objective function) or an automatic optimisation procedure (search algorithm) (MORIASI et al. 2007). The advantage of automatic parameter optimisation in comparison to the manual parameterisation is that the method is time efficient and less subjective. However, a parameter set produced by automatic calibration can e.g. contain unrealistic values for individual parameters so that the processes cannot be correctly illustrated by the model (REFSGAARD & STORM 1996).

A combination of trial and error and automatic parameter optimisation can be used for e.g. an initial adjustment of parameters by a manual calibration to determine the realistic range of parameter values. An automatic calibration can realise a fine adjustment of parameters in the given range. Furthermore, a reverse process is possible (REFSGAARD & STORM 1996). The combined method can be very useful and is increasingly applied in practice (MORIASI et al. 2007).

Whatever method of calibration is selected, parameters interact with each other. Thus, calibration procedures with the same output results may be given by two or more completely different combinations of parameters, none of which can be described as the "right" one (ADDISCOTT 1993).

### Applied method

In the present study, one of the major parts is the calibration of the plant module SI-WAPFLAN. The first step of the calibration is to decide which model parameters should be adjusted. This decision corresponds to the most sensitive parameters which are identified with the sensitivity analysis (HEIDMANN et al. 2008).

Besides the calibration method, the available data set for the adjustment of parameters is decisive. In consideration of the following validation, the parameter adjustment of calibration should use an independent data set of the growing season in the years 2004-2007 for winter wheat, potato and maize. The data set contains crop variables:

- development stages,
- biomass,
- N uptake.

The whole calibration is conducted for three investigated crops - winter wheat, potato and maize - and starts with the sub module 'plant development'. The organisation of the plant module determines this approach as the simulated development stages are passed on to the processes of the sub modules 'Biomass growth' and 'N uptake'. Furthermore, the small numbers of parameters and the stringent structure of the sub module enable a manual calibration. This is performed to obtain the best simulation result of the development stages in comparison to the field data.

The sub module 'Biomass growth' is more complex in comparison to the first sub module. Corresponding to the most sensitive parameters a combination of a manual and automatic calibration of parameters is used. The manual part of calibration determines the realistic range of values for the most sensitive parameter. The following procedure is an automatic optimisation. Hence, an optimiser tool is used realising a fine adjustment of parameters in the identified range of the manual calibration. The optimiser adapts the selected parameters in defined ranges in order to minimise the differences between modelled and measured results of the crop variable biomass. Therefore, an automatic multi-criteria optimisation is used involving computation of prediction error using the least squares method.

The calibration procedure of the sub module 'N uptake' is conducted in a similar way as for the sub module 'Biomass growth'. The organisation of the sub module suggests that a manual calibration could be applied. However, the connection and interaction with the sub module 'Biomass growth' complicates the manual procedure of calibration. Consequently, the crop variables biomass and N uptake are used for the multi-criteria optimisation with the optimiser tool.

The target of the calibration is the minimisation of deviations between model output results and a measured data set. The acceptable limit of a successful calibration concerning all crop variables should be below 20 % (NAIN & KERSEBAUM 2007).

### 4.4.3 Validation

#### **Methodological principles**

Model validation is defined as the process that assesses the calibrated model without changing the parameter values that were determined during calibration (HENRIKSEN et al. 2003). The evaluation process of validation compares the simulated output results with the real system observations using data that are not used in model development or calibration. The model is said to be validated if its accuracy and predictive capability in the validation are proven to lie within the predefined acceptable limits (deviation in observed and simulated variable should be below 20 %). This demonstration shows that the model is acceptable for use, not that it is any absolute truth nor that it is the best model available. The term model validation implies a site-specific validation (REFSGAARD 1996).

Various validation testing procedures exist which are documented in the study of SAR-GENT (2005). The relevance and application of validation tests depend on the available data and the system being modelled (SARGENT 2003). REFSGAARD & STORM (1996) developed four categories of validation tests. The first and second category includes tests of time period assessments (split-sample and proxy-basin test). The third category contains assessments of different areas (proxy-basin differential split-sample test). The fourth validation test combines the period and different areas procedure (proxy-basin differential split-sample test). The split-sample test will be explained in the following section because it bears relevance to the aim of this study.

The split sampling, also called cross-validation, is a classical validation test, on which the model is calibrated and validated with a long time data set, whereas the location conditions remain unchanged. The available data set is divided into two parts. One part is used for the calibration process and, whereas the other part is used for the validation. The calibration of model is based on 3-5 years of data and the validation on another period of similar length (REFSGAARD & STORM 1996). Both, the calibration and the validation results should be in an acceptable limit (POWER 1993).

### **Applied method**

The split sampling represents a classical and common used method to test the applicability of the module. Furthermore, the availability of the data is the basis and the limitation of the chosen method. In addition, the aim is relevant as well. The crop data of the location Bad Lauchstädt (1999-2007) was split in two parts due to the fact that the data set needs to meet the methodological requirements (3-5 years for both procedures).

The validation phase bases on a successful calibration. In this regard with the calibration procedure, the validation of the plant module SIWAPFLAN is conducted using a split sample test. An independent data set for winter wheat, potato and maize of another period (1999-2003) of Bad Lauchstädt is applied.

After the calibration of the sub module 'Plant development', the simulated results of development stages of the years 1999-2003 were compared to the measured field data. Through that the obtained results are assessed using graphical analysis and the below mentioned criteria. In order to validate the sub module 'Biomass growth' the intermediate harvests and main harvest of biomass were considered for assessment. The field data of N uptake on harvest are used to validate the sub module 'N uptake'.

### 4.4.4 Assessment criteria of calibration and validation

Assessment criteria are associated with the model assessment procedures. This method of statistical techniques defines an objective measure of the accuracy, also called goodness of fit, representing quantitative measures of model performance in comparison to the measured data (MORIASI et al. 2007).

The literature shows a plurality of accuracy criteria of simulation. The classification of SMITH & SMITH (2007) includes two types of quantitative analysis. On the one hand, an

analysis of coincidence and its criteria show how different the simulated and measured values are (relative error, RMSE and %RMSE). On the other hand, an analysis of association demonstrates how well trends in measured values are simulated. Most frequently used criteria of association are the index of agreement (IA) and coefficient of determination (R<sup>2</sup>).

The relative error (rel. E) is an indicator for the bias in the total difference between simulation and measurements. It can be used to assess consistent and inconsistent errors in the simulations in respect to observations. Values of zero indicate a perfect fit whereas values approaching 100 indicate incorrect results. The rel. E is calculated with the following formula which is also used in the study of POST et al. (2007):

rel. 
$$E = \frac{100}{n} \sum_{i=1}^{n} \frac{(O_i - P_i)}{O_i}$$
Eq. 28  
O<sub>i</sub> observed values  
P<sub>i</sub> simulated values  
n number of samples

The root mean square error (RMSE) is one of the commonly used error index statistics and indicates the degree of variation in simulated values with respect to the measured values. The RMSE value of zero indicates a perfect fit of the simulation performance. Therefore, a low RMSE value is desirable. Though, a disadvantage of this measure is its sensitivity to outliers. It is defined as shown in following equation (JANSSEN & HEU-BERGER 1995):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}$$
Eq. 29

The RMSE was converted into % errors (%RMSE) by dividing mean average of observation and multiplying by 100. The following equation is applied in NAIN & KERSEBAUM (2007):

$$\% RMSE = (RMSE / \overline{O}) * 100$$
 Eq. 30

Ō mean average of the observed data values

The index of agreement (IA) is a standardised measure of the degree of model prediction error and varies between zero (no agreement) and one (perfect agreement). The dimensionless index was developed by WILLMOTT (1981 cited in MORIASI et al. 2007) and represents the ratio between the mean square error and "potential error". IA can detect additive and proportional differences in the observed and simulated means and variance. An overly sensitivity to extreme values is given due to the squared difference. IA was calculated according to this formula (KERSEBAUM 2007):

$$IA = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (\left| P_i - \overline{O} \right| + \left| O_i - \overline{O} \right|)^2}$$
Eq. 31

Coefficient of determination (R<sup>2</sup>) calculates the proportion of the variance in measured data explained by the model. R<sup>2</sup> ranges from zero to one, with higher values indicating less error variance. MORIASI et al. (2007) state that values greater than 0.5 are considered acceptable. R<sup>2</sup> is calculated with the following equation:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (O_{i} - P_{i})^{2}}{\sum_{i=1}^{n} (O_{i} - \overline{O})^{2}}$$
Eq. 32

For the assessment of the calibration and validation results in comparison to the measured data, the following common used statistical criteria were applied in this study:

- Relative error (rel. E) (Eq. 28)
- Root mean square error (RMSE) (Eq. 29)
- %RMSE (Eq. 30)
- Index of agreement (IA) (Eq. 31)
- Coefficient of determination (R<sup>2</sup>) (Eq. 32)

A mix of assessment criteria, which represent quantitative measures of model performance as well as theoretical (IA, R<sup>2</sup>) and more practically (RMSE) oriented criteria, was selected to identify strengths and weakness of the module performance. Furthermore, the assessment criteria serve as comparison to other models. The %RMSE is the decisive criterion for the deviation of results in an acceptable limit (< 20 %) in the present study.

# **5 RESULTS**

## 5.1 Leaf area index

All results of the LAI were measured with the LAI-2000 Plant Canopy Analyzer. The plant parameter LAI was taken weekly until harvest. Besides the already mentioned values, the height of the plants was manually measured and the development was additionally documented on photos.

The following diagrams (Figure 16, Figure 17, Figure 19) present the LAI of the investigated crops on the organic farming management system along with the measurement range of the LAI and the mean average values on each weekly measurement as well as the height of plants.

The results of the observed LAI were subjected to a statistical analysis in order to assess the obtained values. The statistical characteristic with mean average value, minimum and maximum range, variance, standard deviation and coefficient of variation is summarised in Table 19 to Table 21 (Appendix D).

### 5.1.1 Leaf area index of winter wheat

The results of the LAI of winter wheat are shown in Figure 16. The measurements started at the earliest possible date (3<sup>rd</sup> May 2007) and were taken weekly until harvest. Plant height increased from approximately 60 cm to 95 cm.

The course of winter wheat LAI showed an increase up to a peak on 30<sup>th</sup> May 2007 with the maximum value of 3.01, excluding of the first measurement on 3<sup>rd</sup> May 2007. The LAI value of 2.56 can be explained by random error of measurement. Right after the peak, the LAI decreased along with the change from the flowering of winter wheat to the grain development (DIEPENBROCK et al. 2005). As shown in Figure 16, the range of each measurement, which is the result of eight single measurements on the small plot, amounts to averaged 0.64 about the mean average. This value shows a good homogeneity of the cultivated winter wheat plants. Also, the small coefficients of varia-

tion, which vary from 5.76 to 14.86 %, confirm the statement. Further statistical characteristics of the results obtained by LAI-2000 are given in Table 19 (Appendix D).



Figure 16: Winter wheat-LAI values of the organic farming (LAI data: 11 measurement dates; mean average and range of 8 measured points per date)

### 5.1.2 Leaf area index of potato

The following Figure 17 illustrates all LAI results of the potato. The emergence of the potato gave the starting point of measurements (17<sup>th</sup> May 2007) and then, the plant parameter LAI was taken weekly until removing of the leaves (14<sup>th</sup> August 2007). The course of potato LAI showed an increase up to a climax on 12<sup>th</sup> July 2007 with the value of 3.47 (Figure 17).



Figure 17: Potato-LAI values of the organic farming (LAI data: 14 measurement dates; mean average and range of 8 measured points per date)

The LAI range of 2 on 30<sup>th</sup> May 2007 was even affected by a hail which destroyed some of the leaves. The fourth measurement (5<sup>th</sup> June 2007) was twice higher than the third (30<sup>th</sup> May 2007). This development came along with the change from the leaf development to the heading of the potato plants. The high LAI ranges from 5<sup>th</sup> July to 18<sup>th</sup> July 2007 are results of the heterogeneous plant growth on the small plot. In addition, the rainy weather influenced the LAI measurement, e.g. when the leaves lay down after intense rain.

The range of LAI measurements about the mean average value amounts to 1.63. This result can be explained by the row cultivation, primarily at the beginning of the growing season. Furthermore, the row of potato plants was characterised by different coverage. I.e. the growth was partly very closely and partly very clearly, which is the reason for the high range value. The potato plants are very different in comparison to winter wheat and maize and therefore a comparison is difficult. This fact also shows for potato in the high coefficient of variation with values of 42.11 % (5<sup>th</sup> June) and 39.27 % (12<sup>th</sup> June). The variation coefficients of the first three measurements are not given in Table 20 (Appendix D) because the calculation with zero values causes values of above 100 % and is therefore unsuitable.

Furthermore, Figure 17 shows an abrupt cut in the LAI course of the potato plot. This fact was caused by a plague of potato beetles. Figure 18 emphasises this fact as it compares potato plants on two dates (18<sup>th</sup> July and 26<sup>th</sup> July 2007).



Figure 18: Comparison of potato plants from 18<sup>th</sup> July (a) to 26<sup>th</sup> July 2007 (b)

Manual ablation and the use of organic plant protection product did not help against the explosive reproduction of the beetles. One larva eats 35-40 cm<sup>2</sup> of leaf area. Starting from a threshold of 12 larvae per plant, a noticeable loss of biomass and yield is expected (MEßMER 2007). On 7<sup>th</sup> August 2007, the deletion of the whole leaves on the organic field plot occurred.

#### 5.1.3 Leaf area index of maize

The course of the LAI of maize is illustrated in Figure 19. The measurements started in the middle of may (17<sup>th</sup> May 2007) and were also taken weekly until harvest.



Figure 19: Maize-LAI values of the organic farming (LAI data: 15 measurement dates; mean average and range of 12 measured points per date)

The values of LAI showed an increase from the first to the fourth measurement on 5<sup>th</sup> June 2007. The measured value on 12<sup>th</sup> June 2007 was twice as high as then the week before. The maize plants also developed intensely from the measurement of 12<sup>th</sup> June to 21<sup>st</sup> June 2007 which characterises the beginning of the shoot development of maize. An increase of the LAI was also observed on the next two measurements. The plant height of maize had a similar development. After this, the LAI values of maize stayed at the same level of about 2.75 until harvest. The range of measurements about the mean average value is averaged at 0.74 and demonstrates homogeneities of plant growth despite the influence of weather. The measurement on 30<sup>th</sup> May 2007 was even affected by hail which destroyed some of the leaves. However, the maize plant could compensate these effects in this young development stage. Maize and winter wheat have a similar range since both crops belong to the same plant family of
*Poaceae*. The coefficient of variation is situated between 8.37 and 21.31 %. The higher coefficients are denoted in the phase of LAI increase (Table 21, Appendix D).

### 5.2 Sensitivity analysis for the sub modules of SIWAPFLAN

The calculated sensitivity indices (SI) of the parameters of the plant module SIWAP-FLAN are shown in Table 12 that is divided in the three sub modules: 'Plant development', 'Biomass growth' and 'N uptake'. The reference values and value ranges, on which the analysis is based, are also arranged in this table. Furthermore, the following figures (Figure 20 to Figure 22) show the SI for the three simulation output results concerning each sub module:

- transpiration,
- coverage,
- N uptake.

Parameter	Reference value	Value range of parameter	SI of output results transpiration	SI of output re- sults coverage	SI of output re- sults N uptake
'RIPING'	18000	16200-23400	5.26	0.53	1.82
'BTEMP'	4.8	3.06-6.54	0.02	-0.03	-0.12
'ROOTING'	12000	8400-15600	-0.06	-0.03	-0.02
'PHMAX'	90.0	63.0-117.0	-0.04	-0.03	-0.20
'RDMAX'	18.0	12.6-23.4	0.19	0.03	0.18
Parameter	Reference	Value range	SI of output results	SI of output re-	SI of output re-
i arameter	value	of parameter	transpiration	sults coverage	sults N uptake
'AREAWT'	0.004	0.0028-0.0052	1.26	1.62	1.51
'PHOTSR'	12.5	8.75-16.25	3.05	3.33	3.33
'EXCOEF'	0.3	0.21-0.39	0.31	0.23	0.57
'T_0'	0.0	-3.0-3.0	-0.03	-0.02	-0.04
'T_1'	10.0	7.0-13.0	-0.46	-0.32	-0.66
'T_2'	30.0	21.0-39.0	0	0	0.01
'T_3'	40.0	28.0-52.0	0	0	0
Parameter	Reference	Value range	SI of output results	SI of output re-	SI of output re-
i arameter	value	of parameter	transpiration	sults coverage	sults N uptake
'TKMAX'	1.78	1.25-2.32	0	0	-0.60
'TKMIN'	1.0	0.7-1.3	0	0	0.50
'NCT0'	0.041	0.0287-0.0533	0	0	0.11
'NCT1'	0.009	0.0063-0.0117	-0.01	0	0.97
'NCNF'	0.4	0.28-0.52	0	0	-0.37
'NCKR'	0.002	0.0014-0.0026	0	0	0

# Table 12: Value ranges of sensitivity analysis and sensitivity indices (SI) of the simulation results<br/>transpiration, coverage and N uptake

Indices are classified (non consideration of the sign) in high (> 1), medium (< 1 and > 0.3) and small (< 0.3) SI.

Figure 20 illustrates one clear result. I.e. the parameter 'RIPING' is the most sensitive of the sub module 'Plant development' for the results transpiration and N uptake. Therefore, 'RIPING' will be the focus of the sub module calibration. The parameter 'RDMAX' had a medium sensitivity for the output results transpiration and N uptake. The behaviour of sensitivity is explained by the dependency of water and N uptake through the plant root depth and its possibility of uptake in the reached horizons.



Figure 20: Sensitivity indices of the parameters of the sub module 'Plant development'

The parameters 'PHOTSR' and 'AREAWT' of the sub module 'Biomass growth' had high positive indices (Figure 21). These were all extremely sensitive for all the simulation results. This is decisive for the prediction of biomass production in the module. 'EXCOEF' parameter showed a medium positive sensitivity.



Figure 21: Sensitivity indices of the parameters of the sub module 'Biomass growth'

On the contrary, the parameter 'T\_1' had a negative medium index which lead to the input parameter value changing the output value in the opposite direction. The high and medium values of indices show a necessity for careful calibration of the parameters in order to ensure that the model is behaving as accurate as possible. Little variation in the sensitivity of the parameters 'T\_0', 'T\_2', 'T\_3' was encountered. Thus, these parameters will be neglected in the following calibration steps of the plant module SIWAPFLAN.



Figure 22: Sensitivity indices of the parameters of the sub module 'N uptake'

The parameters of the sub module 'N uptake' showed small sensitivities in comparison to the other sub modules. However, the parameters 'NCT1' and 'TKMIN' with a positive index and the parameters 'TKMAX' and 'NCNF' with a negative index have a priority for the sub module and were thus considered in the calibration.

# 5.3 Parameterisation and calibration for the sub modules of SIWAPFLAN

The following section contains and describes separate steps of the calibration procedure for the three sub modules of SIWAPFLAN.

#### 5.3.1 Sub module 'Plant development'

The first step is the parameterisation of the sub module parameters which are determined from measured and literature data. The parameter 'BTEMP' for the investigated crops, being a central component in the basic function of 'PTU' / 'SUMPTU', were taken from the literature of STOCK & DIEPENBROCK (1999). Furthermore, the parameters 'PHMAX' and 'RDMAX' were derived from measured data of the Bad Lauchstädt experimental field (Table 13).

Parameter	Winter wheat	Potato	Maize
'BTEMP'	5 °C	3° 6	<b>3</b> 8
'RDMAX'	15 dm	9 dm	20 dm
'PHMAX'	95 cm	80 cm	230 cm
'RIPING'	20000 PTU	25500 PTU	22000 PTU
'ROOTING'	6000 PTU	14000 PTU	15000 PTU

Table 13: Parameters of the sub module 'Plant development'

The adjustment of the parameter 'RIPING' for the investigated crops was the first object of the calibration which corresponds to the sensitivity analysis. The preset of 'RIP-ING' influences the course of the plant development. The calibration of the parameter 'RIPING' produced no satisfactory results (%RMSE of 31.10 % and rel. E of -28.86 %). Figure 23 shows an overestimation until the development stage (BBCH / DC) number 30 and the development course was underestimated from stage number 30 on.



Figure 23: Comparison of simulated development stages and observed development stages at the example of maize 2007

An analysis of development stage simulation reveals two problems. On the one hand, the assumption of the linear development with ten HANWAY stages causes difficulties in the simulation of different plant species. This is justified by the development courses which may be shifts in the stages and / or certain stages may even be omitted (MEIER

2001). Winter wheat has a continued development throughout the stages. Maize and potato are crops which omit the same stages in their development (Figure 4, page 14).

The example of maize in Figure 23 emphasises this fact. The measured data show a two-sided polarisation. On the one hand, a high amount of measured data is located between stage 0 and stage 19. On the other hand, a similar data volume exists from stage 50 to stage 90. In addition, stage 34 is mostly present. The failure of data between stage 19 and stage 30 can be explained by the omitting of stages. If tillering occurs earlier than stage 19, the measurements have to be continued with growth stage 30. Furthermore, with an earlier tassel emergence, the development goes on with stages 50 (MEIER 2001). Similar aspects can be observed in the development of potato.

On the other hand, an inconsistency occurred because of the transformation from internal used HANWAY stages in the output result BBCH / DC stages. It is neither linear nor constant which is illustrated in Figure 24. The different inclinations of the curve, that are shown in red lines in Figure 24, cause the %RMSE value in Figure 23.



Figure 24: Schematic comparison of BBCH / DC and HANWAY stages (red lines = inclinations of curve)

A ratio calculation of both development scales (HANWAY and BBCH / DC) (Table 14) and an example should clarify the visual statement in Figure 24. The BBCH / DC development period 30 to 59 includes a number of 30 stages and the same development in HANWAY stages would be the period 2 to 7.7 including a number of 5.7 stages. A ratio of 30 : 5.7 results in a ratio number of 5.26 (period 2). In comparison, the ratio

number of the first period is twice as high as the ratio number of the second period. The third development period has a ratio number of 17.65. The three ratio numbers show the differences which cause difficulties in the calibration process.

	1 <sup>st</sup> Period	2 <sup>nd</sup> Period	3 <sup>rd</sup> Period
development period BBCH / DC	0-29	30-59	60-89
number of including stages	30	30	30
development period HANWAY	0-3	3.1-7.7	7.8-9.5
number of including stages	3	5.7	1.7
ratio of DC to HANWAY	30 : 3	30 : 5.7	30 : 1.7
ratio number	10	5.26	17.65

Table 14: Comparison of BBCH / DC and HANWAY stages

As a result of different main stages in the development courses of the investigated crops and the tripartition of development conversion, the simulation of the plant development in stages was extended by three phases according to the application of the model SPASS by GAYLER et al. (2002). The development stages are summarised into three phases: (1) from germination to shoot; (2) from shoot to flowering; (3) from flowering to ripeness. Considering these results, the following algorithm with plant-specific parameters for phases and factors of ontogenesis was implemented:

 $DEVSTG \le PHASE 1$   $DEVSTG = OF1*\frac{SUMPTU}{RIPING}$   $DEVSTG \ge PHASE 1 \text{ and } \le PHASE 2$   $DEVSTG = OF2*\frac{SUMPTU}{RIPING}$   $DEVSTG \ge PHASE 2$ 

 $DEVSTG = OF3 * \frac{SUMPTU}{RIPING}$ 

Eq. 43

PHASE 1plant-specific parameter for determination of phase (1) and (2)PHASE 2plant-specific parameter for determination of phase (3)OF 1 / OF 2 / OF 3plant-specific parameter: factor of ontogenesis for phase 1 / phase 2 / phase 3

The example in Figure 25 shows that the RMSE is halved and the relative error is reduced to the amount of -3.17 %. For the parameterisation of the phase development parameters, an analysis according to the ontogenesis field data was conducted to determine the parameter values (Table 15).



Figure 25: Comparison of calibration results of the initial and the improved sub module 'Plant development

Furthermore, on the basis of the existing field emergence data, the new parameter 'MAX\_EMERG' was created. 'MAX\_EMERG' controls the simulated emergence. If the development does not reach the development stage 9 (BBCH / DC) after the given days, the emergence of plant is induced.

Parameter	Winter wheat	Potato	Maize
'OF 1' 9.36		4.05	3
'OF 2'	14	20	13.5
'OF 3'	12	12	10.5
'PHASE 1'	2.5	0.9	1.05
'PHASE 2'	8.9	8.9	8.9
'MAX_EMERG'	20 days	45 days	20 days

Table 15: Parameters of the phases development in the sub module 'Plant development'

Afterwards, a systematical comparison of observed and simulated stages of development was accomplished by a manual calibration. In order to find the best solution, the first step was a visual adaptation to 1:1 line in a stepwise approximation. The best results were obtained with the value 20000 PTU of the parameter 'RIPING' (winter wheat), 25500 PTU (potato) and 22000 PTU (maize) for the field plots and the simulation years (2004-2007) of calibration (Figure 26).

The calibration of winter wheat shows the best result with a %RMSE of 13.25 %. The negative relative error indicates that most values are below the 1:1 line. Noticeable for winter wheat in Figure 26 is that the module underestimated the stages in the range

between the observed stage 60 and stage 85. This effect is the result of the unequal conversion from HANWAY to DC stages, despite the extension of phases development.

The calibration of maize development obtains good results either. The %RMSE of 19.76 % is produced by the overestimated simulation of the observed stage number 30 and underestimation from the stage number 50 to 70 and also at stage number 90.

The best calibration of potato DEVSTG shows that most values are below the 1:1 line. A quartering of the potato data set is given. Thus, it appeared that the calibration was difficult. The %RMSE amounts to 18.76 % which is a good calibration result (Figure 26).



Figure 26: Overall result of the calibration of the sub module 'Plant development'

#### 5.3.2 Sub module 'Biomass growth'

The parameters 'AREAWT' and 'PHOTSR', which are most sensitive, were subjected to the calibration process. The considered crop variables for the model calibration were the LAI and the time course of biomass. The total biomass on harvest is a very important objective of agricultural system. Therefore, this study reflects it in a separate way in the calibration process. The provided data of total biomass on harvest for the calibration process of the investigated crops are summarised in Figure 27.



Figure 27: Observed total biomass on harvest for calibration

As demonstrated in Figure 27, the yearly biomasses have a natural variability. The amounts of biomass for winter wheat and potato showed a decreasing trend from 2004 to 2007. Furthermore, the year 2007 was characterised by extremely small biomasses for winter wheat and potato. This fact is explained by pest infestation. The damage done by mice reduced the biomass of winter wheat by half. On the one hand, potato was minimised by the plague of potato beetles and on the other hand by the damage done by mice, mainly after the harvest of winter wheat. In comparison to the biomasses of potato from the year 2004 to 2006, the biomass of the year 2007 amounted to only half its value. Furthermore, the biomass of winter wheat (2007) had a similar amount compared to the potato biomass in this year.

Furthermore, corresponding to the structure and approach of the module, the measured crop variable LAI should be used for the calibration of the sub module 'Biomass growth'. The sub module contains two types of LAI, the green LAI (GRNLAI) and the total LAI (TOTLAI). The LAI measurements in field were conducted over the whole growing season. Thus, the measured LAI values contain not only the green part of LAI. Consequently, the field data of LAI were compared with the simulated values of total LAI (TOTLAI) in the calibration process. The simulated TOTLAI describes an exponential curve which reaches a maximum value and remains constant until harvest. Hence, for the calibration, the course of the measured LAI values could only be used to reach the maxima. The inclination and maximum of simulated LAI could be determined.

#### Calibration process of maize

The calibration of the parameters 'PHOTSR' and 'AREAWT' for maize is based on two crop variables. One of them is the LAI data set of the growing season 2007. In the procedure of calibration, a test phase was conducted and only unsatisfying results of the simulated LAI course were obtained. The "fixed" regulation of the LAI time course is the cause of these results. The original "fixed" regulation contains two approaches. Up to the stage number 2 (HANWAY scale), the flow of assimilates is only used for the leaves. Between the stages number 2 and 5 (HANWAY scale) the partition depends on the development. Consequently, the inflexion points of the LAI course in the module is fixed on two stages. This simulation base produces unrealistic results that are caused by the different plant development of winter wheat, potato and maize. Thus, the structure of the sub module was changed in the following approaches. The stages and thus the inflexion points could be determined by two plant-specific parameters 'D0\_LAI' and 'D1\_LAI' using the original principle. I.e. up to the stage, which is fixed by the parameter 'D0\_LAI', the assimilates are used for the biomass of leaves. The leaf development and the supply of assimilates are finished when transgressing the stage, which is determined by parameter 'D1\_LAI'. Besides, the dependence of development between the selectable stages is maintained. The parameter values were determined by the observed LAI courses of the three investigated crops which are shown in Table 16 (page 77). Figure 28 shows the calibration result of the LAI course of maize with the above mentioned approach.

The visual interpretation of the results shows that there is a good agreement between the simulated and observed LAI of maize. The comparison of simulation and observation with the index of agreement indicates with 0.98 a very good prediction of the trend as well. With a %RMSE of 18.27 %, the calibration is successful.



Figure 28: Calibration result of maize LAI with 95 % confidence interval

The second crop variable for calibration was the biomass data of the period from 2004 to 2007. Figure 29 illustrates the best result of the calibration process for the time courses of the biomass simulated in comparison to the measured values. Different statistical criteria evaluate the accuracy of the biomass description. The parameters used by the sub module are listed in Table 16 (page 77).



Figure 29: Comparison of the simulated and observed time courses of maize biomass in consideration of the measurement range

The sub module shows little deviation in the simulation of the time course of maize biomass with an index of agreement that amounts to 0.99 and 0.92 (Table 23, Appendix E). The RMSE detects the total difference between the simulated and the measured values which ranges between 365 and 2373 kg ha<sup>-1</sup>. The result of the fourth harvest of the year 2005 was overestimated and that causes the RMSE of 2373 kg ha<sup>-1</sup>. The RMSE results 1651 kg ha<sup>-1</sup> (2004) and 2178 kg ha<sup>-1</sup> (2007) are also caused by the over- and underestimation of the fourth intermediate harvest. The RMSE converting into % errors obtains values that exceed 50 %. Despite the larger values of %RMSE (> 20 %), the values of  $R^2$  is comparable with other models in literature (MIRSCHEL & WENKEL 2007).

The calibration results of total biomass on harvest of maize (2004-2007) are illustrated in Figure 30. The comparison between simulation and observation with the 1:1 line justifies the calibration process with a %RMSE of 16.32 % which reflects a successful calibration. The RMSE of all years amounts to 2350 kg ha<sup>-1</sup> which represents a satisfactory result for the calibration. Furthermore, the index of agreement with 0.76 shows an acceptable result. Further accuracy criteria – rel. E and RMSE – for each year are summarised in Table 22 (Appendix E).



Figure 30: Comparison of simulated and observed total maize biomass on harvest in consideration of the measurement range

#### Calibration process of winter wheat

Similar to maize, the process of calibration for winter wheat used the LAI to determine the parameters 'AREAWT' and 'PHOTSR'. The damage done by mice, which is described in section 5.3.2, was observed after the reach of the LAI maximum. Four values of LAI were used for the calibration. Figure 30 illustrates the comparison of the observed and simulated values which are the best result of the calibration. The index of agreement of 0.89 and R<sup>2</sup> of 0.37 show a poor result in comparison to the maize LAI. This fact is caused by the small number of observation and the outlier sensitivity of the accuracy criterion R<sup>2</sup>. The rel. E is very small with 1.02 %. The %RMSE amounts to 6.36 % which shows a successful calibration.



Figure 31: Calibration result of winter wheat LAI with 95 % confidence interval

The continuation of the calibration for winter wheat with the data of biomass required a change of the above mentioned method of calibration. The reason was the observed total biomass on harvest of the year 2007 which were half of the average, as previously explained. A comparison of the fourth intermediate harvest on 5<sup>th</sup> June 2007 with the harvests of the same development stage in the years 2004, 2005 and 2006 lead to the conclusion that the fourth intermediate harvest of 2007 is comparable with the others. Therefore, this harvest of 2007 was used for calibration instead of the main harvest 2007. Furthermore, the total biomass on harvest of the years 2004, 2005 and 2005 and 2006 was used to derive the parameters 'AREAWT' and 'PHOTSR' in the calibration.

The calibration with this changed method also produces unsatisfactory results. I.e. the biomass 2007 was overestimated and the previous years were extremely underestimated (Figure 32). The rel. E for the underestimated years amounts to partly more than - 30 %. The index of agreement with 0.37 corroborates this effect in the calibration. Furthermore, the decisive criterion %RMSE obtains 27.95 % and thus the calibration failed. Due to that, the determination of the parameters 'AREAWT' and 'PHOTSR' was only applied by the biomass data of the years 2004, 2005 and 2006. The parameterisation of the LAI related parameters 'D0\_LAI', 'D1\_LAI' and 'LAIatCD1' remained unchanged to the calibration step above described. Figure 32 documents both calibration results with and without the year 2007. The sub module that includes calibration

without the year 2007 produced an IA of 0.95 and a %RMSE of 4.76 %. The further accuracy criteria changed for the better as well and are summarised in Table 22 (Appendix E).



Figure 32: Comparison of simulated and observed total winter wheat biomass on harvest in consideration of the measurement range (quad symbols = calibration without 2007, quad symbols with cross = calibration with 2007)

The sub module could not exactly simulate the time course of biomass but could capture the temporal pattern of biomass with the index of agreement of 0.80 to 0.86, which indicates deviations in the courses (Figure 33). The criterion R<sup>2</sup>, which gives stronger assessment of accuracy in comparison of IA, shows low values for the simulation of time courses of biomass. The cause is a general underestimation of measurements. RMSE, %RMSE and rel. E are summarised in Table 23 (Appendix E).



Figure 33: Comparison of the simulated and observed time courses of winter wheat biomass in consideration of the measurement range

The higher values of the RMSE and rel. E are also caused by the slower simulation performance of the time courses of winter wheat biomass (Figure 33). Especially, the years 2004 and 2005 showed differences in the simulation quality in the early development.

#### Calibration process of potato

The obtained data of LAI field measurements for potato required a check whether it was possible to use them in the calibration process in spite of the pest infestation. The course of potato LAI was degraded by potato beetles. For an estimation of the reduction of the LAI, a comparison to the conventional management system with and without mineral fertiliser and with chemical plant protection should be given (Figure 34). The values of the LAI were also measured during the same time period. However, this data set was not used for calibration and validation in this study. The fact is that both plots of the conventional system show similar courses of LAI (Figure 34) as on the investigated course of organic farming. Expectedly, the three measured LAI courses reflect the supply with fertiliser. The field plot with mineral fertiliser shows the highest LAI results, whereas the LAI values of the organic fertiliser are lower. The lowest LAI values are observed with the unfertilised variant. The maximum value of all three variants was reached on 12<sup>th</sup> July 2007. Due to this aspect, it is assumed that the damage in the stages of LAI increase on the field plot of organic farming was very small.



Figure 34: LAI of potato – comparison between the values of organic farming and conventional agriculture without and with mineral fertilizer



Figure 35: Weekly photo documentation of the potato development and its LAI

In addition, the first punctiform damage done by potato beetles on a single potato plant was observed on 28<sup>th</sup> June 2007. An increasing damage of the leaves was observed and documented by weekly photos (Figure 35). Despite the damage, an increase of LAI was measured. The major damage is documented after the LAI had reached the maxima. On 12<sup>th</sup> July 2007, the first extensive damage was discovered caused by the increased number of potato beetles. This damage was on the "turned away side" of the measurement. In the photo of 18<sup>th</sup> July 2007, a further increase of damage was identified by means of the bright areas in the "background" on the field plot. The comparison to the other management systems and the photo documentation show that the measured LAI values could be considered as an approximation in the calibration.

The calibration result is illustrated in Figure 36. The underestimation from the 50<sup>th</sup> to the 70<sup>th</sup> day after sowing and the overestimation near the maxima are the causes for the %RMSE of 24.10 %. However, the accuracy criteria IA and R<sup>2</sup> show however very good results in simulation quality. Hence, the calibration can be accepted.



Figure 36: Calibration result of potato LAI with 95 % confidence interval

The calibration for potato was subjected to similar conditions by the crop variable biomass. The observed biomass in the year 2007 was reduced by the potato beetles and furthermore by mice. These damages could be already identified by the fourth intermediate harvest of 2007. Therefore, the biomass values of the year 2007 were not considered for the calibration. The parameter 'AREAWT' and 'PHOTSR' were calibrated with the data of the years 2004, 2005 and 2006. The calibration results in an IA of 0.91 which represents a good agreement between the measured and the simulated values (Figure 37). The RMSE of the calibration period amounts to 1007 kg ha<sup>-1</sup> which means a %RMSE of 13.87 %. The criteria of accuracy of the total biomass calibration are summarised in Table 22 (Appendix E).



Figure 37: Simulated and observed total potato biomass on harvest in consideration of the measurement range

The results of the time course of biomass show differences in the quality of simulation which is also reflected in the values of R<sup>2</sup> that range from 0.35 to 0.65. The rel. E and %RMSE with more than 50 % indicate poor performances (Table 23, Appendix E). One reason for this is that the last intermediate harvests of 2005 and 2006 were underestimated with a high difference in comparison to the measured values. Another reason is that all measured values of 2004 were underestimated (Figure 38).



Figure 38: Comparison of the simulated and observed time courses of potato biomass in consideration of the measurement range

The sub module 'Biomass growth' contains nine parameters: 'AREAWT', 'PHOTSR', 'EXCOEF', 'T\_0',' T\_1', 'T\_2', 'T\_3', 'LAlatCD1', 'HRVI'. All were considered in the parameterisation and calibration procedure. The basic parameters 'T\_0', 'T\_1','T\_2' and 'T\_3' for the optimum temperature curve of assimilation were not changed from the original parameterisation. The temperature values were checked with data of literature for the investigated crops. PETR (1991) and STOCK & DIEPENBROCK (1999) postulate the same temperature thresholds. The parameter 'EXCOEF' was also determined by literature values which are listed in Table 16. 'LAlatCD1', determining the simulated value of LAI with coverage of 100 %, was derived from the weekly measured values of LAI. The parameter 'HRVI' was retained in the original value for the investigated crops.

Parameter	Winter wheat	Potato	Maize	Method of estimation
AREAWT	0.00116	0.00332	0.00209	calibrated by field data
PHOTSR	14.74836	12.45372	19.53679	calibrated by field data
	0.4	0.55	0.49	
EXCOEF	(Schröder	(RITCHIE	(LINDQUIST	parameterised by literature
	1995)	et al. 1995)	et al. 2005)	
T_0	0	0	10	retained by initial parameterisation
T_1	10	10	20	retained by initial parameterisation
T_2	20	20	35	retained by initial parameterisation
T_3	30	30	45	retained by initial parameterisation
LAIatCD1	1.8	2.2	1.5	adapted by field data
HRVI	0.45	0.8	0.1	retained by initial parameterisation
D0_LAI	3	3	2	adapted by field data
D1_LAI	8.9	9.8	8.9	adapted by field data

Table	16:	Parameters	of	the	sub	module	'Biomass	growth'
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After the reflection of each separate calibration step, Figure 39 shows all results of the parameterisation and calibration of the sub module 'Biomass growth'. The descriptions of LAI, total biomass on the harvest and time course of biomass using the sub module with any parameters are listed in Table 16. The calibration shows a reasonable accuracy for the simulated crop variables. The prediction of LAI has a bipolarisation. The early development was underestimated and the development was overestimated. The simulations of the total biomass on the harvest showed a trend of underestimation. The performance of the time courses of biomass produces an unsatisfactory result for all investigated crops (Figure 39) as an underestimation of the measured values occurred in the majority of the cases. Due to that, the validation is based on a successful cali-

bration and the time courses of biomass were not considered in the validation process of the sub module 'Biomass growth'.



Figure 39: Overall result of the calibration of the sub module 'Biomass growth' - LAI, total biomass on the harvest and time course of biomass

#### 5.3.3 Sub module 'N uptake'

The crop variables for the calibration of the sub module 'N uptake' are the N contents in crop that are measured in defined stages and the amounts of the total N uptake on the harvest. The years 2004, 2005 and 2006 were used for the parameterisation and calibration. For parameters of maize, the measured values of the year 2007 were also considered. The N uptake by crop is a calculated value from the N content and the total biomass on harvest. As described previously, the values of winter wheat and potato

biomass in the year 2007 were not useable. Therefore, the values of N uptake for these both crops could not be considered in the calibration process.

The parameterisation of 'NCT0' and 'NCT1' was derived from the measured N contents of the plant in the beginning and in the end of the growing season for the three investigated crops. Both parameters determined the ontogenesis-dependent curve which was controlled by the observed N contents analysed during the growing season. The curve form of N content in the sub module was determined by the parameter 'NCNF'. The value of 'NCNF' was also derived from the measured N content.

A comparison between the observed and simulated amount of total N uptake on harvest was conducted to reinforce the trial and error calibration procedure of the parameter 'NCKR'.

Both parameters 'TKMAX' and 'TKMIN' were in the focus of this calibration. The calibration was based on the data of total N uptake on the harvest. The comparison between simulated and measured values of maize N uptake and the 1:1 line justifies the calibration process with a %RMSE of 11.62 % (Figure 40). The comparison between simulated and measured values of winter wheat showed a very good prediction which also verifies the small %RMSE with 3.72 %. The calibration result of potato has an accuracy of 13.45 % (%RMSE). Therefore, the calibration of the sub module 'N uptake' is successful for all investigated crops (Table 24, Appendix E). The parameters, which were determined by the parameterisation and calibration, are listed in Table 17.



Figure 40: Comparison of simulated and observed total N uptake on harvest in consideration of the measurement range

Parameter	Winter wheat	Potato	Maize	Method of estimation
TKMAX	2.01835	1.79299	2.36730	calibrated by field data
TKMIN	1.04588	0.00624	0.86793	calibrated by field data
NCT0	0.041	0.055	0.085	adapted by field data
NCT1	0.008	0.014	0.01	adapted by field data
NCNF	0.4	0.2	0.3	adapted by field data
NCKR	0.002	0.003	0.005	calibrated by field data

Table 17: Parameters of the sub module 'N uptake'

## **5.4 Validation for the sub modules of SIWAPFLAN**

The simulation of the calibrated sub modules was validated against the independent data set for the three investigated crops which are described in detail in the following three sections. The validation procedure considered the years from 1999 to 2003. The validation of winter wheat contained one year less in comparison to the other two crops. The reason is that in the year 2001 the cultivation of winter wheat was discontinued by reconstruction on the experimental field 'land use experiment' in Bad Lauchstädt.

#### 5.4.1 Sub module 'Plant development'

The crop variable, ontogenesis stages, was used for the evaluation of the sub module 'Plant development'. The results suggest that the simulated development stages of winter wheat were in close agreement with the observed stages. The %RMSE of winter wheat is 5.65 %. This accuracy is very good. However, the %RMSE of the calibration process is twice as much. Therefore, it is assumed that the lower number of compared stages is the cause of the small value of %RMSE.

The result of validation for the maize development stages shows that the comparison of simulation and observation produces a good result. The BBCH / DC stages between number 0 and 20 and between number 50 and 90 are gathered at the 1:1 line. At BBCH / DC stage number 30, the same outliers can be recognised (Figure 41). The simulation quality of this stage shows both under- and overestimation. A similar effect was also noticed in the calibration process. The good agreement of observation and simulation results in a %RMSE of 17.58 %. The outliers cause the higher values of %RMSE.

The validation of potato development stages is similar to maize regarding the accuracy. The result shows the tripolarisation of data (Figure 41). Most values hit the 1:1 line in the comparison between measured and simulated values. Only the data of the year 2000 were continuously overestimated causing a %RMSE of 16.31 %.

Figure 41 shows the evidence that the sub module very well simulates the crop development stages. The sub module 'Plant development' is validated with the help of the reached validation accuracy showing a RMSE between 2.63 and 6.79 stages in the performance of development stages for the three crops.



Figure 41: Overall result of the validation of the sub module 'Plant development'

#### 5.4.2 Sub module 'Biomass growth'

The total biomass on the harvest was the main objective in the comparison of the validation for the sub module 'Biomass growth'. The simulated and measured values of total biomass on the harvest for the three investigated crops are given in Figure 42.



Figure 42: Overall result of the validation of the sub module 'Biomass growth' - comparison of simulated and observed total biomass on harvest in consideration of the measurement range

The total biomass on the harvest was underestimated for nearly all values of the validation period. For the years 1999, 2001 and 2002, the sub module 'Biomass growth' worked satisfactory with RMSE between 221 and 414 kg ha<sup>-1</sup>. Both results of year 2000 and 2003 were underestimated by the sub module with the RMSE of 1502 and 2380 kg ha<sup>-1</sup>. The differences in the simulation quality give a %RMSE of 19.58 % (Table 25, Appendix E). Due to the fact that the accuracy of the result is lower than 20 %, the validation for maize is successful.

Figure 42 shows the relatively good agreement of measured and simulated values for the total biomass on the harvest for winter wheat. The years 2001 and 2003 were not accurately predicted for winter wheat. The %RMSE of these two years ranged from 14.02 to 14.16 %. Considering all the simulation results, despite some serious deviations between simulated and observed values (%RMSE of 22.25 %), the sub module can predict the total biomass on harvest for winter wheat (Table 25, Appendix E).

The validation process for potato indicates for the years 1999, 2000 and 2001 good to acceptable results. The insufficient of validation result is caused by the over- and underestimation of the years 2002 and 2003. The discrepancies produce an inaccuracy

with a %RMSE of 26.41 % (Table 25, Appendix E). Therefore, the assessment of the whole performance results in the assumption that the sub module is not validated for potato.

The reflection of the all validation results for the sub module 'Biomass growth' shows that the year 2003 was underestimated for all the investigated crops. A similar effect could not be established in the calibration. The cause of this effect is assumed in the operative stress factors of the biomass production which will be discussed in section 6. In general, the validation of the sub module 'Biomass growth' shows a reasonable accuracy with some restriction for the simulated crop variable.

#### 5.4.3 Sub module 'N uptake'

The performance of the calibrated sub module 'N uptake' was also validated against the independent data set for the period from 1999 to 2003. The result of the comparison of the measured and simulated values of N uptake is illustrated in Figure 43. The values show a bigger range around the 1:1 line in comparison to the calibration.



Figure 43: Overall result of the validation of the sub module 'N uptake'- comparison of simulated and observed total N uptake on harvest in consideration of the measurement range

The difference between simulated and observed N uptake vary from 0.71 to 18.46 % (%RMSE) for maize. The performance shows underestimated as well as overestimated values. The highest RMSE's of maize are 16.10 kg ha<sup>-1</sup> and 18.65 kg ha<sup>-1</sup>. Despite these differences, the sub module 'N uptake' has an inaccuracy error of less than 20 % documenting the validity of the sub module for maize (Table 26, Appendix E).

The N uptake simulation of winter wheat shows only negative rel. E which is the evidence for underestimation by the sub module. The %RMSE varies from 10.37 % to 31.18 %. The largest differences of simulated N uptake occurred in the years 2001 and 2003 which are the same underestimated years of the total biomass on the harvest in the previously described validation step. These results indicate the connection in the simulation of biomass and N uptake. Therefore, an underestimated biomass in the sub module 'Biomass growth' also influenced the simulated uptake of nitrogen. Due to the inaccuracy of 46.39 % the validation is not successful (Table 26, Appendix E).

The result of the simulation for potato produced overestimated values for the years 1999, 2001 and 2002 which show the %RMSE with a range of 19.27 to 28.62 % (Table 26, Appendix E). On the contrary, the N uptake of 2003 was underestimated. The simulated results of 1999, 2000, 2002 and 2003 indicate that the simulation of N uptake is controlled by the biomass. However, the overestimation of the value of 2001 is contrary to this statement. Due to the fact, that the comparison between observed and simulated values of N uptake revealed too many differences, the sub module 'N uptake' is not validated for potato.

The procedure of validation showed that the sub module 'N uptake' accurately simulated the N uptake of maize. High inaccuracies occurred for the crops winter wheat and potato. Furthermore, the effect of underestimation in the year 2003 was also encountered. The performance of the validation for all the investigated crops, under consideration of the calibration process, will be discussed and assessed in section 6.

# **6 DISCUSSION**

The first part of discussion contains the methodology of the LAI measurement and the methodology of calibration and validation, as both have an important influence on the result. The second part discusses the results of the calibration and validation procedures of the module SIWAPFLAN where gained insights are outlined. The concluding part deals with the applicability of the module regarding the description of crop growth and development processes on the location.

# 6.1 Methodological aspects

#### 6.1.1 Leaf area index

The influences on the accuracy of the LAI measuring method with the LAI-2000 Plant Canopy Analyzer can be categorized in spatial and temporal as well as plant and development-specific aspects.

The first aspect contains the size of the field plots which is 5 x 10 m. The realisation of the LAI measurement must be conducted to compromise with the target sampling areas of the four intermediate harvests. These are also essential for the calibration of the module. Therefore, the present size of the measurement area was accepted enabling the measurements with the non-consideration of the outer-ring number five or four and five. On the one hand, this avoids the detection of objects or gaps outside the small plots. On the other hand, it could cause an underestimation which is effected by the non-detection of leaves.

The temporal aspects depend mainly on the time of measurement realisation. The recommendation of the manufacturer is that the device should be applied during both twilight hours and uniformly clouded weather conditions. This restricts the number of measurable samples that can be measured in one day and forces an intricate planning of the data collection events (WILHELM et al. 2000). The results of HICKS & LASCANO (1995) demonstrate that a more independent realisation time is possible by making observations either during uniformly overcast conditions or around solar noon using the shading method.

The realisation of the LAI measurements in this study considered the given recommendations and results of the investigation studies. Thus measurements were generally taken during morning hours that include a failure of 15 % that is sufficient for most research and crop management purposes (WILHELM et al. 2000). Some measurements took place during direct insolation where the shading method was applied. These measurements can produce a failure of 15-30 %. In addition, the change in brightness during the day causes approximately 10 % failure of the LAI values (WANG 2001).

Besides, the temporal and spatial influences, a general limitation concerning the differentiation of plant-specific aspects of the device, needs to be considered. The analyzer contains an inability to differentiate between leaves and other plant parts such as stems and branches (MALONE et al. 2002). Therefore, different authors postulated that the term 'foliage area index' (WELLES & NORMAN 1991) or 'vegetation area index' (FASSNACHT et al. 1994), rather than LAI, might be a better description of the measured content with the plant canopy analyzer.

A further reason of an inaccuracy regarding the development of plants may occur. SMITH et al. (1993) suggest that a reason for underestimation of the LAI is the inhomogeneous crop stand. This case was observed in this study in the beginning of the maize growing season 2007. To reduce the inaccuracy, the measurement number was increased from eight to twelve. Furthermore, within the four replications during the early development, a great range was noticed. This was caused by greater values underneath the plants and smaller values in between the crop rows. This difference decreases as the plants grow and the crop rows close.

The measuring method with the LAI-2000 is subjected to potential uncertainty / failure which are revealed by the conducted measurements. The results of LAI for the module calibration must be used with the proviso that these are approximate values.

#### 6.1.2 Calibration and validation

In the present thesis, the method of split sample test was used for calibration and validation. This method is commonly used for testing the applicability of agroecosystem modelling. In an optimal case, an equal splitting of the available data set is performed. The lower number of years for calibration or validation results in a relative uncertainty. For the present study, this was not possible as the data set covers a period of nine years. The decision to take four years for the calibration and five years for the validation results in a relatively certain validation. Further restrictions influenced this almost uniform splitting of data set. So, the biomass data for the year 2007 could not be considered for winter wheat and potato which enlarged the uncertainty of the calibration. Concerning the BBCH / DC stages, more observed stages for the calibration period of 2004-2007 were available in comparison to the validation period. That increased the certainty of the calibration, despite the fact that more years are available for the validation.

# 6.2 Parameterisation and calibration results for the sub modules of SIWAPFLAN

#### 6.2.1 Sub module 'Plant development'

The calibration of the sub module 'Plant development' was based on data of BBCH / DC stages. The measurements of plant development stages (BBCH / DC) do not contain the same number of stages every year as it varies from seven to twenty observed stages per year for winter wheat, potato and maize. Hence, calibration and validation include different numbers of observed values. For all investigated crops, the calibration period contains more measured BBCH / DC stages.

The sub module 'Plant development' uses a simple approach to simulate the development stages. The application of temperature and day length calculates the used internal HANWAY scale which is divided in ten single stages. The results of the parameterisation procedure show a systematic underestimation from stage number 60 to 90 (BBCH / DC). This effect is caused by the transformation of the ten-stage HANWAY scale into the FEEKES scale and subsequently into the practice relevant BBCH / DC scale. The scale of HANWAY is not linear and limits the transformation. Therefore, the extension of three plant-specific phases factors, which was compared to the non extended version, corrects in large parts the mentioned underestimation. Winter wheat shows the best result of calibration (13.25 %) which is explained by the continuous development. The calibration for potato was conducted with an error of 18.67 %. The maize calibration of the development stages was calculated with an error of 19.76 %.

The assessment of the result should be regarded under the aspect of important development stages for the three investigated crops. These stages are essential for all crop processes and have a high relevance for practice as well. Concerning winter wheat, the BBCH / DC 10, 31, 51, 65, 75 and 92 are main stages in the development. The BBCH / DC stage 10, which means the emergence of crop, was accurately simulated. Shoot development begins with the stage number 30, one of the most important stages after winter domination of winter cereals. The stage was very well simulated. The second most important stage is reached with number 50 which is the heading of crop. About this stage, a statement of the simulation cannot be given as the number of measurements is not adequate. A similar situation was noticed at stage number 65 (flowering). The simulation accuracy of the fruit development (main stage number 75) is good as only a few values were underestimated. The simulation of stage number 92, which means ripeness, has a good agreement compared to the observation.

The development of potato is concentrated in six important stages (BBCH / DC 9, 19, 51, 59, 69 and 92). However, the measured values of Bad Lauchstädt showed a quartering. At stage number 9 the potato emerges. For the leaf development, stage number 19 was measured. Both stages of early development perform very well in the sub module. Stages number 51 and 59 include the process of potato flowering. A point cloud of simulated values for this period is very close to the observed values. Furthermore, the observed data set contained the stages number 69 and 92, which characterise the end of flowering and the potato ripening. The agreement of observation and simulation is only given at stage number 92. The sub module overestimates the BBCH / DC stage number 69. This might be the result of the scale transformation.

The measured values of maize development stages show a tripolarisation. The essential stages for maize are BBCH / DC stages 11-16, 32, 53, 63, 79 and 89. The leaf development of maize occurs in stages number 11 to 16, which are accurately simulated by the sub module. The stages of heading (BBCH / DC 53) and fruit development (BBCH / DC 79) have a good agreement. The measurements were simulated well except a small underestimation of stages number 63 and 89. It is noticeable that the

stage number 32 was not following a tendency. This fact is the result of an inaccuracy in the sub module structure. The transformation of the internal scale (HANWAY) into BBCH / DC means that Hanway stages 2.0 and 2.5 correspond to the BBCH / DC stage number 30. The same effect is given for BBCH / DC 31 which is described by HANWAY 3.0 and 3.1. Furthermore, the BBCH / DC stages 32 and 33 only show a difference of 0.05 in the internal HANWAY scale. Both phenomena occurred in the calibration of maize as the field documentations for maize contain a detailed observation of the shoot development. E.g. the comparison between the simulation and observation of the BBCH / DC stages number 30, 31, 32 and 33 showed an under- and overestimation for shooting because a BBCH / DC stage correspond to two internal stages or because two BBCH / DC stages are very close together in the internal scale.

The inaccuracy in the comparison between observation and simulation of the BBCH / DC stages of the three investigated crops could be caused by the subjectivity of different persons that were assigned to the recording over the considered 9 years.

Furthermore, the simple approach of PTU used for the description of plant development stages has limitations because some factors of influence (soil moisture and vernalisation) are not considered. However, both factors could effect the deviation of development stages simulation (ROBBERG et al. 2005).

Concluding, a closer examination of the calibration results compared to other similar studies is elaborated to evaluate the applicability of the module. In a similar study, the model CERES was calibrated for wheat using two years and 15 observed stages (NAIN & KERSEBAUM 2007). The calibration results for the development stages are simulated with a %RMSE of 9.3 % and R<sup>2</sup> of 0.99. Both accuracy criteria are comparable with the accuracy of the sub module 'Plant development' as the error values are minimally higher than the results of CERES. Furthermore, the calibration process included 63 observed stages and obtains a %RMSE of 13.25 % and a R<sup>2</sup> of 0.96.

After the reflection of the results for the three investigated crops, the used sub module simulated a very good to good performance for the calibration in spite of the simple approach.

#### 6.2.2 Sub module 'Biomass growth'

The calibration of the sub module 'Biomass growth' relies on two measured crop variables: biomass and LAI. Both variables underlie a natural variability in agricultural systems depending on date and other factors, e.g. extreme weather events. To account for the natural variability, several replications of the crop variables are necessary. SCHRÖDER (1995) discusses that on the field scale, eight replications of biomass measurement were realised for the detection of outliers. The existing biomass data of the small plot scale in Bad Lauchstädt contain two replications which result in the mean average. The realisation of three replications is regarded as desirable because two measured points are not representative for an area. However, it is probably not realisable due to the size of the plot area of  $5 \times 10$  m. Concerning the crop variable LAI, eight replications were necessary in order to identify outliers and to maintain the measuring error.

However, the measurement variability could not be realised within the module. Therefore, the procedure of calibration as well as the evaluation by the statistical criteria was conducted on the basis of mean averages crop variable. Thus, the fluctuation range has constantly to be considered as the mean average value explicitly represents a generalisation. Consequently, the discussion of the calibration results accounts for this aspect.

The measurements of LAI consider for each date a 95 % confidence interval regarding the three investigated crops. Consequently, the simulated values approach the observation. Simulation of potato and winter wheat show better agreement with the measurement considering the confidence interval, whereas the simulation for maize lies outside in four cases (Figure 28, page 69).

In spite of this, the structure and the used equations for LAI simulation show a deficit that results in a general overestimation in the first phase and a general underestimation in the second phase as well. Particularly, the inclination of the curve for maize and potato is inaccurately simulated (Figure 36, page 75). A lower inclination would fit the observed curve more precisely. Concerning the simulation of winter wheat, a clear statement cannot be given as only four measured values are available for comparison (Figure 31, page 71).

The calibration with observed LAI values was decisive because the simulated LAI values could result in unrealistic amounts. This can be explained by the extreme sensitivity of the parameters 'PHOTSR' and 'AREAWT'. A very small change of these two parameters can produce a high 'uncontrolled' reaction of simulated LAI. Therefore, a limitation of simulated LAI in the form of a maximum parameter is desirable, particularly if no measured data are available.

The observed biomass data for the calibration process, as mentioned above, have a natural variability. Therefore, the comparisons of the total biomass on harvest for each investigated crop consider the range of the two measured replications. The values of biomass show a small range about the mean average ( $\pm$  3.22 to 6.01 %), primarily in the main harvest. The range of the intermediate harvests varies between  $\pm$  5.89 to 12.65 % about the mean average. The biomass harvest variability of SCHRÖDER (1995) ranges within 30 % on a field scale approving the given variability of the harvests used in the study.

The calibration over four or three years respectively attempted to predict the mean behaviour of total biomass within an acceptable limit which was successful in the presented cases. However, the comparison indicates that the simulated values are almost in all cases outside the measured range. It shows that not all processes and / or influences are considered in the sub module. This effect can be explained by the intended simplifications and assumptions of the plant module. E.g. if the measured main harvest used for the orientation of the simulation is reduced due to unconsidered influence factors (hail, pests etc.), then the calibration alters the considered factors to compensate the unconsidered influence to finally match the measured result.

The simulated time course results of biomass indicate a high inaccuracy. Even in consideration of the actual values of the two replications, the simulation did not improve. This deficit of the biomass simulation is caused by the used exponential function in the sub module. Generally, the calculation is slow in the beginning. During the calibration of winter wheat and potato, it was attempted to simulate the biomass time course, especially, the first and / or second intermediate harvest, in an accurate way. This could only be realised with unrealistic parameter combinations and resulted in an overestimation of the following harvests. The obtained calibration results of the biomass time courses are comparable with published similar studies. The models THESUS and OPUS simulate a crop rotation with an IA between 0.89 and 0.98 (WEGEHENKEL et al. 2004). The sub module 'Biomass growth' obtained an index of agreement for maize between 0.92 and 0.98, for potato between 0.77 and 0.90, and for winter wheat between 0.80 and 0.85. However, the reflection of the IA is a one-dimensional description of accuracy which needs a second criterion for a distinct detection of simulation accuracy. The comparison with the R<sup>2</sup> relativises the results of the time courses of biomass. The coefficient of determination lies between 0.70 and 0.99 for maize which represents an acceptable result and is comparable to the study of MIRSCHEL & WENKEL (2007) with the model AGROSIM. However, for the time course of biomass for potato and winter wheat R<sup>2</sup> varies between 0.15 and 0.65 which emphasises an imprecise simulation and reinforces the argument of an existing deficit.

The calibrated results of the total biomass on harvest, which are represented in section 5, will be discussed and compared with other studies in the following section. Possible errors of the module concept are identified and explained.

In general, the calibration results of winter wheat and potato show no distinctive features. However, the result values of maize indicate three underestimated years which are still in an acceptable range. The year 2007 shows a contrary result. An explanation can be given by the dynamic of the weather values (air temperature, global radiation, precipitation) which is the driving force of the module SIWAPFLAN. April 2007 had a strong global radiation and a high overall temperature representing no stress factor of temperature for the photosynthesis rate in the module. The beginning of the growing seasons in the years 2004 and 2006 the radiation was weak and according to this the temperature was low. Due to the fact that the optimum curve of photosynthesis is set between 20 and 35  $^{\circ}$  for maize, the module calculat ed small gain of maize biomass. Furthermore, for June 2005 and 2006, only little precipitation could be measured which resulted in water stress for the module.

The reflection of each calibration year for all investigated crops shows that the year 2005 followed the same pattern. The total biomass on harvest was always underestimated. However, the underestimations were partly very small. Thus, it is assumed that the module has a strong reaction on dry conditions during the growing season (June

and July 2005). The simulation of assimilation is reduced by water stress resulting in less biomass gain. The assumed tendency of the module about the reaction of dry conditions must be checked with the validation results.

The obtained results of total biomass on harvest, which were simulated by the sub module 'Biomass growth', show a good performance in comparison to the models HERMES and Expert-N (KERSEBAUM et al. 2007). Both models indicate a RMSE ranging from 1424 to 2726 kg ha<sup>-1</sup>. The sub module results vary in a similar scale (from 488 to 2350 kg ha<sup>-1</sup>). The IA of the calibration results is also comparable with the mentioned studies.

Therefore, it can be said that the sub module 'Biomass growth' relatively accurately simulates the results of the total biomass on harvest. The prediction of the biomass time course indicates an inaccuracy for most cases of the calibration. The deficit can be attributed to the used structure of the sub module that could be improved by a restructuring of the sub module 'Biomass growth'. Due to unsuccessful calibration, the time courses of biomass are not considered in the validation results.

#### 6.2.3 Sub module 'N uptake'

The sub module 'N uptake' was also calibrated by the crop variables being the measured N content and the values of total N uptake on harvest. Both variables are depending on the biomass which was already described in the section 5.3.3. Therefore, the N content is analysed by the two replications of biomass. The N contents in plants have a natural variability. The range amounts to  $\pm 10$  % about the mean average. The values of total N uptake on harvest are the product of the variability of biomass and the N content. Thus, the range of the total N uptake results in  $\pm 4.78$  to 7.26 % about the mean average.

In comparison to the N uptake prediction of other models, the RMSE ranges from 31.2 and 59.9 kg ha<sup>-1</sup> (KERSEBAUM et al. 2007). The sub module performance is accurate because the RMSE are within 3.47 and 22.76 % and thus are even below both values from KERSEBAUM et al. (2007). The obtained indices of agreement (0.84 and 0.90) are also comparable with the other crop growth models.

The calibration result, which is obtained with the sub module 'N uptake', has no noteworthy differences in the simulation and reaches a good quality. The comparison between observation and simulation follows the same pattern as the result of total biomass. This effect can be explained by the interaction of the sub modules 'Biomass growth' and 'N uptake'.

### 6.3 Validation results for the sub modules of SIWAPFLAN

#### 6.3.1 Sub module 'Plant development'

The obtained result of the validation for the crop variable BBCH / DC development stages is depending on the measurements. As previously documented, the number of stages for validation is different in comparison to the calibration. I.e. the difference amounts to twelve values for maize and potato. This fact results from the lower number of observations over growing seasons from the years 1999-2003. Especially, the number of winter wheat stages for validation is very small resulting into a relative uncertainty for the validation procedure. The difference between both procedures is 24 measurements. Therefore, a further assessment of validation in comparison to the calibration for winter wheat is necessary. The assessment method is leaned on the accuracy evaluation for the ontogenesis model SIMONTO (ROBBERG et al. 2005). The BBCH / DC stages are classified in four groups of importance in practice, particularly for the fertilisation and plant protection.

Group	Importance of stage	BBCH / DC stage	Group factor
3	particular important	10, 25, 31, 32, 39, 61, 65	3
2	very important	21, 51, 59	2
1	important	13, 23, 30, 33, 37, 49, 55, 69	1
0	less important	all further stages	0.5

Table 18: Assessment of the validation (changed after ROBBERG et al. 2005)

The comparison of simulated and observed stages is assessed by the deviation in days with error values ( $\pm$  two days deviation = half an error;  $\pm$  six days deviation = one error; > six days deviation = three errors). Each simulated stage has a value of error which is multiplied by the group factor (Table 18). In addition, the sum of the error values is calculated and divided by the number of included stages. The result for valida-
tion amounts to 1.60. The assessment of calibration is 1.27. Both amounts are comparable. In spite of this result, the validation is more certain, as previously described.

On the one hand, the validation result of winter wheat development stages amounts to 5.95 % caused by the small number of comparable BBCH / DC stages (four years). On the other hand, a smaller error value is given by the very good calibration result which has a deviation of five days (13.25 %). The model CERES reaches a %RMSE of 10.38 % for wheat in a validation of one growing season. The error value implies a deviation between zero and 28 days (NAIN & KERSEBAUM 2007). The obtained validation results of potato and maize were 16.31 % and 17.58 %. These differences show a good prediction of development and are comparable with the calibration procedure.

A reflection of the important stages of development in the validation provides more information about the simulation accuracy. Thereby, the most important stages, which were already considered for the calibration results, should be regarded for the validation.

The winter wheat BBCH / DC stages number ten (emergence), 31 (shoot) and 51 (heading) were predicted in an accurate way. Stage number 65 (flowering) was underestimated in three years which supports the given assumption in the parameterisation process about the systematic underestimation caused by the scale transformation. The fruit development (BBCH / DC stages 75) was not available for comparison which is caused by the observation on fewer stages in the validation years. Thus, the ripeness of winter wheat (BBCH / DC 92) was measured and the sub module simulates with a relative accurateness.

For the obtained result of the validation for the potato development stages 9 (emergence), 51, 59 (flowering) and 92 (ripeness) a good simulation was performed. The prediction of the leaf development (BBCH / DC 19) was underestimated. The stage number 69 was not observed. Therefore, the overestimation of the calibration process cannot be confirmed. The validation result of the year 2000 was overestimated for three measured stages. A reason could be the very warm beginning of the growing season 2000 where the PTU approach (temperature / day length) reacts with too fast development. The simulated development stages of maize show a good agreement in the beginning of development (BBCH / DC 11-16). Stage 32 is only documented in the year 2003. However, the under- / overestimation tendency of the shoot development is noticeable. A statement about the stages 53 (heading) and 79 (fruit development) are not possible since no measured values are available. A relatively good performance is simulated for the stages 63 (flowering) and 89 (ripening) as the simulated values are close to the 1:1 line.

The validation results show good performances for all investigated crops. The systematic under- / overestimation from stage number 60 to 90, which was detected in the beginning of the calibration, could be corrected with extension of the phases development in the major part of the simulation. Furthermore, the non-continuous development and omitting of stages, which are characteristic for maize and potato, can be explained and predicted by the sub module. The deficit of stage number 32 (under- / overestimation) could be eliminated by a check of the used scales and its implementation in the sub module. The PTU approach with the 'phases' extension produces a good accuracy for the modelling of plant ontogenesis.

Concluding, the obtained results of the sub module 'Plant development' can be applied for the simulation of behaviour of plant development for the investigated crops in Bad Lauchstädt. In addition, the accurate simulation of the development stages is the basis of the sub modules 'Biomass growth' and 'N uptake'. The stages control all processes of the module SIWAPFLAN which are initiated, stopped, accelerated or slowed down by plant development. Furthermore, the partitioning of biomass and the time course biomass depends on the plant development stages. The practical relevance, e.g. timing of fertilisation and plant protection, can also be predicted with the sub module 'Plant development'.

## 6.3.2 Sub module 'Biomass growth'

The validation results are based on the crop variable biomass. The comparison between simulated and measured values also considers the natural variability range. The two replicated measurements of biomass vary in a small way (between  $\pm 2.98$  and 3.83 % about the mean average). The consideration of the measured range shows a closer agreement between simulation and observation in some cases. The validation results of the total biomass on main harvest are also discussed in this section concerning the insights gained in calibration. In addition, the comparison to similar studies provides information about the applicability of the sub module.

The years 1999, 2001 and 2002 of total biomass of maize were well reflected by the sub module. The remaining years were underestimated. The results of winter wheat showed an analogous effect in the validation. Similar results were obtained for potato. However, only one year was below the 1:1 line. All three investigated crops followed the same trend. I.e. the year 2003 was always underestimated by the sub module. The simulation of total biomass of maize and winter wheat in the year 2000 also calculated lower values than the measured values. The reason in this case is assumed in the reduction factors of the simulated biomass: temperature and water stress. The reduction by temperature can be excluded as the temperature of the growing season 2003 was 20 % above the long-time average.

The reduction of simulated biomass by water stress is depending on the simulated soil moisture which is directly linked to the input precipitation. An increase of the simulated soil moisture is transformed to no water stress in the module SIWAPFLAN. Low soil moisture values result in high water stress in the module. However, the agreement between the measured and simulated soil moisture is decisive and it shows that CANDY very well predicts the observed soil moisture including the year 2003. With this insight, the water stress can also be excluded as a cause of biomass reduction in the sub module 'Biomass growth'.

Since two possible biomass underestimation reasons of the year 2003 were tested and could be excluded, the reason for this effect can only be attributed to the structural simplification and assumptions of the sub module. The crop variable biomass is a result of different sub-processes and factors of influence. Analysing the sub-processes in detail could improve the resulting biomass output. An approach could be that e.g. the natural plant assimilation is measured in the field. Those measurements could subsequently be used to verify the simulation of assimilation in the sub module.

A trend in validation results could be detected by the comparison to the annual records of the growing seasons. The simulation of the year 2002 was overestimated for potato and winter wheat. This effect can be explained by the damage by pests for both crops. The sub module reacts only on the driving forces allowing a better production of biomass. The natural reduced behaviour of pests is not included in the sub module 'Biomass growth' and therefore, it cannot be explained by the sub module.

The validation results of the total biomass on harvest obtain a RMSE between 1772 and 2863 kg ha<sup>-1</sup> for the investigated crops. In a similar study using the OPUS model, the RMSE regarding total biomass ranged from 2708 to 2942 kg ha<sup>-1</sup> (WEGEHENKEL & MIRSCHEL 2006). In other studies, that evaluated the performance of the models THE-SUS and OPUS, the IA for the biomass varied from 0.64 to 0.99 and from 0.69 to 0.82 (WEGEHENKEL & MIRSCHEL 2004). The standard criteria IA for the simulation with the sub module 'Biomass growth' ranged within 0.37 and 0.61. These unsatisfying results are caused by the underestimation of the years 2000 and 2003. Without the consideration of the year 2003 the IA increased by an amount comparable to the models THE-SUS and OPUS.

In summary, the validation of the sub module 'Biomass growth' in this study already shows an acceptable simulation result. Analysing each year, the deficits, which cause a reduction of the performance quality, could be detected. Against this background where the sources of deficit are known, it can be said that the sub module 'Biomass growth' simulates the crop growth behaviour of Bad Lauchstädt well.

#### 6.3.3 Sub module 'N uptake'

The validation results are also based on the crop variable total N uptake on harvest. The variability of the measured values is comparable to calibration. The range of the total N uptake amounts to  $\pm 5.47$  to 7.36 % about the average.

The validation results of the three crops are very different. The validation years of maize are good. The two years, which close to the 1:1 line, are still in an acceptable range (< 20 %). The difference of the year 1999 can be explained by the cultivation of another variety in comparison to the other years. The inaccurate simulations of the years 1999 and 2001 for potato are also caused by different cultivated varieties. The underestimation of the total amount of maize N uptake (2001) is caused by a low N supply in soil which is simulated with the soil module of CANDY.

The cause of the approximate underestimation of the year 2000 is the interaction of the sub module 'Biomass growth' and 'N uptake'. The simulation of biomass in this year

was too small and thus, the values for N uptake as well. This value is also controlled by the underestimated biomass. The obtained validation results for potato and winter wheat (2003) underlie the same effect. The remaining years of the winter wheat N uptake were also underestimated. These differences could be caused by the inaccuracy of the N simulation in the soil module. Winter wheat is an ambitious, "decompose" crop which needs the fixed N of the residues of alfalfa. The model implementation of this N utilisation is complex and can cause discrepancies. Furthermore, the investigated crops were analysed without consideration of crop rotation effects.

In comparison to the N uptake performance of other models, the RMSE ranges from 24.2 and 63.4 kg ha<sup>-1</sup> and the IA varies between 0.51 and 0.91 (KERSEBAUM et al. 2007). The RMSE of maize (27.59 kg ha<sup>-1</sup>) and the IA of 0.82 are comparable with the study. In the investigation study of winter wheat, the model AGROSIM performs with a RMSE of 36.4 kg ha<sup>-1</sup> and an index of agreement of 0.51. The comparison with the AGROSIM shows a greater inaccuracy in the prediction of winter wheat. The N uptake is calculated with a RMSE 56.48 kg ha<sup>-1</sup> and an IA of 0.21. For potato, similar criteria are determined (RMSE 39.56 kg ha<sup>-1</sup> and IA of 0.35).

The validation of the sub module 'N uptake' is only successful for maize. For potato and winter wheat sources of inaccuracy are partly given by the sub module 'Biomass growth' and the soil module of CANDY. With elimination of the failures, the sub module 'N uptake' is capable in depicting N uptake accurately.

# 7 CONCLUSION AND OUTLOOK

The present study assessed and improved the applicability of the plant module SI-WAPFLAN regarding the description of crop growth and development.

In a first step, natural plant-relevant and agroecosystem-relevant processes were analysed as a base of the present study. The gained insights of processes were transferred onto the following tasks and represented the base for the assessment of the achieved results.

The analysis of implemented processes in SIWAPFLAN and CANDY showed that the processes generally stand the test. In the plant module SIWAPFLAN, detailed extensions were conducted, e.g. the phases plant development and inflexion points of the LAI. The structural subdivision in three sub modules according to the main processes was reasonable.

The already available data and particularly, the enlargement of the LAI data, made a good contribution to the first application of the plant module SIWAPFLAN. It was demonstrated that a time series of ten years is eligible, since certain events can occur that eminently influence the measurements. However, the temporal resolution of the existing data set was inconstant resulting in a visible impact of the model output.

The results of calibration showed that the sub module 'Plant development' very well predicts the simulation of plant development stages. Regarding the total biomass on harvest, the sub module 'Biomass growth' simulated a good performance. The time course of biomass in the calibration procedure illustrated discrepancies between simulation and measurement which excluded its reflection in the validation. The obtained results of the total N uptake on harvest in the calibration indicated a very good agreement with the measured values.

The validation of the sub module 'Plant development' resulted in a good to very good performance. This shows that the module can be applied for the simulation of plant behaviour at the location of Bad Lauchstädt. In view of the acceptable performance of the sub module 'Biomass growth' for simulating total biomass on harvest, it can be

used to predict crop growth behaviour on the investigated location. The results of the validation for the total amount of N uptake indicate deficiencies which still made this part of the module SIWAPFLAN insufficient for the application.

In general, it can be concluded that the present study was the first step of an application of the module SIWAPFLAN and can be divided in two forms of insights. On the one hand good performances were simulated, and on the other hand sources of inaccuracy were detected, e.g. structure / equation of sub module 'Biomass growth' and simulations of N supply.

Therefore, further future tasks should be focussed on the elimination of inaccuracy sources. This could be achieved by an extension of the data basis that could also improve the split sample test as an equal splitting could be possible. In addition, the extended data could be used to assess sub-processes in the module. Another task could be to simulate a whole crop rotation of organic farming is an important task in the future as only this constellation of crops represents the primary rules and aims of organic farming which should be considered in the simulation of the plant module SIWAP-FLAN. Furthermore, a test of the plant module for other management systems and other locations would complete the applicability of the module.

The assessment and improvement of the applicability of SIWAPFLAN, in consideration of the gained insights, showed that the plant module is able to reproduce the plant-relevant processes and its variables. Therefore, SIWAPFLAN adequately extends the model CANDY for tasks which include plant processes regarding the influence of environmental conditions.

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# **9 APPENDIX**

#### Appendix A: List of modelling-specific abbreviations

Abbreviations	Description	Module function
AET	Actual evapotranspiration	Output result
'AREAWT'	Leaf area per weight of leaf dry matter	Plant-specific parameter
ASLOPE	Slope of the light curve	Internal value
ASSIM (A)	Actual assimilation	Internal value
ASSIM (P)	Potential assimilation	Internal value
'BTEMP'	Base temperature	Plant-specific parameter
'D0_LAI',	Supply of assimilates for leaves on time T 0	Plant-specific parameter
'D1_LAI'	Supply of assimilates for leaves on time T 1	Plant-specific parameter
DAYLGT	Day length	Driving force
DEVSTG	Development stages	Output result
DMGAIN	Fraction of dry matter gain	Internal value
DRYMAT	Dry matter of biomass	Output result
'EXCOEF'	Extinction coefficient of global radiation	Plant-specific parameter
EXPAR	Reduction coefficient of the light	Internal value
FBULK	Gain fraction of the plant without leaves and roots	Internal value
FDEADL	Fraction of the dead leaves	Internal value
FRDMAT	Fraction of root dry matter	Internal value
GBULK	Gain fraction of plant organ without roots and leaves	Internal value
GLOB	Global radiation	Driving force
GRNLAI	Area index of green leaves	Output result
'HRVI'	Harvest index	Plant-specific parameter
kf	Regulation variable of transpiration coefficient	Internal value
'LAIatCD1'	Leaf area index at 100 % coverage	Plant-specific parameter
'MAX_EMERG'	Control value of the emergence	Plant-specific parameter
NCACT	Actual nitrogen content	Internal value
'NCKR'	Critical nitrogen concentration	Plant-specific parameter
'NCNF'	Factor of the nitrogen concentration curve	Plant-specific parameter
NCOPT	Optimum nitrogen content	Internal value
NCREL	Relative nitrogen content	Internal value
'NCT0'	Nitrogen concentration on time T 0	Plant-specific parameter
'NCT1'	Nitrogen concentration on time T 1	Plant-specific parameter
NDEM	Daily demand of nitrogen	Output result

NSTRESS	Growth-limiting factor through nitrogen deficiency	Internal value
NUPACC	Accumulated amount of N uptake	Internal value
'OF 1'	Factor of ontogenesis for phase 1	Plant-specific parameter
'OF 2'	Factor of ontogenesis for phase 2	Plant-specific parameter
'OF 3'	Factor of ontogenesis for phase 3	Plant-specific parameter
PASYMP	Asymptotic limit of "crop stand light curve of assim."	Internal value
PH	Plant height	Output result
'PHASE 1'	Determination of ontogenesis phase 1 and 2	Plant-specific parameter
'PHASE 2'	Determination of ontogenesis phase 3	Plant-specific parameter
'PHMAX'	Maximal height of plant	Plant-specific parameter
PHOTR	Asymptotic limit of assimilation	Internal value
'PHOTSR'	Maximum photosynthetic rate of leaf	Plant-specific parameter
PSLOPE	Slope of crop stand light curve of the assimilation	Internal value
PTU	Photo thermal units	Internal value
RD	Root depth	Output result
'RDMAX'	Maximal depth of root	Plant-specific parameter
RESP	Fraction of respiration	Internal value
'RIPING'	SUMPTU that is necessary for the plant ripeness	Plant-specific parameter
'ROOTING'	SUMPTU that is necessary for PHMAX or RDMAX	Plant-specific parameter
SLOPE	Slope of the light curve	Internal value
STRESS	Growth-limiting factors of water / nitrogen deficiency	Internal value
SUMPTU	Sum of photo thermal units	Internal value
'T_0'	Factor 0 for temperature function	Plant-specific parameter
'T_1'	Factor 1 for temperature function	Plant-specific parameter
'T_2'	Factor 2 for temperature function	Plant-specific parameter
'T_3'	Factor 3 for temperature function	Plant-specific parameter
TEMP	Mean air temperature	Driving force
TFUNC	Function of temperature	Internal value
'TKMAX'	Maximum of transpiration coefficient	Plant-specific parameter
'TKMIN'	Minimum of transpiration coefficient	Plant-specific parameter
TOTLAI	Total leaf area index	Output result
TRANSKO	Transpiration coefficient	Internal value

#### Appendix B: Management data for the simulation of all small plots from 1996 to 2007

Small plot 1: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 01.09.1997 emergence alfalfa (perennial) 538,7 dt/ha 28.05.1998 harvest, crop res. removed alfalfa (perennial) 234,7 dt/ha 06.07.1998 harvest, crop res. removed alfalfa (perennial) 196,5 dt/ha 17.08.1998 harvest, crop res. removed alfalfa (perennial) 107,5 dt/ha 18.01.1999 ploughing up (fallowing) unspez. 25 cm 24.03.1999 soil tillage unspez. 10 cm 20.04.1999 emergence alfalfa (perennial) 382.3 dt/ha 23.06.1999 harvest, crop res. removed alfalfa (perennial) 194,3 dt/ha 10.08.1999 harvest, crop res. removed alfalfa (perennial) 121,7 dt/ha 28.09.1999 harvest, crop res. removed alfalfa (perennial) 66,3 dt/ha 12.10.1999 soil tillage unspez. 28 cm 14.10.1999 (sowing) w. wheat V522(\*) 08.11.1999 emergence w. wheat V522(\*) 58 dt/ha 01.03.2000 mineral N fertilizer calcium ammonium nitrate 22 kg N/ha 04.08.2000 harvest, crop res. removed w. wheat V522(\*) 58 dt/ha 20.09.2000 soil tillage unspez. 28 cm 04.10.2000 emergence winter barley 72,7 dt/ha 13.07.2001 harvest, crop res. removed winter barley 72,7 dt/ha 10.08.2001 soil tillage unspez. 12 cm 04.09.2001 soil tillage unspez. 12 cm 17.11.2001 organic manure farm yard manure, fr(10%C) 253 dtFM/ha 21.11.2001 soil tillage unspez. 25 cm 09.04.2002 (sowing) potato V522(\*) 17.05.2002 emergence potato V522(\*) 274,6 dt/ha 02.09.2002 harvest, crop res. removed potato V522(\*) 274,6 dt/ha 06.09.2002 soil tillage unspez. 10 cm 13.10.2002 emergence dinkel 60,38 dt/ha 11.07.2003 harvest, crop res, removed dinkel 60.38 dt/ha 26.09.2003 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 16.10.2003 soil tillage unspez. 28 cm 23.04.2004 (sowing) silo maize V522(\*) 04.05.2004 emergence silo maize V522(\*) 520 dt/ha 10.09.2004 harvest, crop res. removed silo maize V522(\*) 520 dt/ha 13.10.2004 soil tillage unspez. 28 cm 06.04.2005 emergence oats 60,42 dt/ha 14.07.2005 harvest, crop res. removed oats 60,42 dt/ha 17.08.2005 soil tillage unspez. 10 cm 26.08.2005 emergence alfalfa (perennial) 129,32 dt/ha 11.05.2006 harvest, crop res. removed alfalfa (perennial) 35,28 dt/ha 03.07.2006 harvest, crop res. removed alfalfa (perennial) 34,04 dt/ha 01.08.2006 harvest, crop res. removed alfalfa (perennial) 22,59 dt/ha 31.08.2006 harvest, crop res. removed alfalfa (perennial) 37,35 dt/ha Small plot 2: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha

<sup>01.09.1997</sup> emergence alfalfa (perennial) 542,2 dt/ha

28.05.1998 harvest, crop res. removed alfalfa (perennial) 220,2 dt/ha 06.07.1998 harvest, crop res. removed alfalfa (perennial) 194,7 dt/ha 17.08.1998 harvest, crop res. removed alfalfa (perennial) 127,3 dt/ha 14.09.1998 soil tillage unspez. 25 cm 20.10.1998 soil tillage unspez. 10 cm 21.10.1998 (sowing) w. wheat V522(\*) 10.11.1998 emergence w. wheat V522(\*) 87,5 dt/ha 03.08.1999 harvest, crop res. removed w. wheat V522(\*) 87,5 dt/ha 30.08.1999 soil tillage unspez. 10 cm 24.09.1999 soil tillage unspez. 25 cm 03.10.1999 emergence winter barley 43,6 dt/ha 29.06.2000 harvest, crop res. removed winter barley 43,6 dt/ha 25.10.2000 organic manure farm yard manure fr(10%C) 400 dtFM/ha 03.11.2000 soil tillage unspez. 25 cm 26.04.2001 emergence potato V522(\*) 25.05.2001 emergence potato V522(\*) 405 dt/ha 14.09.2001 harvest, crop res. removed potato V522(\*) 405 dt/ha 10.10.2001 soil tillage unspez. 10 cm 29.10.2001 emergence dinkel 15,19 dt/ha 31.07.2002 harvest, crop res. removed dinkel 15,19 dt/ha 25.10.2002 organic manure farm yard manure, fr(10%C) 253 dtFM/ha 28.10.2002 soil tillage unspez. 25 cm 13.04.2003 (sowing) silo maize V522(\*) 05.05.2003 emergence silo maize V522(\*) 489,5 dt/ha 18.08.2003 harvest, crop res. removed silo maize V522(\*) 489,5 dt/ha 16.10.2003 soil tillage unspez. 28 cm 02.04.2004 emergence oats 86,83 dt/ha 28.07.2004 harvest, crop res. removed oats 86,83 dt/ha 04.10.2004 emergence alfalfa (perennial) 457,73 dt/ha 25.05.2005 harvest, crop res. removed alfalfa (perennial) 71,73 dt/ha 30.06.2005 harvest, crop res. removed alfalfa (perennial) 28,44 dt/ha 09.08.2005 harvest, crop res. removed alfalfa (perennial) 42,83 dt/ha 15.09.2005 harvest, crop res. removed alfalfa (perennial) 22,43 dt/ha 22.05.2006 harvest, crop res. removed alfalfa (perennial) 103,07 dt/ha 03.07.2006 harvest, crop res. removed alfalfa (perennial) 97,84 dt/ha 01.08.2006 harvest, crop res. removed alfalfa (perennial) 41,92 dt/ha 31.08.2006 harvest, crop res. removed alfalfa (perennial) 48,84 dt/ha 29.09.2006 (sowing) w. wheat V522(\*) 08.10.2006 emergence w. wheat V522(\*) 75 dt/ha 16.07.2007 harvest, crop res. removed w. wheat V522(\*) 85 dt/ha 17.07.2007 soil tillage unspez. 10 cm Small plot 3: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 01.10.1997 (sowing) w. wheat V522(\*) 10.10.1997 emergence w. wheat V522(\*) 38,5 dt/ha 07.08.1998 harvest, crop res. removed w. wheat V522(\*) 38,5 dt/ha 11.09.1998 soil tillage unspez. 25 cm 29.09.1998 emergence winter barley 48,6 dt/ha 12.07.1999 harvest, crop res. removed winter barley 48,6 dt/ha 04.08.1999 organic manure straw (corn) 40,7 dtFM/ha 05.11.1999 organic manure farm yard manure, fr(10%C) 400 dtFM/ha 05.11.1999 soil tillage unspez. 25 cm 21.03.2000 soil tillage unspez. 10 cm 20.04.2000 (sowing) potato V522(\*) 06.05.2000 emergence potato V522(\*) 304,2 dt/ha

29.08.2000 harvest, crop res. removed potato V522(\*) 304,2 dt/ha 23.10.2000 emergence triticale 2.24 V522 64,6 dt/ha 25.07.2001 harvest, crop res. removed triticale 2.24 V522 64,6 dt/ha 27.07.2001 organic manure straw triticale V522 46 dtFM/ha 04.09.2001 soil tillage unspez. 12 cm 17.11.2001 organic manure farm yard manure, fr(10%C) 253 dtFM/ha 21.11.2001 soil tillage unspez. 25 cm 26.04.2002 (sowing) silo maize V522(\*) 11.05.2002 emergence silo maize V522(\*) 472,9 dt/ha 01.06.2002 mineral N fertilizer calcium ammonium nitrate 85 kg N/ha 30.08.2002 harvest, crop res. removed silo maize V522(\*) 472,9 dt/ha 06.09.2002 soil tillage unspez. 10 cm 28.10.2002 soil tillage unspez. 25 cm 04.04.2003 emergence oats 37,39 dt/ha 14.07.2003 harvest, crop res. removed oats 37,39 dt/ha 14.08.2003 soil tillage unspez. 25 cm 07.04.2004 emergence alfalfa (perennial) 594,8 dt/ha 04.05.2004 harvest, crop res. removed alfalfa (perennial) 6.55 dt/ha 17.06.2004 harvest, crop res. removed alfalfa (perennial) 80,84 dt/ha 29.07.2004 harvest, crop res. removed alfalfa (perennial) 66,42 dt/ha 15.09.2004 harvest, crop res. removed alfalfa (perennial) 58,17 dt/ha 25.05.2005 harvest, crop res. removed alfalfa (perennial) 151,2 dt/ha 30.06.2005 harvest, crop res. removed alfalfa (perennial) 131,1 dt/ha 09.08.2005 harvest, crop res. removed alfalfa (perennial) 60,9 dt/ha 08.09.2005 harvest, crop res. removed alfalfa (perennial) 39,6 dt/ha 13.09.2005 soil tillage unspez. 20 cm 30.09.2005 (sowing) w. wheat V522(\*) 10.10.2005 emergence w. wheat V522(\*) 57,25 dt/ha 17.07.2006 harvest, crop res. removed w. wheat V522(\*) 57,25 dt/ha 18.07.2006 soil tillage unspez. 6 cm Small plot 4: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 02.10.1997 emergence winter barley 35,5 dt/ha 15.07.1998 harvest, crop res. removed winter barley 35.5 dt/ha 15.08.1998 organic manure straw (corn) 36,2 dtFM/ha 18.01.1999 soil tillage unspez. 25 cm 16.04.1999 (sowing) potato V522(\*) 17.05.1999 emergence potato V522(\*) 199,4 dt/ha 02.09.1999 harvest, crop res. removed potato V522(\*) 199,4 dt/ha 27.09.1999 soil tillage unspez. 25 cm 05.10.1999 emergence triticale 2.24 V522 64,7 dt/ha 31.07.2000 harvest, crop res. removed triticale 2.24 V522 64,7 dt/ha 03.11.2000 soil tillage unspez. 25 cm 26.04.2001 (sowing) silo maize V522(\*) 09.05.2001 emergence silo maize V522(\*) 411,2 dt/ha 05.09.2001 harvest, crop res. removed silo maize V522(\*) 411,2 dt/ha 06.09.2001 soil tillage unspez. 12 cm 21.11.2001 soil tillage unspez. 25 cm 22.04.2002 emergence oats 34,2 dt/ha 31.07.2002 harvest, crop res. removed oats 34,2 dt/ha 22.08.2002 soil tillage unspez. 25 cm 02.10.2002 ploughing up (fallowing) unspez. 10 cm 24.10.2002 emergence alfalfa (perennial) 0 dt/ha 17.03.2003 ploughing up (fallowing) unspez. 10 cm 02.04.2003 emergence alfalfa (perennial) 706,75 dt/ha

23.06.2003 harvest, crop res. removed alfalfa (perennial) 110,18 dt/ha 25.07.2003 harvest, crop res. removed alfalfa (perennial) 93,92 dt/ha 26.08.2003 harvest, crop res. removed alfalfa (perennial) 73,52 dt/ha 04.05.2004 harvest, crop res. removed alfalfa (perennial) 130,84 dt/ha 17.06.2004 harvest, crop res. removed alfalfa (perennial) 109,56 dt/ha 29.07.2004 harvest, crop res. removed alfalfa (perennial) 110,45 dt/ha 25.08.2004 harvest, crop res. removed alfalfa (perennial) 78,28 dt/ha 09.09.2004 soil tillage unspez. 30 cm 28.09.2004 (sowing) w. wheat V522(\*) 08.10.2004 emergence w. wheat V522(\*) 63,54 dt/ha 14.07.2005 harvest, crop res. removed w. wheat V522(\*) 63,54 dt/ha 14.07.2005 soil tillage unspez. 6 cm 13.09.2005 soil tillage unspez. 20 cm 14.09.2005 soil tillage unspez. 6 cm 21.09.2005 emergence winter barley 43,68 dt/ha 03.07.2006 harvest, crop res. removed winter barley 43,68 dt/ha 02.04.2007 (sowing) potato V522(\*) 17.05.2007 emergence potato V522(\*) 50 dt/ha 14.09.2007 harvest, crop res. removed potato V522(\*) 177 dt/ha Small plot 5: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 05.11.1997 organic manure farm yard manure, fr(10%C) 400 dtFM/ha 14.04.1998 (sowing) potato V522(\*) 14.05.1998 emergence potato V522(\*) 264,8 dt/ha 31.08.1998 harvest, crop res. removed potato V522(\*) 264,8 dt/ha 06.11.1998 emergence triticale 2.24 V522 64,2 dt/ha 03.08.1999 harvest, crop res. removed triticale 2.24 V522 64,2 dt/ha 05.11.1999 soil tillage unspez. 25 cm 25.04.2000 (sowing) silo maize V522(\*) 04.05.2000 emergence silo maize V522(\*) 401,4 dt/ha 08.09.2000 harvest, crop res. removed silo maize V522(\*) 401,4 dt/ha 03.11.2000 soil tillage unspez. 25 cm 24.04.2001 emergence sp. durum 1.76 V522 29,1 dt/ha 09.08.2001 harvest, crop res. removed sp. durum 1.76 V522 29,1 dt/ha 02.09.2001 soil tillage unspez. 25 cm 03.10.2001 emergence alfalfa (perennial) 0 dt/ha 27.03.2002 ploughing up (fallowing) unspez. 10 cm 17.04.2002 emergence alfalfa (perennial) 854,9 dt/ha 28.06.2002 harvest, crop res. removed alfalfa (perennial) 39 dt/ha 14.08.2002 harvest, crop res. removed alfalfa (perennial) 96,5 dt/ha 13.09.2002 harvest, crop res. removed alfalfa (perennial) 120,3 dt/ha 20.05.2003 harvest, crop res. removed alfalfa (perennial) 224,3 dt/ha 23.06.2003 harvest, crop res. removed alfalfa (perennial) 173,44 dt/ha 25.07.2003 harvest, crop res. removed alfalfa (perennial) 138,96 dt/ha 26.08.2003 harvest, crop res. removed alfalfa (perennial) 62,4 dt/ha 08.09.2003 soil tillage unspez. 25 cm 29.09.2003 (sowing) w. wheat V522(\*) 11.10.2003 emergence w. wheat V522(\*) 67,25 dt/ha 28.07.2004 harvest, crop res. removed w. wheat V522(\*) 67,25 dt/ha 09.09.2004 soil tillage unspez. 30 cm 19.09.2004 emergence winter barley 43,94 dt/ha 04.07.2005 harvest, crop res. removed winter barley 43,94 dt/ha 30.08.2005 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 18.10.2005 soil tillage unspez. 28 cm 06.04.2006 soil tillage unspez. 6 cm

11.04.2006 (sowing) potato V522(\*) 17.05.2006 emergence potato V522(\*) 327,64 dt/ha 05.09.2006 harvest, crop res. removed potato V522(\*) 327,64 dt/ha Small plot 6: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 02.10.1997 emergence triticale 1.33 V522 46 dt/ha 07.08.1998 harvest, crop res. removed triticale 1.33 V522 46 dt/ha 18.01.1999 soil tillage unspez. 25 cm 29.04.1999 (sowing) silo maize V522(\*) 12.05.1999 emergence silo maize V522(\*) 405,7 dt/ha 13.09.1999 harvest, crop res. removed silo maize V522(\*) 405,7 dt/ha 05.11.1999 soil tillage unspez. 25 cm 17.04.2000 emergence sp. durum 1.76 V522 28 dt/ha 04.08.2000 harvest, crop res. removed sp. durum 1.76 V522 28 dt/ha 03.11.2000 soil tillage plough 25 cm 26.04.2001 emergence alfalfa (perennial) 610,65 dt/ha 12.07.2001 harvest, crop res. removed alfalfa (perennial) 91,95 dt/ha 28.08.2001 harvest, crop res. removed alfalfa (perennial) 65 dt/ha 16.05.2002 harvest, crop res. removed alfalfa (perennial) 163,4 dt/ha 01.07.2002 harvest, crop res. removed alfalfa (perennial) 118,3 dt/ha 14.08.2002 harvest, crop res. removed alfalfa (perennial) 70,6 dt/ha 13.09.2002 harvest, crop res. removed alfalfa (perennial) 101,4 dt/ha 16.09.2002 soil tillage unspez. 10 cm 25.09.2002 soil tillage unspez. 25 cm 01.10.2002 (sowing) w. wheat V522(\*) 15.10.2002 emergence w. wheat V522(\*) 79,5 dt/ha 15.07.2003 harvest, crop res. removed w. wheat V522(\*) 79,5 dt/ha 26.08.2003 soil tillage plough 25 cm 22.09.2003 emergence w. barley 1.91 V522 57,3 dt/ha 14.07.2004 harvest, crop res. removed w. barley 1.91 V522 57,3 dt/ha 09.09.2004 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 13.10.2004 soil tillage unspez. 28 cm 05.04.2005 soil tillage unspez. 10 cm 05.04.2005 (sowing) potato V522(\*) 17.05.2005 emergence potato V522(\*) 353,74 dt/ha 01.09.2005 harvest, crop res. removed potato V522(\*) 353,74 dt/ha 10.10.2005 emergence dinkel 35,31 dt/ha 17.07.2006 harvest, crop res. removed dinkel 35,31 dt/ha 18.07.2006 soil tillage unspez. 6 cm 10.08.2006 soil tillage unspez. 5 cm 17.08.2006 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 17.08.2006 soil tillage unspez. 6 cm 19.10.2006 soil tillage plough 28 cm 12.03.2007 soil tillage unspez. 5 cm 23.04.2007 soil tillage unspez. 6 cm 23.04.2007 (sowing) silo maize V522(\*) 30.04.2007 emergence silo maize V522(\*) 428 dt/ha 27.08.2007 harvest, crop res. removed silo maize V522(\*) 428 dt/ha Small plot 7: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 27.04.1998 (sowing) silo maize V522(\*)

11.05.1998 emergence silo maize V522(\*) 501,5 dt/ha 15.06.1998 mineral N fertilizer calcium ammonium nitrate 55 kg N/ha 08.09.1998 harvest, crop res. removed silo maize V522(\*) 501,5 dt/ha 18.01.1999 soil tillage unspez. 25 cm 02.04.1999 emergence sp. durum 2.66 V522 34,6 dt/ha 03.08.1999 harvest, crop res. removed sp. durum 2.66 V522 34,6 dt/ha 05.11.1999 soil tillage unspez. 25 cm 05.04.2000 soil tillage unspez. 10 cm 19.04.2000 emergence alfalfa (perennial) 553,6 dt/ha 11.08.2000 harvest, crop res. removed alfalfa (perennial) 117,3 dt/ha 05.10.2000 harvest, crop res. removed alfalfa (perennial) 53,6 dt/ha 22.05.2001 harvest, crop res. removed alfalfa (perennial) 202,05 dt/ha 12.07.2001 harvest, crop res. removed alfalfa (perennial) 118,25 dt/ha 28.08.2001 harvest, crop res. removed alfalfa (perennial) 62,4 dt/ha 02.09.2001 soil tillage unspez. 12 cm 27.09.2001 soil tillage unspez. 25 cm 24.10.2001 (sowing) w. wheat V522(\*) 20.11.2001 emergence w. wheat V522(\*) 37,6 dt/ha 31.07.2002 harvest, crop res. removed w. wheat V522(\*) 37,6 dt/ha 06.09.2002 soil tillage unspez. 25 cm 27.09.2002 emergence winter barley 55,39 dt/ha 03.07.2003 harvest, crop res. removed winter barley 55,39 dt/ha 26.09.2003 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 16.10.2003 soil tillage unspez. 28 cm 06.04.2004 (sowing) potato V522(\*) 15.05.2004 emergence potato V522(\*) 217,33 dt/ha 01.09.2004 harvest, crop res. removed potato V522(\*) 217,33 dt/ha 10.10.2004 emergence dinkel 74,48 dt/ha 14.07.2005 harvest, crop res. removed dinkel 74,48 dt/ha 30.08.2005 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 18.10.2005 soil tillage unspez. 25 cm 25.04.2006 soil tillage unspez. 6 cm 25.04.2006 (sowing) silo maize V522(\*) 08.05.2006 emergence silo maize V522(\*) 369,8 dt/ha 16.08.2006 harvest, crop res. removed silo maize V522(\*) 369,8 dt/ha 17.08.2006 soil tillage unspez. 6 cm Small plot 8: 08.10.1996 emergence w. barley 2.19 V521 70 dt/ha 13.03.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 05.05.1997 mineral N fertilizer calcium ammonium nitrate 30 kg N/ha 25.07.1997 harvest, crop res. removed w. barley 2.19 V521 70 dt/ha 18.08.1997 soil tillage unspez. 30 cm 01.04.1998 emergence sp. durum 2.66 V522 40 dt/ha 07.08.1998 harvest, crop res. removed sp. durum 2.66 V522 40 dt/ha 18.01.1999 soil tillage unspez. 25 cm 20.04.1999 emergence alfalfa (perennial) 983,9 dt/ha 23.06.1999 harvest, crop res. removed alfalfa (perennial) 199,2 dt/ha 10.08.1999 harvest, crop res. removed alfalfa (perennial) 154,9 dt/ha 28.09.1999 harvest, crop res. removed alfalfa (perennial) 82,6 dt/ha 29.09.1999 soil tillage unspez. 30 cm 10.05.2000 harvest, crop res. removed alfalfa (perennial) 183,3 dt/ha 21.06.2000 harvest, crop res. removed alfalfa (perennial) 162,3 dt/ha 11.08.2000 harvest, crop res. removed alfalfa (perennial) 131 dt/ha 05.10.2000 harvest, crop res. removed alfalfa (perennial) 97,2 dt/ha 26.10.2000 soil tillage unspez. 25 cm 07.12.2000 ploughing up (fallowing) unspez. 10 cm 22.03.2001 emergence sp. durum 1.76 V522 40,25 dt/ha 09.08.2001 harvest, crop res. removed sp. durum 1.76 V522 40,25 dt/ha 04.09.2001 soil tillage unspez. 12 cm

27.09.2001 soil tillage unspez. 25 cm 22.10.2001 emergence winter barley 57,4 dt/ha 04.07.2002 harvest, crop res. removed winter barley 57,4 dt/ha 25.10.2002 organic manure farm yard manure, fr(10%C) 253 dtFM/ha 28.10.2002 soil tillage unspez. 25 cm 14.04.2003 (sowing) potato V522(\*) 17.05.2003 emergence potato V522(\*) 321,88 dt/ha 15.06.2003 mineral N fertilizer calcium ammonium nitrate 23 kg N/ha 25.08.2003 harvest, crop res. removed potato V522(\*) 321,88 dt/ha 22.09.2003 emergence dinkel 42,55 dt/ha 28.07.2004 harvest, crop res. removed dinkel 42,55 dt/ha 09.09.2004 organic manure farm yard manure, fr(10%C) 250 dtFM/ha 13.10.2004 soil tillage unspez. 28 cm 20.04.2005 (sowing) silo maize V522(\*) 09.05.2005 emergence silo maize V522(\*) 408 dt/ha 31.08.2005 harvest, crop res. removed silo maize V522(\*) 408 dt/ha 18.10.2005 soil tillage unspez. 28 cm 21.04.2006 emergence oats 60,4 dt/ha 21.07.2006 harvest, crop res. removed oats 60,4 dt/ha 21.07.2006 soil tillage unspez. 6 cm

08.08.2006 soil tillage unspez. 20 cm

14.08.2006 emergence alfalfa (perennial) 100 dt/ha

#### Appendix C: Calculation of leaf area index

The LAI can be calculated from the gap fraction. The fraction of diffuse radiation transmittance, which passes through a plant canopy, for each view angle ( $\theta$ ) and can be summarised in the following equation:

$$T(\theta) = \frac{\text{Diffuse radiation below the canopy at the view angle }(\theta)}{\text{Diffuse radiation above the canopy at the view angle }(\theta)}$$
(Eq. 1a)

The mean light transmittance  $T(\theta)$  can also be written in equation 1a, according to the Beer-Lambert Law. Thus  $T(\theta)$  depends on foliage density  $\mu$  (m<sup>2</sup> foliage per m<sup>3</sup> canopy), path length S( $\theta$ ) through the canopy and foliage orientation:

$$T(\theta) = \exp(-G(\theta)\mu \ S(\theta))$$
(Eq. 2a)

$$G(\theta)$$
 fraction of foliage projected toward angle  $\theta$ 

The above mentioned equation can be rewritten by adopting MILLER'S (1967 cited in LI-COR 1992b) theorem of contact frequency:

$$G(\theta) * \mu = -\frac{\ln(T(\theta))}{S(\theta)} = K(\theta)$$
(Eq. 3a)
$$\ln T(\theta) / S(\theta)$$
the ratio is the contact number (m<sup>-1</sup>)
contact number or frequency

MILLER (1967 cited in HYER & GOETZ 2004) developed a solution for the foliage density  $\mu$ :

$$\mu = 2 \int_0^{\pi/2} \frac{\ln T(\theta)}{S(\theta)} \sin \theta \, d\theta \tag{Eq. 4a}$$

The foliage density  $\mu$  is related to the LAI and the plant height z. Furthermore path length S is proportional to plant height by the angle  $\theta$ :

$$LAI = z * \mu$$
 (Eq. 5a)

$$S(\theta) = \frac{z}{\cos \theta}$$
(Eq. 6a)

The LAI is formulated from the equations 5a and 6a and the canopy height cancels out  $(S(\theta) = 1/\cos(\theta))$ :

$$LAI = -2\int_{0}^{\pi/2} \ln(T(\theta)) \cos\theta \sin\theta \,d\theta \tag{Eq.7a}$$

The equation is used in the analyzer including the five rings (i stands for each ring with view angle):

$$LAI = -2\sum_{i=1}^{5} \ln(T(\theta_i)) \cos \theta_i \ w(\theta_i)$$
(Eq. 8a)

w(θ)<sub>i</sub>

 $\sin\theta$  d  $\theta,$  constant weight factor for each ring

Appendix D: Statistical characteristics	of	LAI
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		3 <sup>rd</sup> May	9 <sup>th</sup> May	17 <sup>th</sup> May	23 <sup>rd</sup> May	30 <sup>th</sup> May	5 <sup>th</sup> June	12 <sup>th</sup> June	21 <sup>st</sup> June	28 <sup>th</sup> June	5 <sup>th</sup> July	12 <sup>th</sup> July
Panga	Min.	2.23	1.87	2.19	2.41	2.37	2.44	2.43	2.14	1.69	1.47	1.48
Range	Max.	2.8	2.77	2.73	3.09	3.3	3.36	2.99	2.58	1.96	2.1	1.98
Mean av of LAI	verage	2.56	2.45	2.55	2.80	3.01	2.85	2.68	2.32	1.84	1.76	1.76
Varianco	9	0.06	0.10	0.03	0.05	0.10	0.09	0.05	0.02	0.01	0.07	0.03
Standar deviatio	d n	0.24	0.32	0.16	0.23	0.31	0.30	0.21	0.15	0.11	0.26	0.16
Coefficit of variat	ent tion (%)	9.44	13.13	6.36	8.08	10.37	10.44	8.02	6.44	5.76	14.86	9.27

 Table 19: Statistical characteristic of the LAI measurements for winter wheat

Table 20: Statistical characteristic of the LAI measurements for pota	to
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		17 <sup>th</sup>	23 <sup>rd</sup>	30 <sup>th</sup>	5 <sup>th</sup>	12 <sup>th</sup>	21 <sup>st</sup>	28 <sup>th</sup>	5 <sup>th</sup>	12 <sup>th</sup>	18 <sup>th</sup>	26 <sup>th</sup>	31 <sup>st</sup>
		May	May	May	June	June	June	June	July	July	July	July	July
Pango	Min.	0	0	0	0.52	0.7	1.5	1.64	1.85	1.78	2.03	0.69	0.29
Range	Max.	0.71	1.53	1.93	1.84	2.14	2.43	3.5	4.49	5.27	4.88	1.34	0.51
Mean av of LAI	verage	0.12	0.28	0.55	1.07	1.29	1.92	2.38	2.98	3.48	3.37	1.08	0.39
Varianc	е	0.06	0.31	0.58	0.20	0.26	0.12	0.37	0.82	1.35	0.96	0.04	0.01
Standar deviatio	d on	0.25	0.56	0.76	0.45	0.51	0.34	0.61	0.90	1.16	0.98	0.20	0.07
Coeffici variatio	ent of n (%)	-	-	-	42.11	39.27	17.96	25.55	30.26	33.40	29.08	18.05	18.46

#### Table 21: Statistical characteristic of the LAI measurements for maize

		17 <sup>th</sup>	23 <sup>rd</sup>	<b>30</b> <sup>th</sup>	5 <sup>th</sup>	12 <sup>th</sup>	21 <sup>st</sup>	28 <sup>th</sup>	5 <sup>th</sup>	12 <sup>th</sup>	18 <sup>th</sup>	<b>26</b> <sup>th</sup>	31 <sup>st</sup>	7 <sup>th</sup>	14 <sup>th</sup>	21 <sup>st</sup>
		May	May	May	June	June	June	June	July	July	July	July	July	Aug.	Aug.	Aug.
Pango	Min.	0	0	0	0	0.33	1.27	1.53	1.71	2.12	2.39	2.49	2.16	2.2	2.33	2.22
Range	Max.	0.53	0.41	0.52	0.68	1.22	1.79	2.13	3.01	3.13	2.8	3.07	3.08	2.9	3.29	3.29
Mean a of LAI	verage	0.09	0.09	0.20	0.33	0.86	1.51	1.76	2.29	2.56	2.63	2.75	2.71	2.70	2.74	2.66
Varianc	e	0.04	0.02	0.05	0.26	0.13	0.10	0.07	0.24	0.17	0.06	0.05	0.19	0.07	0.11	0.26
Standa deviatio	rd on	0.19	0.16	0.22	0.51	0.37	0.32	0.26	0.49	0.42	0.24	0.23	0.44	0.27	0.34	0.51
Coeffic variatio	ient of on (%)	-	-	-	-	42.63	21.31	14.96	21.34	16.31	9.15	8.37	16.23	10.03	12.28	19.01

## Appendix E: Assessment of the calibration and validation accuracy

Maize	2004	2005	2006	2007	total
Relative error (%)	-16.21	-16.34	-15.19	16.42	-
RMSE (kg ha <sup>-1</sup> )	1491	1071	934	1133	2350
%RMSE (%)	8.10	8.17	7.59	8.21	16.32
Winter wheat	2004	2005	2006	2007	total
Relative error (%)	-23.08	-30.77	-20.69	16.28	-
RMSE (kg ha <sup>-1</sup> )	1559	1848	1039	808	2752
%RMSE (%)	13.32	17.76	11.95	9.40	27.95
Winter wheat	2004	2005	2006	2007	total
Relative error (%)	0.01	-5.95	6.63	-	-
RMSE (kg ha <sup>-1</sup> )	20	397	333	-	488
%RMSE (%)	0.01	3.43	3.83	-	4.76
Potato	2004	2005	2006	2007	total
Relative error (%)	14.34	-9.47	-17.93	-	-
RMSE (kg ha <sup>-1</sup> )	712	416	579	-	1007

Table 22: Accuracy criteria of the total biomass on harvest (calibration)

Table 23: Accuracy criteria of the time courses of biom	ass (calibration)
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Maize	2004	2005	2006	2007
R <sup>2</sup>	0.93	0.80	0.99	0.70
IA	0.98	0.98	0.93	0.92
RMSE (kg ha <sup>-1</sup> )	1651	2373	365	2178
%RMSE (%)	36.50	51.91	10.99	51.44
Relative error (%)	72.29	17.66	29.54	22.20
Winter wheat	2004	2005	2006	
R <sup>2</sup>	0.15	0.47	0.28	
IA	0.80	0.86	0.85	
RMSE (kg ha <sup>-1</sup> )	3207	2404	2123	
%RMSE (%)	45.97	37.50	25.90	
Relative error (%)	49.23	43.38	25.81	
Potato	2004	2005	2006	
R <sup>2</sup>	0.65	0.60	0.35	
IA	0.90	0.77	0.80	
RMSE (kg ha <sup>-1</sup> )	2465	2800	2328	
%RMSE (%)	52.71	83.19	91.84	
Relative error (%)	68.37	57.56	67.67	

Maize	2004	2005	2006	2007	total
Relative error (%)	-5.58	-18.43	-10.86	11.00	-
RMSE (kg ha <sup>-1</sup> )	6.45	16.40	9.30	11.00	22.76
%RMSE (%)	2.79	7.92	4.03	6.18	11.63
Winter wheat	2004	2005	2006	2007	total
Relative error (%)	0.01	-6.34	0.9	-	-
RMSE (kg ha <sup>-1</sup> )	0.01	3.41	0.46	-	3.47
%RMSE (%)	0.01	3.66	0.54		3.72
Potato	2004	2005	2006	2007	total
Relative error (%)	-5.76	-20.18	1.17	-	-
RMSE (kg ha <sup>-1</sup> )	3.93	13.28	0.52	-	13.86
%RMSE (%)	3.32	11.65	0.67		13.45

Table 24: Accuracy criteria of the total N uptake on harvest for maize, winter wheat and potato(calibration)

Table 25: Accuracy criteria of the total biomass on harvest (validation)

Maize	1999	2000	2001	2002	2003	total
Relative error (%)	-3.74	-38.57	-6.39	-3.31	-21.27	-
RMSE (kg ha <sup>-1</sup> )	233	2380	414	221	1502	2863
%RMSE (%)	1.67	17.25	2.86	1.48	9.51	19.58
Winter wheat	1999	2000	2001	2002	2003	total
Relative error (%)	-8.08	-	-28.31	18.92	-28.05	-
RMSE (kg ha <sup>-1</sup> )	432	-	1139	652	1444	1999
%RMSE (%)	4.04	-	14.16	9.46	14.02	22.25
Potato	1999	2000	2001	2002	2003	total
Relative error (%)	18.30	-5.79	0.10	41.78	-44.20	-
RMSE (kg ha <sup>-1</sup> )	414	189	4	953	1423	1772
%RMSE (%)	8.18	2.59	0.05	18.69	19.77	26.41

Table 26: Accuracy criteria of the total N uptake on harvest for maize, winter	r wheat and potato
(validation)	

Maize	1999	2000	2001	2002	2003	total
Relative error (%)	41.29	16.07	-27.07	1.58	-10.14	-
RMSE (kg ha <sup>-1</sup> )	18.65	8.05	16.10	1.12	9.39	27.59
%RMSE (%)	18.46	7.19	12.11	0.71	4.54	19.40
Winter wheat	1999		2001	2002	2003	total
Relative error (%)	-37.62		-62.35	-20.74	-42.30	-
RMSE (kg ha <sup>-1</sup> )	26.90		42.40	9.85	23.90	56.48
%RMSE (%)	18.81		31.18	10.37	21.15	46.39
Potato	1999	2000	2001	2002	2003	total
Relative error (%)	43.09	-6.61	51.18	64.00	-25.93	-
RMSE (kg ha <sup>-1</sup> )	13.10	3.22	25.18	24.33	12.52	39.56
%RMSE (%)	19.27	2.95	22.89	28.62	11.59	41.20