

WAVE: a mathematical model for simulating
water and agrochemicals in the soil and vadose
environment

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Preface

The need for more careful management of our planet's land and water resources is quickening. This results from two clashing realities: the growing numbers of fellow humans with their increasing expectations for a more bountiful life, and the limitations of the planet's natural resources and ability to absorb environmental abuse.

Excessive use of agrochemicals in many industrialized countries endanger the quality of land and water resources and will do so if no drastic measures are taken. In Europe for example the drinking water quality standard of 50 ppm nitrates is exceeded at several locations. Legislation measures for controlling fertilizer, pesticide and herbicide applications are currently considered at regional, national and transnational levels. Several authorities have already enacted different measures to reduce nitrate pollution. Most of these measures are based on rough estimations of nitrogen leaching risk, which not always consider the interaction between climate, crop, soil and geo-hydrology. Even if these effects are considered, it is not clear what the long term effect of regulative measures will be. Both the developments of regulations and the assessment of their long term effects would be substantially simplified by the availability of comprehensive and tested simulation models. Such models can help the decision makers to define about when, where and how much fertilizer or pesticide to apply on agricultural land to ensure that the soil, surface and groundwater resource system are least effected.

The foregoing requires good understanding of the transfer and transformation processes of solutes as they migrate through the soil, and as such requires a good knowledge of the physical, chemical and biological laws governing the changes in the atmosphere-plant-soil continuum. Although considerable expertise has been gained in each of these domains, only recently due to the development of simulation models the interactions of the different processes effecting the fate of chemicals in the vadose environment are studied. As a result, a tremendous interest in system studies, using mathematical modelling, has emerged the last decade. Mathematical modelling is increasingly applied in environmental studies because it enables to get a better insight in processes, integrate knowledge of different disciplines, analyse complex problems in a holistic way, and predict short and long-term impacts of changes in climate and farming on the environment.

The major purpose of this reference and user's manual is to convey a modular modelling system for studying the transport and transformations of matter and

energy in the soil, crop and vadose environment. The version of the WAVE model, presented herein, is based on the SWATRER (the extended and revised version of the Soil Water and Actual Transpiration Rate model of Feddes et al., 1978 (Dierckx et al., 1986)). After 1986, this version was regularly upgraded and extended within the frame of different doctoral research projects of the Institute for Land and Water Management of the K.U.Leuven. This resulted in several upgrades of the SWATRER programme and the development of models like SWATNIT (Vereecken et al., 1989). The latter is a programme for modelling the behaviour of nitrogen species in the soil-plant continuum. However, due to the different upgrading and adding of new sections the programme became rather complex and difficult to manipulate. Therefore, it was decided to completely restructure and rewrite the code of the programme to improve its transparency and user friendliness. The programme has been structured so that it will be easy to add new modules if knowledge of other soil processes than those already present in the programme, and relevant for the analysis of the fate and transfer of chemicals in soils, becomes available. The new programme code was given the name WAVE, which stands for simulation of the substances Water and Agrochemicals in the soil, crop and Vadose Environment.

To simplify the use of the reference and user manual, the chapters are presented in the sequence the WAVE-model describes the different processes. Furthermore, most of the analytical material is presented in a brief form with limited attention given to the derivation of the equations presented. This has been done to focus on the synthesis of the entire process rather than concentration on the analysis of the individual steps along the way. Throughout the different sections of the reference manual special emphasis is given to different parametric models for the description of model parameters. In addition, the manual contains extensive tables with published values of difficult to measure parameters and factors. In this way the manual serves also the objective of providing a comprehensive literature review of parametric models used to describe certain model parameters and value ranges for model parameters. Besides a description of the main transport modules (water, solutes and energy), the crop growth and the nitrogen fate module, the reference and user's manual devotes quite some attention to the model 'input' and 'output', and the description of the structure of the programme code and the variables used.

First and foremost, this is a reference and user's manual for both teachers, researchers and students. Its objective is to present and convey the state-of-the-art in the field of modelling some physical, chemical and biological processes in the vadose environment, which control the fate and transfer of agrochemicals. Therefore, the emphasis is on approaches for conceptualizing, applying, and synthesizing basic underlying concepts. For the convenience of engineers there is an extensive section on how to use the programme code, and in rewriting the code considerable attention is given in adding special check routines for controlling the consistency of the model input.

The reference and user's manual is written from the perspective of authors with scientific background in soil physics, agronomy and computer science and skill in the measurement of static and dynamic soil properties, and the monitoring of complex laboratory and field experiments. In addition, the authors are experienced in fields such as model calibration and validation, and in quan-

tifying the effect of poor concept formulation and random input uncertainty on model output. Furthermore, they have gone through several exercises of using the WAVE-model for engineering purposes. The manual integrates the efforts of the Institute for Land and Water Management on grappling during 20 years of how best to understand and model some dominant processes in the vadose environment. Since continuous developments and research findings will become available, the authors are convinced that this reference and user's manual in future will be replaced by new updates.

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Chapter 1

Introduction

1.1 Background and ORIGIN

Expansion of human activities causes dispersion of pollutants in the subsurface environment. Today, acid rain, hazardous chemical wastes, fertilisers, pesticides, heavy metals, nuclear deposits, solvents and sewage sludge are amongst other things, a serious threat to soil and groundwater quality. Therefore, existing groundwater and soil conservation policies and strategies are reconsidered, while new are developed. For the development of adequate and durable measures the system analytic approach offers many interesting features. A system approach, encompassing the development and validation of simulation models, can help decision makers and scientists to get better insights in the complexity and the interaction of the different processes affecting the fate of chemicals in the dynamic soil-crop environment. As a result, a tremendous interest in system studies, especially through mathematical modelling, has emerged the last decade. Mathematical modelling is an important part of many current environmental studies and it is believed that there is still a lot of scope for model development as long as new insights in processes will emerge and computing facilities improve.

The WAVE-model (Water and Agrochemicals in soil, crop and Vadose Environment), is an example of such a mathematical tool. The model describes the transport and transformations of matter and energy in the soil, crop and vadose environment. The model is mainly process-based, since physical, chemical and biological laws were considered when developing the model. The model is deterministic, by which is meant that one set of input data always yields the same model output values. The model is numerical, since finite difference techniques were used for the solution of the differential equations describing matter and energy transport in the soil-crop continuum. The model is holistic, which means that an attempt was made to integrate the different sub-processes (and hence sub-models) ruling the transfer and fate of different state variables in the complex soil-crop environment. The model is one-dimensional, because it is assumed that governing transport processes of matter and energy in the soil subsystem occur essentially in the vertical direction. The model is an explanatory model because it helps to understand the different processes and process

interactions governing e.g. pollutants in the soil. However, results from these explanatory studies can always be used in extrapolation or prediction studies for decision making. Hence, the current model is one of the ad-hoc tools available to improve current management of the soil-crop environment. It is a unique tool for the better understanding of the processes controlling the transfer and fate of chemicals in soils, the evaluation of experimental field data, the prediction of short and long-term impact of farming strategies on the quality of soil and the groundwater and the development of soil specific environmental measures for the application of fertilisers.

The present WAVE-model is the output of different research projects which aimed at the development, calibration and validation of mathematical models for the quantitative description of matter and energy in soils and environment. These projects were funded by the Institute for the Encouragement of Scientific Research in Agriculture and Industry, Belgium (I.W.O.N.L.) and the Directorates General VI and XII of the European Union. The projects output is, amongst other things, a model consisting of different modules simulating respectively the fate of water, solute, heat, or nitrogen in the soil environment and crop growth. The model is structured in a modular way, enabling the user to use only those modules required to analyse his problem. This allows also the extension of the present model with other modules without the need to adapt the model structure or existing input files of the model. It offers the possibility to exchange modules when new concepts and insights of certain processes becomes available. Fig. 1 present the different modules and the arrows indicate the 'uses-relationships' among them. For example, the solution of the solute flow equation needs to be proceeded by the solution of the water flow equation. Hence the solute module 'uses' the water flow module, which is indicated by the direction of the arrow.

Fig. 1: Schematic presentation of the modules in WAVE (release 1.0). Full line arrows represents obligatory 'uses-relations', dashed lines are optional

The WAVE-model is a software package developed by the Institute for Land and Water Management of the K.U.Leuven, Belgium. The present version of the model integrates earlier models and packages developed by the Institute or developed and published by other scientific institutes. The model is a revised version of the SWATNIT-model (Vereecken et al., 1990; 1991), which integrates the SWATRER-model (Feddes et al., 1978; Belmans et al., 1983; Dierckx et al., 1986), a nitrogen model based on the SOILN-model (Bergstrom et al., 1991), a heat and solute transport model based on the LEACHN-model (Wagenet and Hutson, 1989) and the universal crop growth model SUCROS (van Keulen et al., 1982; Spitters et al., 1988). New modules, considering macroporous flow, pesticide flow, amongst other things are in current development, and will be added after extensive validation. The WAVE-model is written in MS-FORTRAN 5.10 and can be run either under UNIX or MS-DOS.

The user's manual is a revised form of the report of Vanclooster et al. (1993). In the user's manual an attempt is made to describe in detail all the process formulations. Special emphasis is given to the quotation of recent and relevant literature and to the listing of default values for model parameters and

constants. This information together with the integration of automatic data quality control checks in the input files and the use of menus will certainly facilitate the use of the WAVE-model.

1.2 Space and time scales

WAVE is essentially a 1-D model for the description of matter and energy flow in the soil and crop system. Mass and energy fluxes in the soil system are known to be strong non-linear processes. The numerical solution of the 3-D transport problem for unsteady state boundary conditions is, from a computational point of view, still an arduous task. Hence the model is conceived to describe flow only in 1-D systems, as in soil laboratory columns or field lysimeters. The model can also be used to describe transport at the field scale (or a small pedon) if transport is mainly vertical and if effective (1-D) parameters are used. If not, the model describes only flow for a horizontally isolated pedestals (Fig. 2).

Fig. 2: Concept of the horizontal space scale in the WAVE-model

In the vertical direction, the model considers the existence of heterogeneity in the form of soil layers within a soil profile (Fig. 3). The soil layers are subdivided in space intervals called the soil compartments. Halfway each soil compartment a node is identified, for which state variable values are calculated using finite difference techniques. All soil compartments have the same thickness and the user can specify the thickness depending on the desired accuracy. Increasing the compartment thickness will decrease the calculation time but also the numerical accuracy.

Fig. 3: Concept of the vertical space scale

The WAVE-model uses a time step smaller than a day to calculate the different system state variables, for processes which are strongly dynamic (water transport, heat transport, solute transport, solute transformations). The time step is variable, and is chosen as to limit mass balance errors induced by solving the water flow equation. However, the time step size criterion can be input to change the model's robustness. For less dynamic processes (crop growth) a fixed daily time step is often used. The model input is specified on a daily basis and flux type boundary conditions, are assumed constant within the time span of a day. This means, for example, that the daily precipitation is distributed equally within the day. State variables are integrated after each day to yield daily output. The simulation period should not exceed one single year. The simulation starts at midnight of the specified starting date and ends at midnight of the specified ending date.

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Chapter 2

The water transport module

2.1 The soil water flow equation

In the absence of plants, the soil field water balance can simply be written as:

$$\Delta W = (P + I + U) - (R + E + D) \quad (2.1)$$

where ΔW is the change in water content (mm) in the soil volume (set equal to the soil profile volume), P the precipitation (mm), I the irrigation depth applied (mm), U the upward capillary flow into the soil profile (mm), R the water depth lost by runoff (mm), E the actual evaporation (mm) and D the percolation or drainage depth. Generally, P and I are known system input, while U , R , E and D are unknown terms of the water balance. In order to quantify the unknown terms of the water balance, the soil water flow equation is solved.

For homogeneous isotropic isothermal rigid porous media one-dimensional water transport in an infinitesimal small soil element can be described using the Richards equation (Jury et al., 1991):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(K(\theta) \left(\frac{\partial h}{\partial z} + 1 \right) \right) \quad (2.2)$$

where θ is the volumetric water content ($\text{m}^3 \text{m}^{-3}$); z is the vertical co-ordinate (cm) defined as positive upward; t is the time (day); $K(\theta)$ is the hydraulic conductivity (cm day^{-1}); h is the soil water pressure head (cm).

Equation (2) combines the Darcian water flow equation with the water mass conservation law. By introducing the differential water capacity $C(h) = \partial \theta / \partial h$, which represents the slope of the water retention curve, and by expressing the hydraulic conductivity as a function of the pressure head one can convert Eq. (2) to a differential equation with only one unknown h :

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left(K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right) \quad (2.3)$$

Equation (3) is applicable for both unsaturated and saturated flow conditions. In the first case this equation is parabolic, whereas in the second case

($C(h)=0$) it reduces to an elliptic differential equation. Because both the hydraulic conductivity and the differential water capacity are non linear functions of h , Eq.(3) is non-linear. Analytical solutions of Eq.(3) only exist for specific boundary conditions (see Philip et al., 1957; amongst others). To handle more general flow situations, a numerical solution is applied in the WAVE- model to solve the soil water flow equation.

2.2 The soil hydraulic properties

2.2.1 The soil moisture retention characteristic

To solve the flow equation Eq. (3), the moisture retention ($MRC = \theta(h)$) and hydraulic conductivity ($HCC = K(\theta)$ or $K(h)$) functions need to be specified. A parametric model is available to describe the shape of the MRC. In addition to the widely used non-hysteretic retention models, some parametric hysteresis models are available in WAVE. Since the beginning of the century (Haines, 1930), it is known that the MRC of a soil is hysteretic i.e. the moisture content corresponding to a certain pressure head depends on the drying or wetting history. Hysteresis is caused by the irregular geometry of a pore, air inclusions in the soil matrix, shrinking and swelling characteristics (Childs, 1969). It has been observed that the occurrence of hysteresis substantial influence on the calculated water fluxes (Russo et al., 1990; Jones et al., 1990).

When no hysteresis is assumed, moisture retention in the WAVE-model is described using the power function model of van Genuchten (van Genuchten, 1980; van Genuchten and Nielsen, 1985):

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{(1 + (\alpha|h|)^n)^m} \quad (2.4)$$

where θ_s is the saturated volumetric soil water content ($m^3 m^{-3}$); θ_r is the residual volumetric soil water content ($m^3 m^{-3}$); α is the inverse of the air entry value (m^{-1}); and n , m are shape parameters (-). Fig. 5 illustrates a physical interpretation of the parameters of Eq.(4) with exception of the m parameter which characterises the asymmetry.

Fig.5: Moisture retention characteristic as described by the van Genuchten model (van Genuchten et al., 1980)

When modelling the water balance of a field soil, the correct definition of the parameters of the MRC is crucial. If simultaneously measured moisture content and pressure head data are available, one can use these measurements to fit the parameters of Eq.(4) using non-linear optimisation techniques. Therefore, one can develop his own programmes using e.g. statistical software or spreadsheet programmes. Alternatively, one can use special softwares (e.g. van Genuchten, 1991).

In many cases, no measurement data of the MRC are available and so one needs an indirect estimate of the MRC parameters. For a range of soils, Vereecken et al. (1989) found that the MRC can reasonably well be estimated

by assuming a symmetrical moisture retention characteristic (or $m=1$). Pedo-transfer functions, relating the remaining parameters of Eq.(4) to basic soil properties such as texture, soil organic carbon and others, were developed and validated (Vereecken et al., 1989; Vereecken et al., 1992; Tietje and Tapkenhins, 1993). The following multiple regression pedo-transfer functions, taken from Vereecken et al., (1989) can be used to estimate the parameters of Eq.(4):

$$\begin{aligned}
 \theta_s &= 0.81 - 0.283(Bd) + 0.001(Cl) \\
 \theta_r &= 0.015 + 0.005(Cl) + 0.0014(C) \\
 \ln(\alpha) &= -2.486 + 0.025(Sa) - 0.351(C) - 0.2617(Bd) - 0.023(Cl) \\
 \ln(n) &= 0.053 - 0.009(Sa) - 0.013(Cl) + 0.00015(Sa)^2
 \end{aligned} \tag{2.5}$$

where Bd is the soil bulk density (g cm^{-3}); C = the carbon content (perc) Sa = the sand content (fraction 50-2000 μm in perc); Cl = the clay content (fraction 2 μm in perc).

When hysteresis of the MRC is considered, four types of relations should be distinguished. If desorption starts from saturation, the main drying branch of the MRC (θ^d) is obtained. Branching from this curve results in a primary wetting curve (θ_1^w) which in turn leads to a secondary drying curve (θ_2^d) upon drying. All curves that once originated from the main drying curve are either uneven order wetting curves (θ_n^w , with $n=1,3,\dots$) or even order drying curves (θ_n^d , with $n=2,4,\dots$). In the same way, branching from the main wetting curve (θ^w) can only result in uneven drying curves (θ_n^d , with $n=1,3,\dots$), or even wetting curves (θ_n^w , with $n=2,4,\dots$).

In the WAVE-model, the second model reported by Mualem (1974) is included to describe the MRC. This model was found to be one of the most accurate in a comparative study of hysteresis models (Viaene et al., 1994). Mualem's model is a two branch, conceptual model. The conceptual foundation for the model is the independent domain theory of hysteresis (Nel, 1942-1943). As a two branch model, the model describes the moisture content on a curve of the MRC as a function of the moisture content on the two main curves. In the comparative study of hysteresis models, it was found that the main loop can be considered as a primary wetting loop without significant loss of accuracy. This implies that only two groups of scanning curves need to be considered: uneven order wetting curves and even order drying curves. For an uneven order wetting scanning curve branching from a drying curve at $\theta_{n-1}(h_\Delta)$, the moisture content $\theta_n^w(h)$ can be calculated as:

$$\theta_n^w(h) = \theta_{(n-1)}^d(h_\Delta + (\theta^w(h) - \theta^w(h_\Delta)) \left(\frac{\theta_s - \theta^d(h_\Delta)}{\theta_s - \theta^w(h_\Delta)} \right) \tag{2.6}$$

where $q_{dn-1}(hD)$ and hD are respectively the water content and pressure head at the transition from the previous drying curve to the present wetting curve; $q_w(h)$ is the main wetting curve; $q_d(h)$ is the main drying curve; and q_s , the saturated moisture content. Similarly, an even order drying scanning curve branching from a wetting curve at $q_{wn-1}(hD)$ can be calculated as:

$$\theta_n^d(h) = \theta_{(n-1)}^w(h_\Delta - (\theta^w(h_\Delta) - \theta^w(h)) \left(\frac{\theta_s - \theta^d(h)}{\theta_s - \theta^w(h)} \right) \quad (2.7)$$

where θ_{n-1}^w and h_Δ are respectively the water content and the pressure head at the transition from the previous wetting curve to the present drying curve; and $\theta_{n-1}^w(h)$ is the previous wetting curve.

The $\theta^d(h)$ and $\theta^w(h)$ relationships are described with the van Genuchten model (Eq.(4)). Assuming a closed main loop implies the same residual and saturated moisture content for the main drying and wetting curve. Practical application of the model revealed that a different choice of n and m for the main curves results in numerical errors. Therefore the n and m parameters are default equal for both main retention curves. A hysteresis model needs to be combined with a $K(\theta)$ model since the $K(h)$ relationship is also hysteretic. A common choice is the use of Mualem's conductivity model (cf. infra). For the use of this model, and hence for the use of Mualem's hysteretic retention model, the m parameter is restricted to $m = 1 - 1/n$. So, the only parameter differing between the main wetting and drying curve is a . For the main drying curve, a_d is the inverse of the air entry point, while for the main wetting curve a_w is the inverse for the water entry point. If Mualem's two branch model is used, one needs to input a_w as additional parameter to the parameters of Eq.(4). In Fig.6 the effect of different values of n , m , a_w and a_d are illustrated for the main loop and a small primary wetting - secondary drying loop. Notice the increase of the main loop area when a large a^w/a^d and large n , m are selected.

Fig. 6: Examples of hysteretic moisture retention characteristic, for a range of a_d , a_w and n , m values

In many situations only the main drying curve of the MRC is determined. In those cases the rule of thumb $a_w/a_d = 2$ can be used (Kool and Parker, 1987). Alternatively, one can use Mualem's universal hysteresis model to estimate the main drying loop from the main wetting (Mualem, 1977):

$$\theta_d(h) = (2 \cdot \theta_s - \theta_w(h) - \theta_r) \cdot \left(\frac{\theta_w(h) - \theta_r}{\theta_s - \theta_r} \right) + \theta_r \quad (2.8)$$

This model is available in the WAVE-model. As input for this MRC model, the user specifies the parameters of Eq. (4) for the main wetting curve.

When applying Eq.(4), it is assumed that the pore-size distribution of the soil matrix follows a mono-modal distribution. Multi-porosity systems, assuming that the matrix system is the combination of different mono-modal systems, are more flexible in describing accelerated flow phenomena (preferential flow) in soils (Gerke and van Genuchten, 1993; Durner, 1994). The multi-porosity model available in the WAVE-model, assumes that the complete MRC curve in a multi-porous system can be described by the sum of separate mono-modal MRC's, similar to Eq.(4):

$$Se = \sum_{i=1}^n \frac{w_i}{(1 + (\alpha_i h)^{n_i})^{m_i}} = \sum_{i=1}^n w_i S_i \quad (2.9)$$

where w_i are the weights of the individual partial MRC's S_i , with $\sum w_i = 1$. The saturation degree is a dimensionless moisture content and is defined as:

$$Se = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (2.10)$$

An example of a multi-porous MRC is given in the Fig.7. When using the multi-porous MRC, a_i , n_i , m_i and w_i parameter need to be specified for each partial MRC, while q_r and q_s are needed to rescale Se back to volumetric moisture contents θ .

Fig. 7: Bi-modal moisture retention characteristic as described with the sum of two van Genuchten equations

2.2.2 The hydraulic conductivity relationship

Just like for the MRC, conceptual, empirical or hybrid parametric models have been cited in literature to describe the hydraulic conductivity (HCC) functions of soils. The HCC can be expressed in terms of pressure head (h), volumetric moisture content (θ) or effective saturation (Se). The different mono-modal models for the HCC which are available in the WAVE-model are listed in Table 1.

Model Equation	Parameter	References
$K_h = \frac{K_{sat}}{1+(b h)^N} \quad (2.11)$	Ksat, b, N	Gardner(1958)
$K_h = K_{sat} \cdot e^{\alpha h} \quad (2.12)$	Ksat, alpha	Gardner (1958)
eq	Ksat, c	Gillham et al (1976)
eq	Ksat, l	Brooks and Corey (1964)
eq	ksat, lambda, m	van Genuchten (1980), Mualem (1976)

Table 1: Hydraulic conductivity models available in the WAVE-model

The parameters of the HCC again can be fitted using optimisation techniques if measurements of the HCC at different moisture contents (or h or Se) are available. Different field and laboratory techniques are at hand to measure discrete points of the HCC, though still no standardised technique is available to yield an effective HCC. All parametric models use Ksat (the saturated hydraulic conductivity value) as first point of the hydraulic conductivity curve. The definition of an effective saturated conductivity is a tedious task. Ksat is strongly influenced by structural phenomena resulting from e.g. worm activity, crop roots, etc. So, the Ksat is behaving as a random variable rather than a deterministic property within the field. Hence, measurements of Ksat are varying tremendously within a field. Therefore it is suggested to measure Ksat slightly below saturation to exclude wormholes or cracks. This value can be obtained

from e.g. sorption infiltrometer data.

When comparing different conductivity models for the description of the HCC, Gardner's model (1958) turned out to perform well for Belgian conditions (Vereecken et al., 1990), though the exponential Gardner model is more widely used to describe the HCC of undisturbed soils. For the Gardner model (1958), the following pedo-transfer function can be used if no good measurement of K_{sat} is available:

$$\begin{aligned} \ln(K_{sat,e}) &= 20.62 - 0.96 \cdot \ln(Cl) - 0.66 \ln(Sa) - 0.46 \cdot \ln(C) - 8.43 \cdot bd \\ \ln(b) &= -.73 - 0.01877 \cdot Sa + 0.058 \cdot Cl \\ \ln(N) &= 1.186 - 0.194 \cdot \ln(Cl) - 0.0489 \cdot \ln(Si) \end{aligned} \quad (2.13)$$

where $K_{sat,e}$ is the estimate of the saturated hydraulic conductivity (cm day⁻¹), Cl , Sa and Si the clay ($< 2\mu$), sand ($50 - 2000\mu$) and silt ($2 - 50\mu$) content (perc), Bd the soil bulk density (g cm⁻³) and C the organic carbon content (perc). The explanation of the pedo-transfer function of the observed variation increases if a measurement of the saturated hydraulic conductivity is included as predictor variable. In this case the following equations can be used to estimate Gardner's parameters:

$$\begin{aligned} \ln(K_{sat,e}) &= \ln(K_{sat,m}) \\ \ln(b) &= -2.640 - 0.019 \cdot Sa + 0.05 \cdot Cl + 0.506 \cdot \ln(K_{sat,m}) \\ \ln(N) &= 1.186 - 0.194 \cdot \ln(Cl) - 0.0489 \cdot \ln(Si) \end{aligned} \quad (2.14)$$

where $K_{sat,m}$ is the measurement of the saturated hydraulic conductivity curve (cm day⁻¹).

The theoretical HCC model of van Genuchten (1980) is a particular solution of the general statistical pore size distributed conductivity model of Mualem (1976). It uses the same parameters as for the MRC, though with the restriction that m must be equal to $1-1/n$. This HCC model is theoretically well elaborated. In practice, however, the resulting $K(\theta)$ -curve is very susceptible to the K_{sat} value. If only K_{sat} is measured, the typical difficulties with K_{sat} measurements (effect of sample size, high short-range variation, continuous cracks/pores through samples) can yield unrealistic $K(\theta)$ -curves. So one should be tremendously careful when using this indirect estimation model to estimate the HCC.

When modelling the field water balance with a multi-porosity system, the closed form expression of the van Genuchten-Mualem HCC needs to be replaced by the general Mualem model (Mualem, 1976):

$$K(h) = K_{sat} \cdot Se^\lambda \left(\frac{\int_0^{Se} \frac{1}{h(Se)} dSe}{\int_0^1 \frac{1}{h(Se)} dSe} \right)^2 \quad (2.15)$$

where the $h(Se)$ curve is the inverse of the MRC curve. When a multi-modal MRC is assumed, the inverse of the MRC, $h(Se)$, cannot be calculated directly.

Therefore, the integrals in Eq.(19) need to be solved numerically. Substituting Eq. (9) in the denominators of Eq.(19) yields:

$$\int_0^{Se} \frac{1}{h(Se)} dSe = \int_{-\infty}^h \frac{1}{h(Se)} \cdot \frac{\partial Se}{\partial h} \cdot dh \quad (2.16)$$

which can be reduced to

$$\int_{-\infty}^h \frac{1}{h(Se)} \left(\sum w_i \frac{\partial Si}{\partial h} \right) dh = \sum w_i \int_{-\infty}^h \frac{1}{h(Se)} \left(\frac{\partial Si}{\partial h} \right) dh$$

and finally into

$$\sum w_i \int_{-\infty}^{Si} \frac{1}{h(Se)} dSi$$

or the integral of the multi-porous $1/h$ curve is the weighed sum of integrals for the partial $1/h$ curves. The integral of the partial $1/h$ curve can be solved by inversion (van Genuchten and Nielsen, 1985):

$$\int_0^{Si} \frac{1}{h(Se)} dSi = \int_0^{Si} \left(\frac{x^{1/m}}{1 - x^{1/m}} \right)^{1/n} dx \quad (2.17)$$

The substitution $x = y^m$ reduces Eq.(21) to:

$$\int_0^{Si} \frac{1}{h(Se)} dSi = m \int_0^{Si^{1/m}} y^{m-1+1/n} (1-y)^{-1/n} dy = m I_\zeta(p, q) \cdot B(p, q) \quad (2.18)$$

where $I_\zeta(p, q)$ is the Incomplete Beta function and $B(p, q)$ is the Complete Beta function, and $\zeta = Se(1/m)$, $p = m+1/n$ and $q = (1-1/n)$. The Incomplete Beta function in the WAVE-model is evaluated numerically using continued fractions (see e.g. van Genuchten, 1991):

$$I_\zeta(p, q) \quad (2.19)$$

where

$$d_{2m+1} = \frac{-(p+q)(p+q+m)}{(p+2m)(p2m+1)} \cdot \zeta \quad (2.20)$$

$$d_{2m} = \frac{m(q-m)}{(p+2m-1)(p2m)} \cdot \zeta \quad (2.21)$$

2.3 Numerical solution of the water flow equation

2.3.1 The solution procedure

In order to solve Eq.(3) numerically, the soil profile is discretised into a number of compartments and the total time period into discrete time increments (time steps) of unequal lengths. The soil compartments are grouped in different

pedological layers (cf. Fig. 3). For each soil layer, the parameters of the MRC and HCC are specified. In this way, the partial derivatives of Eq.(3) can be approximated as ratio's of finite differences. An implicit discretisation scheme with explicit linearisation of the conductivity and the differential moisture capacity is used. In a comparative study of 6 different discretization methods, Haverkamp et al. (1977) found that the implicit schemes are superior in terms of applicability and efficiency. Furthermore Huwe and van der Ploeg (1988) observed that the explicit methods fail in case of saturated conditions. With this implicit difference scheme Eq.(3) can be approximated as:

$$C_i^j \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{K_{i-1/2}^j \left(\frac{h_{i-1}^{j+1} - h_i^{j+1}}{\Delta z_i^*} + 1 \right) - K_{i+1/2}^j \left(\frac{h_i^{j+1} - h_{i+1}^{j+1}}{\Delta z_{i+1}^*} + 1 \right)}{\Delta z_i} \quad (2.22)$$

where :

$$\Delta z_i = z_{i-1/2} - z_{i+1/2} \quad (2.23)$$

is the thickness of the i-th compartment (mm);

$$\Delta z_i^* = Z_{i-1} - z_i \quad (2.24)$$

is the distance between the nodes (mm); and

$$\Delta t = t^{j+1} - t^j \quad (2.25)$$

is the length of the time step (day).

Pressure heads are considered only at specific nodes in the time-depth space. The subscript i refers to the depth position, whereas j refers to the position on the time axis. The position of the variables h, K, and C in the numerical solution grid is illustrated in Fig. 8. Nodal points are situated in the middle of the compartments.

Fig. 8: Numerical grid, with location of pressure heads h (o), hydraulic conductivity K (x) and differential water capacity (+) as used in the finite difference equation (Eq. 26)

For the hydraulic conductivity between the nodal points, the geometric mean is taken as proposed by Vauclin et al. (1979):

$$\begin{aligned} K_{i-1/2}^j &= \sqrt{K(h_{i-1}^j) \cdot K(h_i^j)} \\ K_{i+1/2}^j &= \sqrt{K(h_i^j) \cdot K(h_{i+1}^j)} \end{aligned} \quad (2.26)$$

As can be seen in Eq. 26 and Fig.8, the term $\partial h / \partial z$ is evaluated at the end of the time step (implicit discretisation), whereas K and C are set equal to their values at the beginning of the time step (explicit linearisation of K and C). This scheme implies that the equation, which can be written for node i, contains three unknowns (h_{i-1}^{j+1} , h_i^{j+1} and h_{i+1}^{j+1}). Rearranging Eq.(26) in terms of these unknowns, yields:

$$-d_i h_{i-1}^{j+1} + b_i h_i^{j+1} - a_i h_{i+1}^j + 1 = e_i \quad (2.27)$$

where:

$$\begin{aligned} a_i &= \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} K_{i+1/2}^j \\ b_i &= C_i^j + \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} K_{i+1/2}^j + \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} K_{i-1/2}^j \\ c_i &= \frac{\Delta t}{\Delta z_i \Delta z_i^*} K_{i-1/2}^j \\ e_i &= C_i^j h_i^j - \frac{\Delta t}{\Delta z_i} K_{i+1/2}^j + \frac{\Delta t}{\Delta z_i} K_{i-1/2}^j \end{aligned} \quad (2.28)$$

Equation (31) is written for each node, except for the top and bottom one. As will be explained later, a similar equation can be developed for these boundary nodes. For the top node, Eq.(26) reduces to:

$$b_1 h_1^j + 1 - a_1 h_2^{j+1} = e_1 \quad (2.29)$$

where for the bottom node:

$$-d_n h_{n-1}^{j+1} + b_n h_n^{j+1} = e_n \quad (2.30)$$

In this way, the n pressure head values at the end of each time step (subscript j+1) are derived from the pressure head profile at the beginning of the time step and information of the boundary conditions, by solving a system of n equations having the following form:

$$\begin{pmatrix} b_1 & -a_1 & 0 & \cdot & \cdot & 0 \\ -d_2 & b_2 & -a_2 & 0 & \cdot & \cdot \\ 0 & -d_3 & b_3 & -a_3 & 0 & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -d_i & b_i & -a_i & \cdot \\ \cdot & \cdot & 0 & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & -d_{n-1} & b_{n-1} & -a_{n-1} \\ 0 & \cdot & \cdot & 0 & 0 & -d_n \end{pmatrix} \cdot \begin{pmatrix} h_1^{j+1} \\ h_2^{j+1} \\ h_3^{j+1} \\ \cdot \\ h_i^{j+1} \\ \cdot \\ h_{n-1}^{j+1} \\ h_n^{j+1} \end{pmatrix} = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ \cdot \\ e_i \\ \cdot \\ e_{n-1} \\ e_n \end{pmatrix} \quad (2.31)$$

To solve this tridiagonal system of linear equations, the Thomas algorithm which is a direct non-iterating solution technique is used (see e.g. Remson et al., 1971). Once the pressure head profile at the end of the time step is calculated, the corresponding water content profile is obtained by using the MRC. Next, the whole procedure is repeated for the next time step.

However, as a result of the explicit linearisation of the differential water capacity, mass balance errors occur, especially in case of large water content changes and nearly saturated moisture conditions. As stated before, the q/t derivative in Eq.(2) has been replaced by C(h).h/t (Eq.(3)), which in turn is approximated by its finite difference analog (Eq.(26)):

$$C(h) \frac{\partial h}{\partial t} \approx C_i^j \frac{h_i^{j+1} - h_i^j}{\Delta t} \quad (2.32)$$

Hence, a mass balance error resulting from this explicit linearisation of C is made which is equal to:

$$(\theta_i^{j+1} - \theta_i^j) - C_i^j (h_i^{j+1} - h_i^j) \quad (2.33)$$

In order to reduce these mass balance errors, the Newton-Raphson solution technique is used in the WAVE-model. The Newton-Raphson technique (see e.g. Carnahan et al., 1969) is an iterating solution method for a system of non-linear equations, and has the following form:

$$F_i(\bar{X}) = 0 \quad (2.34)$$

for $i=1, \dots, n$; with $\bar{X} = (x_1, \dots, x_n)$ the vector of unknowns. If the function values are known for a given vector $t = (x_1^\tau, \dots, x_n^\tau)$, the function values F_1, \dots, F_n for a vector $t+1$ in the neighbourhood of the first one can be approximated by using a first order Taylor series expansion around t :

$$F_i(\bar{X}^{\tau+1}) = F_i(\bar{X}^\tau) + \sum_{k=1}^n \frac{\partial F_i(\bar{X}^\tau)}{\partial x_k} (x_k^{\tau+1} - x_k^\tau) \quad (2.35)$$

If t is known as approximate solution of Eq.(26), an improvement can be obtained by solving $F_i(t+1)=0$, using the Taylor expansion given by Eq.(39). This means that successive improvements of the solution can be obtained by solving the following system of linear equations:

$$\begin{pmatrix} F_1(\bar{X}^{\tau+1}) \\ \vdots \\ F_n(\bar{X}^{\tau+1}) \end{pmatrix} + \begin{pmatrix} \frac{\partial F_1(\bar{X}^\tau)}{\partial x_1} & \dots & \frac{\partial F_1(\bar{X}^\tau)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_n(\bar{X}^\tau)}{\partial x_1} & \dots & \frac{\partial F_n(\bar{X}^\tau)}{\partial x_n} \end{pmatrix} \cdot \begin{pmatrix} x_1^{\tau+1} - x_1^\tau \\ \vdots \\ x_n^{\tau+1} - x_n^\tau \end{pmatrix} = 0 \quad (2.36)$$

where $\bar{X}^{\tau+1} = (x_1^{\tau+1}, \dots, x_n^{\tau+1})$ being the unknowns.

Let's consider the q-formulation of the water flow equation given by Eq.(2). The finite difference analog of this equation is similar to Eq.(26) and is rearranged in the form $F_i(H) = 0$ with $H = (h_1^{j+1}, \dots, h_n^{j+1})$ being the vector of unknown pressure heads:

$$F_i(\bar{H}) = \frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} - \frac{K_{i-1/2}^j \left(\frac{h_{i-1}^{j+1} - h_i^{j+1}}{\Delta z_i^*} + 1 \right) - K_{i+1/2}^j \left(\frac{h_i^{j+1} - h_{i+1}^{j+1}}{\Delta z_{i+1}^*} + 1 \right)}{\Delta z_i} \quad (2.37)$$

This finite difference equation for node i is in fact the mass balance equation for compartment i . The solution of this system of equations yields an exact

internal mass balance. Because q_{ij+1} is strongly dependent on the unknown $h_{i+1,j}$ (non-linear $q(h)$), this equation is non-linear and the Newton-Raphson method offers the possibility to solve it in an iterative way. Assume $H_{j+1,t} = (h_{1j+1,t}, \dots, h_{nj+1,t})$ is the t -th approximate solution of the systems of non-linear equations. A better solution is obtained by solving:

$$F_i(\bar{H}^t) + \sum_{k=1}^n \frac{\partial F_i(\bar{H}^t)}{\partial h_k} (h_k^{j+1,t+1} - h_k^{j+1,t}) = 0 \quad (2.38)$$

Equation (42) is obtained by combining Eq. (40) with (41). The partial derivatives can easily be derived from Eq.(41):

$$\begin{aligned} \frac{\partial F_i(\bar{H}^{j+1})}{\partial h_i^{j+1}} &= \frac{1}{\Delta t} \frac{\theta_i^{j+1}}{\partial h_i^{j+1}} + \frac{K_{i-1/2}^j}{\Delta z_i \Delta z_i^*} + \frac{K_{i+1/2}^j}{\Delta z_i \Delta z_{i+1}^*} \\ \frac{\partial F_i(\bar{H}^{j+1})}{\partial h_{i-1}^{j+1}} &= \frac{K_{i-1/2}^j}{\Delta z_i \Delta z_i^*} \\ \frac{\partial F_i(\bar{H}^{j+1})}{\partial h_{i+1}^{j+1}} &= \frac{K_{i+1/2}^j}{\Delta z_i \Delta z_{i+1}^*} \\ \frac{\partial F_i(\bar{H}^{j+1})}{\partial h_k^{j+1}} &= 0 \end{aligned} \quad (2.39)$$

for $k < i - 1$ or $k > i + 1$

After replacing the partial derivatives in Eq.(42) and rearranging in terms of the unknowns $h_1^{j+1,t+1}, \dots, h_n^{j+1,t+1}$ one obtains an improved approximation by solving the following tridiagonal system of linear equations :

$$-d_i(h_{i-1}^{j+1})^{t+1} + b_i(h_i^{j+1})^{t+1} - a_i(h_{i+1}^{j+1})^{t+1} = e_i \quad (2.40)$$

for $i = 2, \dots, n - 1$

where:

$$\begin{aligned} a_i &= \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} (K_{i+1/2}^{j+1})^t \\ b_i &= (C_i^{j+1})^t + \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} (K_{i+1/2}^{j+1})^t + \frac{\Delta t}{\Delta z_i \Delta z_{i+1}^*} (K_{i-1/2}^{j+1})^t \\ d_i &= \frac{\Delta t}{\Delta z_i \Delta z_i^*} (K_{i-1/2}^{j+1})^t \\ e_i &= (C_i^{j+1} h_i^j)^t - ((\theta_i^{j+1})^t - \theta_i^j) - \frac{\Delta t}{\Delta z_i} (K_{i+1/2}^{j+1})^t + \frac{\Delta t}{\Delta z_i} (K_{i-1/2}^{j+1})^t \end{aligned} \quad (2.41)$$

Equation (44) is very similar to Eq.(31), the only difference is the additional $(q_i, j+1, t - q_i, j)$ term in coefficient e_i , and the fact that C and K are now evaluated at time $j+1$. Again, two additional equations, similar to Eq.(33) and Eq.(34) are written for the top and bottom nodes. The resulting tridiagonal system consists of n linear equations with n unknowns which are solved directly by the same Thomas algorithm. The set of equations is solved for each iteration loop within

the same time step. After each iteration, function values $Fi(H)$, which are in fact the mass balance errors for the different compartments (m³ m⁻³ day⁻¹), can be calculated. The iteration procedure continues as long as one or more internal mass balance errors exceed a predefined threshold value ERR_{max} . The solution algorithm is summarized as follows:

1. Given H_j , the pressure head profile at the beginning of the time step, the first approximation $H_{j+1,1}$ is calculated by solving Eq.(26).
2. Repeat the following steps for $t = 1, \dots, NITER_{max}$.
 - (a) Calculate the internal mass balance errors $Fi(H^t)$ if all $Fi(H_j + 1, t) < ERR_{max}$, end iteration loop and go to the next time step; else continue the iteration loop.
 - (b) Calculate an improved solution $H_{j+1, t+1}$ by solving the system of linear equations given by Eq.(44) and the additional equations for the top and bottom nodes.
3. If the desired accuracy is not reached within $NITER_{max}$ iterations, then halve the time step size and repeat the calculations starting from step 1.

2.3.2 Definition of the upper boundary condition

As stated before, it is necessary to construct an additional equation for the first compartment, which has a form given by Eq.(33). The flow situation at the soil surface is determined by the infiltration or the evaporative flux. As long as the flow conditions at the soil surface are not limiting, the flux through the soil surface Q_s equals:

$$Q_s = E_{pot} - \left(Rain + Irr + \frac{Pond - Intc}{\Delta t} \right) \quad (2.42)$$

where: Q_s is the potential flux through the soil surface, defined as positive upward (cm day⁻¹); E_{pot} is the potential soil evaporation rate (cm day⁻¹) as determined by weather conditions and soil cover; Rain is the precipitation rate (cm day⁻¹); Irr is the irrigation amount (cm day⁻¹); Pond is the ponding depth at the soil surface (cm) and Intc the storage capacity of the canopy (m).

Most of the time, the boundary condition at the top is a flux condition (Neuman condition), with the flux calculated from Eq.(3):

$$K(h) \left(\frac{\partial h}{\partial z} + 1 \right) = -Q_s(t) \quad (2.43)$$

for $z = 0$

However, in case of high rainfall (or irrigation) intensities, the soil surface becomes saturated and the infiltration capacity ($=K_{sat} \cdot \text{gradient}$) limits the infiltration rate. If no ponding is assumed, the excess water runs off immediately. In this case, the pressure head at the surface is put to zero. When ponding occurs, the pressure head at the soil surface increases until a maximal ponding depth, specified by the user, is reached. The maximal ponding depth reflects the surface micro-catchment when the soil surface roughness is high. When the

maximal ponding depth is reached, the excess water runs off. In both cases, the flux type boundary condition switches to a pressure head condition (Dirichlet) for the node at the surface ($h_s=0$ or $h_s=\text{ponding depth}$).

A similar phenomenon is encountered in case of prolonged soil evaporation without rewetting. In the beginning the upward flux is equal to the evaporative demand. At a given moment the top soil becomes so dry (low hydraulic conductivity) that the upward flux through the soil surface becomes smaller than the evaporative demand. This implies that the actual soil evaporation rate (E_{act}) becomes smaller than the potential rate (E_{pot}). Reduction of the potential evaporation is simulated by changing from a flux to a pressure head condition. When the pressure head at the surface tends to become more negative than a value h_{airdry} , corresponding with the potential of the air ($1/\text{font} -106 \text{ cm}$), the pressure head is fixed ($h_s = h_{airdry}$). The value h_{airdry} is specified by the user.

With the above concept, the appropriate top boundary condition for each time step depends on the moisture condition in the top soil at the beginning of the time step and the value of the flux Q_s during that step. At the beginning of a time step, the program assumes the same condition as used in the foregoing time-step. After the soil moisture equation is solved accordingly, it is checked whether the choice was justified. In case of a flux condition, the pressure head at the surface is calculated using Darcy's equation:

$$h_s = h_1 + \Delta z_1^* \left(-\frac{Q_s}{K_0} - 1 \right) \quad (2.44)$$

where

$$K_0 = \frac{K(h_s) + K(h_1)}{2}$$

As long as the calculated h_s remains within the interval $(h_{airdry}, 0)$, the choice for a flux condition is correct. If not, the calculations for the given time step are repeated with the appropriate pressure head condition.

If a pressure head condition is adopted, the flux through the surface is calculated using the Darcy equation and compared to the 'potential' flux Q_s . In case of run-off and ponding (h_s , fixed), the actual infiltration should always be smaller than the potential infiltration rate (actual flux $> Q_s$, both fluxes being negative). A similar criterion is used in the case of a reduction of the soil evaporation in dry conditions. In this case the actual soil evaporation should remain smaller (less positive) than the potential rate (actual flux $< Q_s$). If these conditions are not fulfilled, calculations are repeated with a flux condition.

With this algorithm, the soil moisture equation is solved with either a Dirichlet or a Neuman condition at the top. In case of a Dirichlet condition, the finite difference equation for the first node is the same as for the other ones (Eq.(26)), with the exception that the node above the first node is located at the surface (at a distance of half the compartment size), and that its pressure head is known ($h_{i-1} = h_s$):

$$C_i^j \frac{h_1^{j+1} - h_1^j}{\Delta t} = \frac{K_0 \left(\frac{h_s^{j+1} - h_1^{j+1}}{\Delta z_1^*} + 1 \right) - K_{i+1/2}^j \left(\frac{h_1^{j+1} - h_2^{j+1}}{\Delta z_2^*} + 1 \right)}{\Delta z_1} \quad (2.45)$$

Rearranging in terms of the two unknowns, h_1^{j+1} and h_2^{j+1} , yields the following expressions:

$$b_1 h_1^{j+1} - a_1 h_2^{j+1} = e_1 \quad (2.46)$$

where

$$\begin{aligned} a_1 &= \frac{\Delta t}{\Delta z_1 \Delta z_2^*} K_{1+1/2}^j \\ b_1 &= C_1^j + \frac{\Delta t}{\Delta z_1 \Delta z_2^*} K_{1+1/2}^j + \frac{\Delta t}{\Delta z_1 \Delta z_1^*} K_0^j \\ e_1 &= C_1^j h_1^j - \frac{\Delta t}{\Delta z_1} K_{1+1/2}^j + \frac{\Delta t}{\Delta z_1} K_0^j + \frac{\Delta t}{\Delta z_1 \Delta z_1^*} K_0^j h_s^{j+1} \end{aligned} \quad (2.47)$$

In case of a *flux condition*, the equation for node 1 is written as:

$$C_1^j \frac{h_1^{j+1} - h_1^j}{\Delta t} = \frac{-Q_s - K_{1+1/2}^j \left(\frac{h_1^{j+1} - h_2^{j+1}}{\Delta z_2^*} + 1 \right)}{\Delta z_1} \quad (2.48)$$

As for the Dirichlet condition, this equation again contains only two unknowns, and can be written in the form:

$$b_1 h_1^{j+1} - a_1 h_2^{j+1} = e_1 \quad (2.49)$$

where

$$\begin{aligned} a_1 &= \frac{\Delta t}{\Delta z_1 \Delta z_2^*} K_{1+1/2}^j \\ b_1 &= C_1^j + \frac{\Delta t}{\Delta z_1 \Delta z_2^*} K_{1+1/2}^j \\ e_1 &= C_1^j h_1^j - \frac{\Delta t}{\Delta z_1} K_{1+1/2}^j - \frac{\Delta t}{\Delta z_1} Q_s \end{aligned} \quad (2.50)$$

2.3.3 Definition of the Bottom boundary condition

To solve the water flow equation for the n nodes of a soil profile, the flow at the bottom boundary needs to be quantified. It is evident that the flow at the bottom of the soil profile is controlled by the geo-hydrological conditions. In the WAVE-model the flow situation at the bottom of the flow domain can be specified in seven different ways. These seven options are divided into four groups:

1. A groundwater table is present:
 - the groundwater level is given as a function of time;
 - the flux through the bottom of the soil profile is given as a function of time, the groundwater level is calculated;
 - the flux through the bottom of the soil profile is calculated with a flux-groundwater level relationship; the groundwater level is calculated.
2. The pressure head at the bottom is known as a function of time.

3. The flux through the bottom is known at each time step:

- assumption of free drainage at the bottom;
- zero flux.

4. Lysimeter with free outflow at the bottom.

The bottom boundary options offer the possibility to simulate a wide variety of flow situations. Before describing the options in detail, the formulation of the bottom boundary conditions as a flux or pressure head condition is given.

If the flux at the bottom of the flow domain is known (Neuman condition), the boundary condition is given by:

$$K(h) \left(\frac{\partial h}{\partial z} \right) = -Q(t) \quad (2.51)$$

where $Q(t)$ represents the flux (cm day⁻¹, positive upward) at the bottom of the flow domain ($z=-L$). When combining Richards equation with Eq.(53), the following implicit finite difference equation for the bottom node n is obtained:

Figure 9 gives the location of the variables involved in the finite difference equation.

Fig. 9: Numerical grid, showing the location of the variables involved in the finite difference equation for the bottom compartment in case of a Neuman condition

Rearranging in terms of the unknowns $h_{n-1/2}^{j+1}$ and $h_{n+1/2}^{j+1}$ yields:

$$-d_n h_{n-1}^{j+1} + b_n h_n^{j+1} = e_n \quad (2.52)$$

where

$$\begin{aligned} b_n &= C_n^j + \frac{\Delta t}{\Delta z_n \Delta z_n^*} K_{n-1/2}^j \\ d_n &= \frac{\Delta t}{\Delta z_n \Delta z_n^*} K_{n-1/2}^j \\ e_n &= c_n^j h_n^j + \frac{\Delta t}{\Delta z_n} Q_{n+1/2}^{j+1} + \frac{\Delta t}{\Delta z_n} K_{n-1/2}^j \end{aligned}$$

In case of a *pressure head condition* at the bottom of the flow domain (Dirichlet condition), the finite difference equation for the bottom node n is identical to the equations for the other nodes:

$$C_n^j \frac{h_n^{j+1} - h_n^j}{\Delta t} = \frac{K_{n-1/2}^j \left(\frac{h_{n-1}^{j+1} - h_n^{j+1}}{\Delta z_n^*} + 1 \right) - K_{n+1/2}^j \left(\frac{h_n^{j+1} - h_{n+1}^{j+1}}{\Delta z_{i+1}^*} + 1 \right)}{\Delta z_i} \quad (2.53)$$

In this case the new pressure head at node $n+1$ is already known. Rearranging in terms of the two unknowns h_{n-1}^{j+1} and h_n^{j+1} yields:

$$b_n = C_n^j + \frac{\Delta t}{\Delta z_n \Delta z_n^*} K_{n-1/2}^j \quad (2.54)$$

$$d_n = \frac{\Delta t}{\Delta z_n \Delta z_n^*} K_{n-1/2}^j$$

$$e_n = C_n^j h_n^j + \frac{\Delta t}{\Delta z_n \Delta z_{n+1}^*} K_{n+1/2}^j h_{n+1/2}^{j-1} - \frac{\Delta t}{\Delta z_i} K_{n+1/2}^j + \frac{\Delta t}{\Delta z_i} K_{n-1/2}^j \quad (2.55)$$

In the next section it will be shown how, for each of the seven bottom boundary options, the flow situation can be reduced to a flux or pressure head condition.

Option 1: A constant or time variant groundwater level is present and the water level depth (mm) is specified by the user as a function of time When a groundwater level is given, the pressure head at the groundwater depth is exactly known ($h=0$) but no information is available regarding the flow conditions at the bottom of the soil profile. The characterisation of the bottom boundary condition proceeds as follows. Initially, the unsaturated node above the water level is considered as bottom node during the current day. Next, the pressure head at the underlaying (saturated) node ($n+1$) is calculated assuming equilibrium (zero hydraulic gradient) with the water level :

$$h_{n+1}^{j+1} = W^{j+1} - z_{n+1} \quad (2.56)$$

where W_{j+1} is the position of the groundwater level (cm) and z_{n+1} is the position of the first saturated node (cm) (z -axis is defined positive upward, $z=0$ at the surface). The foregoing means that the bottom of the unsaturated flow domain is determined by a Dirichlet condition. Further, the flow equation is solved for the unsaturated nodes (node 1 up to n). The error resulting from the assumption of zero gradient becomes negligible compared to the accuracy of the groundwater level data. Once the new pressure head profile and corresponding fluxes for the unsaturated zone have been calculated, the fluxes in the saturated compartments are calculated by assuming mass conservation for each saturated compartment. Finally, the (positive) pressure heads in the saturated zone are calculated by applying Darcy's equation, starting from node $n+1$.

Option 2 : A groundwater table is present and the flux through the bottom compartment of the soil profile is given In this case the user specifies the flux through the bottom of the soil profile for each day of the simulation period. This flux at the bottom of the soil profile is kept constant throughout a simulation day. The flow situation at the bottom of the soil profile is characterised by a Neuman boundary condition and the flow equation can be solved for all compartments in which

the soil profile has been discretized. The new position of the water table is calculated from the pressure head profile at the end of each time step.

Option 3: A groundwater table is present and a flux-ground water level relationship is available For the sandy soils in the eastern part of the Netherlands, the following relationship between the groundwater level and the discharge Q_b has been derived:

$$Q_b = a \cdot e^{bf} \quad (2.57)$$

where f is the groundwater level (m) and a , b are regression coefficients. Examples of such measurements are given by Ernst and Feddes, (1979). Also for this case the flow situation at the bottom of the soil profile is determined by a Neuman condition.

Option 4: The pressure head at the bottom of the soil profile is given In this case the pressure head is known for a nodal point outside the considered flow domain at the lower boundary of the soil profile (Dirichlet condition).

Option 5: Free drainage condition is assumed at the bottom of the soil profile When free drainage occurs, the flux through the bottom of the soil profile is always negative (=downwards) and equal to the hydraulic conductivity of the bottom compartment:

$$Q_{n+1/2} = -K_n \quad (2.58)$$

According to this assumption the pressure head at the bottom of the soil profile is constant with depth and the flow of water is only controlled by gravity. This assumption is valid for conditions of a deep water table. Furthermore, the profile depth has to be chosen such that infiltration profiles never reach the bottom. Once again a Neuman condition exists at the bottom of the soil profile. To estimate the first approximate solution of the water flow equation, the bottom flux yields:

$$Q_{n+1/2}^{j+1} = -K_n^j \quad (2.59)$$

For the successive Newton-Raphson iterations, the following expression holds:

$$Q_{n+1/2}^{j+1, \tau+1} = -K_n^{j, \tau} \quad (2.60)$$

Option 6: Zero flux through the bottom of the soil profile This boundary condition needs no further comment because the situation at the bottom of the soil profile is a typical Neuman condition.

Option 7: Lysimeter bottom boundary condition Lysimeters often have a drainage system or an outlet at the bottom, allowing free outflow

when saturation occurs at the bottom. None of the foregoing conditions apply to this special case. When a small positive pressure is build up at the bottom, water will flow out. In this case the pressure head of the bottom node ($h_{n+1/2}$) is fixed to zero (Dirichlet), as if we had a water table at the bottom. The situation is however different from a water table, because upward flow can never occur in a free draining lysimeter. Therefore, every time step it is checked whether the flux through the bottom is still negative (downward). If not, the boundary condition is specified as a zero flux condition (Neuman) instead and this condition is maintained as long as $h_{n+1/2}$ remains negative.

2.4 Modelling of the water transport in cropped soils

2.4.1 Introduction

When modelling the water balance of cropped soils crop transpiration and interception are part of the water balance. In the WAVE-model the interception capacity of the crop is input in the model. The potential transpiration rate is calculated as a fraction of the maximum potential evapotranspiration. The latter is obtained by multiplying the potential evapotranspiration of the reference crop or surface with a crop specific coefficient which varies as a function of the crop development stage (Doorenbos and Pruitt, 1977; Raes et al., 1986; Feddes, 1987). The fraction of the potential evapotranspiration allocated to the transpiration is calculated according to the leaf area index. Finally, the potential transpiration is reduced to an actual level, based on moisture conditions in the root zone.

There are two possibilities to specify crop development in the WAVE-model: (i) the leaf area and root development are specified as model input or (ii) leaf area and root growth are calculated using a crop growth model. Taking the first approach, only the water uptake mechanism in the root zone is dynamically represented in the model. Other processes are not explicitly considered in the simulated system. Hence the leaf area and rooting depth are needed as input variables to the model. Yet, when also simulating the crop development and growth, the crop system and the soil water system are completely integrated, offering a framework with many more possibilities for including feed back mechanisms of soil moisture and nutrient availability on crop development. Before describing in detail the integrated crop growth model, the canopy interception model, the transpiration model, and the macroscopic root water uptake model will be discussed at length. These models assume that the crop root length, LAI and potential evapotranspiration are simulated/measured as a function of time.

2.4.2 Crop interception

Interception can be quite considerable in crops like corn or forests. Yet, detailed data on the interception capacity as a function of development stage, for a range of crops and climate conditions are lacking. The interception capacity of water by the crop is not modelled in the WAVE-model, but specified as input. At a specified time step, the storage of water in the canopy, is calculated as the minimum of the sum of the potential precipitation and irrigation during that day and the specified potential interception capacity reduced with that water that is still stored from the previous time step. In calculating the actual transpiration (see later), the amount stored in the canopy is assumed to evaporate first. Hence, this amount is subtracted from the potential transpiration calculated with Eq. 62 (see *infra*).

2.4.3 Calculation of the potential evapotranspiration of a crop

The potential evapotranspiration of a disease free crop (ET_{crop}), grown under optimal soil water and fertility conditions is calculated in the WAVE-model by multiplying the potential evapotranspiration of a reference surface (ET_0) with a crop coefficient K_c . This procedure actually originates from irrigation science and is rather empirical. Since the rainfall surplus is one of the main driving mechanisms of transport in the soil, it is extremely important to try to correctly estimate the ET_{crop} . In this context, it should be noted that the K_c -factors used are the ones derived for a given calculation procedure of the potential evapotranspiration for a specific reference surface. The K_c -value varies throughout the growing season and its value depend on the crop development stage and the climatic conditions.

When the Penman equation is used to calculate potential evapotranspiration with grass as a reference surface, the K_c -factors of Doorenbos and Pruitt (1977) can be used to estimate ET_{crop} . In the approach of Doorenbos and Pruitt, the growing season is subdivided into 4 stages: the initial, the crop development, the mid-season and the late season stage (see Fig. 10). For bare soil conditions, or if the crop ground cover is less than 10 perc, evapotranspiration is mainly controlled by the moisture content in the top soil. The soil evaporation decreases as the soil dries. This effect is accounted for in the approach of Doorenbos and Pruitt by assuming a small value for K_c . Since the reduction of the evaporation is accounted for when solving the water flow equation, a K_c -factor of 1 should be used during the crop initial stages (from germination until the ground cover index is equal to 10 perc). During mid-season (from effective full ground cover until start of maturing) and at maturity K_c -values as reported in Tables 2 and 3 are recommended to calculate the potential crop evapotranspiration, if grass is the reference surface. The value of the K_c -factor for the crop development phase (end of initial stage until attainment of effective full ground cover) is obtained by linear interpolation between the K_c -factor of the initial stage (which is mostly equal to 1.0) and the K_c -factor of the crop mid-season stage. The K_c -factor of the late-season

stage (end of mid-season, until attainment of crop maturity) is obtained by linear interpolation between the mid-season and maturity Kc-value. The assumed Kc-development is given in Fig. 10.

Table 2: Kc-factors during the mid-season stage for different crop and different prevailing climatic conditions according Doorenbos and Pruitt (1977). The value of the Kc-factor is related to ET0 with grass as a reference surface

Table 3: Kc-factors at the end of the late-season stage for different crop and different prevailing climatic conditions according Doorenbos and Pruitt (1977). The values of the Kc-factor is related to ET0 with grass as a reference surface

Fig. 10: Time course of the crop Kc-factor as standard used in the WAVE-model

As an alternative to the Doorenbos and Pruitt approach, one can also use tabular Kc-values. The tables 4 and 5 list monthly Kc-values for a few crops under Dutch conditions. Table 4 gives crop factors to be used in combination with open water evaporation (reference surface = water).

Table 4: Crop factors as related to the Penman open water evaporation equation, for different crops and different decades during the crop season (source: Feddes (1987))

The aerodynamic term in the Penman formula is badly defined. Therefore, more simple but empirical approaches are often used (Makkink, 1957; Priestly and Taylor, 1972). When using the Makkink formula for calculating ET0 of a grass reference surface, the Kc-factors as reported in Table 5 should be used.

Table 5: Crop factors as related to the Makkink reference crop evapotranspiration for grass, for different crops and different decades during the crop season (source: Feddes (1987))

2.4.4 Estimation of the potential transpiration and evaporation

The potential transpiration and evaporation are obtained by splitting the potential crop evapotranspiration, using the LAI as division parameter:

$$\begin{aligned} E_p &= f \cdot e^{-c \cdot LAI} \cdot ET_{crop} \\ T_p &= ET_{crop} - E_p - \frac{CanStor}{1day} \end{aligned} \quad (2.61)$$

where E_p is the potential soil evaporation (mm day⁻¹); T_p is the potential crop transpiration (mm day⁻¹); ET_{crop} is the potential evapotranspiration (mm day⁻¹); CanStor, the amount of water which has been intercepted and is now released from the crop canopy (mm), and f, c are crop specific parameters (-). In the WAVE-model, the f is set fixed to 1 and c equal to 0.6. Eq. (62) implies that, if interception has occurred during the previous day, this water is allowed to evaporate fully during the current day. Furthermore, transpiration only starts after all intercepted water has been evaporated. The sum of soil evaporation, evaporated interception water and transpiration can of course not exceed the ET_{crop} .

2.5 Description of the root water uptake

Water uptake by roots is the result of a complex process which is controlled by soil, plant and atmospheric conditions. To simplify the description of the root water uptake, Feddes et al. (1978) introduced the maximal root water uptake rate as a function of depth $S_{max}(z)$ (day⁻¹). In the WAVE-model the relation $S_{max}(z)$ with depth is input. Note that this relation summarizes the influence of both crop and soil on root water uptake. A compilation of literature data for the $S_{max}(z)$ functions, for cereals and grass, is given by Diels (1994), and is depicted in the Figs. 11 and 12.

Fig. 11: Maximum root extraction rates for cereals as a function of depth. The symbols represent literature data from field experiments with wheat (from Ehlers (1976); + from Gregory et al.(1978); \downarrow from Strebel(1978)) and barley (x from Maul and Chanasyk (1986); D from McGowan et al.(1980)). The solid lines represent extreme curves and a reference curve halfway between both extreme curves

Fig 12: Maximum root extraction rate for grass as a function of depth. The symbols represent literature data from laboratory experiments (from Belmans (1979); \downarrow tropical grass data from Badji (1984)) and a field experiment (+ from Flhler et al.(1975)). The solid lines represent extreme curves and a reference curve halfway between both extreme curves

As can be observed from the Figs.11 and 12, an exponential or linear function could be adopted to describe $S_{max}(z)$. In the WAVE-model, the linear function is available :

$$S_{max}(z) = A - Bz \quad (2.62)$$

where A (day⁻¹), and B (day⁻¹ mm⁻¹) are model input parameters. Alternatively one can input S_{max} -values for each soil compartment separately. Water uptake is strongly reduced at high pressure head values, near saturation, due to anaerobiosis, and at low pressure heads, due to moisture stress. This phenomenon is described in the WAVE-model by specifying the dimensionless reduction function $\alpha(h)$, which reduces the maximum extraction rate according:

$$S(z, h) = \alpha(h)S_{max}(z) \quad (2.63)$$

The $\alpha(h)$ in the WAVE-model is characterized by the pressure head values h_0 , h_1 , h_2 , and h_3 (cm) (Fig.13). When the pressure head in the soil exceeds h_0 (near saturation), water uptake ceases due to lack of oxygen in the root system. Between, h_1 and h_2 , water uptake is optimal ($a=1$). Below h_3 , water uptake stops due to drought stress. The $a(h)$ -function between h_2 and h_3 can be selected to be linear or hyperbolic. The parameters h_2 and h_3 are less sensitive if drainage calculations are of concern (Diels, 1994). The wilting point value ($h_3 = -16000$ cm, $pF = 4.2$) is often taken as a lower limit for the $a(h)$ curve, while h_2 often is set equal to -500 cm. The values of h_0 and h_1 , reflecting anaerobiosis, should be selected with caution. Bakker et al. (1987) presented O_2 -diffusion coefficients of different soils at different air contents. Minimal air contents necessary for a minimal oxygen diffusion ranged between 0.03 - 0.10 m^3 m^{-3} . This corresponds to pressure head values ranging between 20 and 200 cm. The h_0 , and h_1 values should be selected in these ranges.

Fig. 13: General shape of the dimensionless sink term variable a expressed in terms of pressure head (left) and pF (right). Both a linear (top) and hyperbolic (bottom) decrease of $a(h)$ below the threshold pressure head h_2 are depicted. Curve 1 and 2 are the curves for low and high atmospheric demand, respectively. h_0 : threshold pressure head (cm) above which uptake ceases due to anaerobiosis; h_1 : threshold pressure head below which water uptake is not reduced; h_{2l} : threshold pressure head below which water uptake decreases (linearly or hyperbolically) for low atmospheric demand; h_{2h} : threshold pressure head below which water uptake decrease (linearly or hyperbolically) for high atmospheric demand; h_3 : threshold pressure head below which water uptake ceases due to wilting

The $\alpha(h)$ -factor which expresses the effect of pressure head on the root water uptake, is insufficient to describe actual root water uptake. It is still necessary to specify at which depths water will be extracted. Several experiments have shown that water is preferentially extracted near the soil surface. Only when moisture stress occurs is water extracted at larger depths. In the root extraction model of Hoogland et al. (1980) a similar process is mimicked by integrating the root water uptake term from the soil surface to an increasing depth z less or equal to the rooting depth L_r , until the integral becomes equal to the potential transpiration rate. If the integration over the complete rooting depth is insufficient to explain the potential transpiration rate, water stress is considered to occur and the actual transpiration rate is set equal to the integral of $S(h,z)$ over the rooting depth. This concept is written as:

$$T_a = \int_0^{z < L_r} S(h, z) dz \leq T_p \quad (2.64)$$

where T_a is the actual transpiration rate (mm day^{-1}); T_p is the potential transpiration rate (mm day^{-1}); and L_r is the rooting depth (mm). Finally, the root water uptake in each soil compartment is accounted for in the soil water flow equation by adding Eq.(64) to the right hand side of the

flow equation.

Effects of root senescence or severe moisture stress on root water uptake, is simulated in the WAVE-model by specifying an inactivity zone near the surface where the root water uptake is set equal to zero. The date when the roots start to show inactivity and a date when maximum inactivity is reached, is input. In between these dates, the inactivity zone expands linearly with depth, from 0 until a specified depth.

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Chapter 3

The solute transport module

3.1 Introduction

The water transport in soils imposes a convective motion on solutes. Local variations in water flow velocity, induces dispersion of the solute plume during transport. Chemical diffusion, induced by concentration gradients, causes a similar effect. Chemical and physical interactions between solute and soil matrix can retard the overall solute transport. The transfer of solutes is further dispersed by plant uptake and biological transformations. Those processes in turn are strongly controlled by soil temperature and moisture. As a consequence, the transfer of solutes in the soil system is a highly variable and unsteady process.

Before discussing the processes controlling the transfer of solutes in soils, it is relevant to define what is meant by a solute in this context. A solution is a mixture of water and constituents of various chemical composition, which are partially or completely soluble in the soil water phase (De Marsily, 1986). Components in the water phase are normally ionized in proportion to the ionic charge of the element. However, dissolved substances can also be present in an electrically neutral chemical form or aggregated with other molecules and/or ions to form complex substances. Furthermore, it has been observed that salts, considered to be insoluble, can move in a dissolved state as tracers. In the same way, constituents in the form of large molecular aggregates such as colloids, might be present in the soil and move with the liquid phase. All the substances which, in one way or another form part of the soil fluidum, are known as soil solutes as long as they are not part of a mobile phase distinct from the transporting fluid. For many chemical substances on the other hand, a complete mixture with the soil water system does not exist. As such, the transport of many organics is closely related to multiphase flow. In this case processes like volatility, immiscibility and hydrophobicity may complicate the

description of the fate of the chemical compound.

The transport of a decaying and sorbing solute in field soils is described numerically with the solute transport module of the WAVE-model. The included solute transport equation is defined in a macroscopic way, indicating that the state variables (e.g. solute concentration) and material characteristics (e.g. soil transport volume) are defined as averages over a Representative Elementary Volume (REV) (Bear, 1972). The developed solute transport model is referred to as the two component or two region convection dispersion model. The model assumes the existence of immobile or stagnant soil water regions, situated at the intra-aggregate or dead end pores and mobile soil water regions. When considering two regions, no complete mixing of the solute in the soil water phase is assumed but rather a solute exchange, which is diffusion limited, controls solute exchange between both soil regions. Transport in the two component medium is described with a couple of equations. For the mobile soil region the convection-dispersion equation holds. In both regions adsorption is assumed to occur reversibly and linearly. Although the theoretical framework for describing the solute transport phenomena at field scale is still in development, a deterministic point model like the two component model which is developed at the laboratory scale, can be used with variable success to describe solute transport under field conditions.

3.2 The soil solute transport equation

Figure 14 illustrates the conceptualisation of the soil system when developing the solute transport equation. Distinction is made between the soil volume occupied by air, the mobile soil water region, the immobile soil water region, the static soil complex defined as the soil complex with adsorption sites in contact with the immobile soil region and the dynamic soil complex with sorption sites in contact with the mobile soil region.

Fig. 14: Conceptualisation of the soil system (after van Genuchten and Wierenga, 1976)

First the solute transport in the mobile soil region is discussed. Transport of solute in the mobile soil region is determined by chemical diffusion, convection and hydrodynamic dispersion. The term diffusion refers to the movement of solute as a result of Brownian motion. The thermal energy causes the particles to move randomly in the phase that contains them. Given a mass of solute in a stagnant water reservoir, then the diffusion flux in water q_{dl} ($\text{kg m}^{-2} \text{ day}^{-1}$) can be defined as the (macroscopic) solute mass going through a unit area across the water reservoir per unit of time. Fick's first law can be used to relate solute flux and concentration gradient:

$$q_{dl} = -Dif \cdot \frac{\partial C_m}{\partial x} \quad (3.1)$$

where C is the soil solute concentration (kg m^{-3}); x is the space co-ordinate (m); and Dif is the chemical diffusion coefficient of the considered solute

in pure water (m² day⁻¹). When solute moves by diffusion in the water phase of the soil, the cross sectional area available for diffusion is only a fraction of the total cross sectional area. Due to the tortuous nature of the pores, the diffusion process results in a slower macroscopic vertical spreading than in a pure water system. For this reason an effective diffusion coefficient, D_e (Dif) (m² day⁻¹), which depends on the mobile soil water content, θ_m (m³ m⁻³), is used to describe diffusive solute transport in the mobile soil region:

$$q_{ds} = -D_e \cdot \theta_m \cdot \frac{\partial C_m}{\partial x} \quad (3.2)$$

where q_{ds} is the diffusional solute flux in the soil mobile region (kg m⁻² day⁻¹).

The value of D_e can be estimated by the equation of Kemper and Van Schaik (1966):

$$D_e = \frac{Dif \cdot a \cdot e^{b \cdot \theta_m}}{\theta_m} \quad (3.3)$$

where a and b are empirical constants reported to be approximately $b = 10$ and $0.005 \leq a \leq 0.01$ (Olsen and Kemper, 1968). The chemical diffusion coefficient in pure water, Dif , and the parameters a and b are model input. The term convection refers to the phenomenon where dissolved substances are carried along by the movement of water. Solutes that are carried by the moving water are said to undergo convective, viscous, or mass flow. As such, mass flow is perfectly related to the law determining the transport of water and which was described in a previous chapter of this reference manual. Hence, the convective solute flux going through a unit area equals:

$$q_{cw} = C_m \cdot \theta_m \cdot V_m = C_m \cdot q_w \quad (3.4)$$

where q_{cw} is the convective solute flux density (kg m⁻² day⁻¹) imposed by the convective water flow; q_w is the Darcian water flux (m³ m⁻² day⁻¹); V_m is the average macroscopic pore water velocity (m day⁻¹); and C_m is the solute concentration in the mobile soil region (kg m⁻³). Owing to the porous nature of the soil, the microscopic pore velocity in the mobile soil region is not equal to macroscopic pore water velocity. The microscopic pore velocity is distributed around the average macroscopic value, in a manner that depends on the pore size and shape. Flow in larger pores is faster than in the small ones and is much faster at the center of a pore than near the periphery. In this way the complexity of the pore system causes mixing of the soil solution along the flow direction, and hence dispersion of the solute. This phenomenon, often referred to as mechanical dispersion is induced by randomly distributed pore velocities and results in a net flow of solute proportional to the velocity. On the basis of the assumption of randomness, one can describe mechanical dispersion in a similar way as chemical diffusion using Fick's law with the diffusion coefficient D_e or Dif replaced by a mechanical dispersion coefficient, denoted D_m (m² day⁻¹). The latter is assumed to be proportional to the effective average macroscopic pore water velocity:

$$D_m = \lambda \cdot V_m \quad (3.5)$$

where λ (m) is the soil solute dispersivity.

The total macroscopic convective transport of a solute in the mobile soil region is described commonly with an equation that takes into account two modes or components of transport: (i) the average flow velocity component (given by Eq. (69)) and (ii) the mechanical dispersion component (Fick's law with D_m). Adding the two components together yields the total convective flux equation, q_{ct} (kg m⁻² day⁻¹):

$$q_{ct} = \theta_m \cdot C_m \cdot V_m + \theta_m \cdot \lambda \cdot V_m \cdot \frac{\partial C_m}{\partial x} \quad (3.6)$$

By adding the diffusive flux (Eq.(67)) to the convective flux (Eq.(71)), a relation is obtained for the total solute flux travelling along the mobile soil region, q_{tm} (kg m⁻² day⁻¹):

$$q_{tm} = q_{ds} + q_{ct} = -\theta_m \cdot (D_e + D_m) \frac{\partial C_m}{\partial x} + V_m \cdot \theta_m \cdot C_m \quad (3.7)$$

At high flow velocities, or when considerable heterogeneity occurs, the dispersion term is much larger than the diffusion term and Eq.(72) simplifies to:

$$q_{tm} = -\theta_m \cdot D_m^* \frac{\partial C_m}{\partial x} + V_m \cdot \theta_m \cdot C_m \quad (3.8)$$

where D_m^* is the apparent diffusion coefficient in the mobile soil region (m² day⁻¹). Table 6 reports on literature values for pore water velocities, apparent dispersion coefficients, dispersivities, and mobile water contents for undisturbed partially saturated soil.

Table 6: Literature review of solute transport parameters. Values between brackets represent possible ranges (Beven et al., 1993)

When a solute is adsorbed, then the total solute mass in a unit soil volume equals the sum of the mass dissolved in the soil solution phase and the mass adsorbed on the soil complex. Both are related according to the equation:

$$C_m = f \cdot \rho \cdot C_{sm} + \theta_m \cdot C_m \quad (3.9)$$

where C_m is the total solute mass in the mobile region (kg solute m⁻³ dry soil); C_{sm} is the adsorbed solute mass on the soil complex (kg kg⁻¹ dry soil); ρ is the soil bulk density (kg m⁻³); and f is the fraction of the adsorption sites situated in contact with the mobile soil region (-). For linear and reversible adsorbing species, the distribution constant is used to relate solute in the soil solution and on the sorption sites or:

$$C_{sm} = k_d \cdot C_m \quad (3.10)$$

where k_d is the solute distribution constant (m³ kg⁻¹). Hence Eq. (74) simplifies to:

$$C_{tm} = C_m \cdot (\theta_m + f \cdot \rho \cdot k_d) \quad (3.11)$$

The parameters f , k_d and ρ are model input. Reasonable simulations can be obtained if all sorption sites are assumed to be situated in the mobile soil region ($f = 1$). The distribution constants k_d can be derived from batch sorption experiments or the analysis of breakthrough curve data. The latter method should be preferred, since it enables to identify retardation parameters on undisturbed, scale independent, soil samples. For pesticides, the k_{oc} approach is often used. If this is the case, the k_d value is obtained by multiplying k_{oc} with the fraction of organic carbon. Literature data of different k_{oc} and k_d values are extensively reviewed by Montgomery et al., 1993.

So far, no interaction between the mobile and the immobile soil region was considered. If however diffusion between both soil regions occur, then this diffusion solute flux, q_{fl} (kg m⁻³ day⁻¹) is proportional to the solute concentration difference:

$$q_{fl} = \alpha^* \cdot (C_m - C_{im}) \quad (3.12)$$

where α^* is an empirical transfer coefficient (day⁻¹); and C_{im} is the solute concentration in the immobile soil region (kg m⁻³ solution).

The continuity equation for the solute in the soil mobile region, for an infinitesimal small volume of soil is written as:

$$\frac{C_{tm}}{\partial t} = \frac{q_{tm}}{\partial x} + q_{fl} \quad (3.13)$$

In combination with Eqs. (73,76,77), Eq. (78) reduces to the solute transport equation for the mobile soil region:

Similarly, mass conservation in the immobile soil region yields:

$$\begin{aligned} \frac{\partial(\theta_m C_m)}{\partial t} + \frac{\partial(f \cdot \rho \cdot k_d \cdot C_m)}{\partial t} &= \frac{\partial}{\partial x} \left(\theta_m \cdot D_m^* \frac{\partial C_m}{\partial x} \right) - \frac{\partial(q_w \cdot c_m)}{\partial x} + \alpha^* (C_m - C_{im}) \\ \frac{\partial(\theta_{im} \cdot C_{im})}{\partial t} + (1 - f) \cdot \rho \cdot k_d \frac{\partial C_{im}}{\partial t} &= -\alpha^* (C_m - C_{im}) \end{aligned} \quad (3.14)$$

When no immobile water is present, then Eq.(79) simplifies to the classical convection dispersion equation (Warrick et al., 1971; Bresler, 1972).

3.3 Numerical solution of the solute transport equation

3.3.1 The solution Procedure

In order to solve Eqs. (79) and (80) by finite difference technique, the same time and space discretisation as for the water flow equation is adopted. The following parameters and state variables are initialised for each soil compartment: the soil moisture content (q); the soil pore water velocity

(Vm); the soil bulk density (ρ); the chemical diffusion parameters (Dif, a, b); the hydrodynamic dispersivity (l); the ratio mobile versus total moisture content (qm/q); the transfer coefficient between the mobile and the immobile soil region (a^*); the mass distribution coefficient (kd) and the fraction of the sorption sites in the mobile or immobile soil region (f).

The solute transport equations (Eqs.(79) and (80)) are expanded in finite difference formulations. To ensure convergence and to minimise numerical dispersion, a Crank Nicolson numerical scheme is used to solve the transport equation in the mobile soil region. Second order terms are included in the discretisation scheme. Full details of the discretization scheme are given in Tillotson et al. (1980). Expanding the first term of Eq. (79) yields:

where i denotes the space index from the i -th compartment; and j the time index. The second term of Eq.(79), the adsorption term, is discretised as follows:

$$f_i \cdot \rho_i \cdot kd_i \left(\frac{C_{m_i}^{j+1} - C_{m_i}^j}{\Delta t} \right) \quad (3.17)$$

The term containing the apparent diffusion coefficient is developed according to:

$$\frac{D_{m_{i-1/2}}^{j+1/2} \theta_{m_{i-1/2}}^{j+1/2}}{2 \cdot \Delta z^2} \cdot (C_{m_{i-1}}^{j+1} + C_{m_{i-1}}^j - C_{m_i}^{j+1} - C_{m_i}^j) - \frac{D_{m_{i+1/2}}^{j+1/2} \theta_{m_{i+1/2}}^{j+1/2}}{2 \cdot \Delta z^2} \cdot (C_{m_i}^{j+1} + C_{m_i}^j - C_{m_{i+1}}^{j+1} - C_{m_{i+1}}^j) \quad (3.18)$$

while expansion of the convection term results in:

$$\begin{aligned} & -\beta_1 \frac{q_{w_{i-1/2}}^{j+1/2}}{2\Delta x} (C_{m_{i+1}}^j + C_{m_{i-1}}^{j+1}) + \beta_2 \frac{q_{w_{i+1/2}}^{j+1/2}}{2\Delta x} (C_{m_i}^j + C_{m_i}^{j+1}) \\ & -\beta_3 \frac{q_{w_{i+1/2}}^{j+1/2}}{2\Delta x} (C_{m_{i+1}}^j + C_{m_{i-1}}^{j+1}) + \beta_4 \frac{q_{w_{i-1/2}}^{j+1/2}}{2\Delta x} (C_{m_i}^j + C_{m_i}^{j+1}) \end{aligned} \quad (3.19)$$

If the flux in the i -th compartment is negative, then $\beta_1 = 1$ and $\beta_4 = 0$. If, however, this flux is positive, then $\beta_1 = 0$ and $\beta_4 = 1$. A positive flux in the $i+1$ -th compartment results in $\beta_3 = 1$ and $\beta_2 = 0$; while the opposite results in $\beta_3 = 0$ and $\beta_2 = 1$. Defining the following variables:

$$\begin{aligned}
AB_i &= \frac{D_{m_{i-1/2}}^{j+1/2} \cdot \theta_{m_{i-1/2}}^{j+1/2}}{2\Delta x^2} + \frac{\Delta t \cdot V_{m_i}^{j+1/2} \cdot V_{m_{i-1/2}}^{j+1/2} (\theta_{m_i}^{j+1} - \theta_{m_i}^j)}{16\Delta x^2} \\
BB_i &= \frac{D_{m_{i+1/2}}^{j+1/2} \cdot \theta_{m_{i+1/2}}^{j+1/2}}{2\Delta x^2} + \frac{\Delta t \cdot V_{m_i}^{j+1/2} \cdot V_{m_{i+1/2}}^{j+1/2} (\theta_{m_i}^{j+1} - \theta_{m_i}^j)}{16\Delta x^2} \\
CB_i &= \frac{q_{w_{i-1/2}}^{j+1/2}}{2\Delta x} \\
DB_i &= \frac{q_{w_{i+1/2}}^{j+1/2}}{2\Delta x}
\end{aligned} \tag{3.20}$$

$$\begin{aligned}
AB_i &= \frac{D_{m_{i-1/2}}^{j+1/2} \cdot \theta_{m_{i-1/2}}^{j+1/2}}{2\Delta x^2} + \frac{\Delta t \cdot V_{m_i}^{j+1/2} \cdot V_{m_{i-1/2}}^{j+1/2} (\theta_{m_i}^{j+1} - \theta_{m_i}^j)}{16\Delta x^2} \\
BB_i &= \frac{D_{m_{i+1/2}}^{j+1/2} \cdot \theta_{m_{i+1/2}}^{j+1/2}}{2\Delta x^2} + \frac{\Delta t \cdot V_{m_i}^{j+1/2} \cdot V_{m_{i+1/2}}^{j+1/2} (\theta_{m_i}^{j+1} - \theta_{m_i}^j)}{16\Delta x^2} \\
CB_i &= \frac{q_{w_{i-1/2}}^{j+1/2}}{2\Delta x} \\
DB_i &= \frac{q_{w_{i+1/2}}^{j+1/2}}{2\Delta x}
\end{aligned} \tag{3.21}$$

and substituting, yields the finite difference analogue of Eq.(79):

$$\begin{aligned}
&\frac{\theta_{m_i}^{j+1} C_{m_i}^{j+1} - \theta_{m_i}^j C_{m_i}^j}{\Delta t} - AB_i (C_{m_{i-1}}^{j+1} + C_{m_{i-1}}^j - C_{m_i}^{j+1} - C_{m_i}^j) \\
&+ BB_i (C_{m_i}^{j+1} + C_{m_i}^j - C_{m_{i+1}}^{j+1} - C_{m_{i+1}}^j) + f_i \cdot \rho_i \cdot k_{di} \left(\frac{C_{m_i}^{j+1} - C_{m_i}^j}{\Delta t} \right) \\
&= -\beta_1 \cdot CB_i (C_{m_{i-1}}^j + C_{m_{i-1}}^{j+1}) + \beta_2 \cdot DB_i (C_{m_i}^j + C_{m_i}^{j+1}) \\
&+ \beta_3 \cdot DB_i (C_{m_{i+1}}^j + C_{m_{i+1}}^{j+1}) - \beta_4 \cdot CB_i (C_{m_i}^j + C_{m_i}^{j+1}) - \alpha^* (C_{m_i}^j - C_{m_i}^{j+1})
\end{aligned} \tag{3.22}$$

Rearranging the terms in Eq.(86) yields the following equation:

$$AL_i \cdot C_{m_{i-1}}^{j+1} + BL_i \cdot C_{m_i}^{j+1} + CL_i \cdot C_{m_{i+1}}^{j+1} = DL_i \tag{3.23}$$

where:

$$\begin{aligned}
AL_i &= -AB_i + \beta_1 \cdot CB_i \\
BL_i &= \frac{\theta_{m_i}^{j+1}}{\Delta t} + AB_i + BB_i + \frac{f_i \cdot \rho_i k_{di}}{\Delta t} - \beta_2 \cdot DB_i + \beta_4 \cdot CD_i \\
CL_i &= -BB_i - \beta_3 \cdot DB_i \\
DL_i &= C_{m_{i-1}}^j (AB_i - \beta_1 \cdot CB_i) + C_{m_i}^j \left(\frac{\theta_{m_i}^{j+1}}{\Delta t} - AB_i - BB_i + \beta_2 \cdot DB_i - \beta_4 \cdot CD_i \right) \\
&+ C_{m_{i+1}}^j (BB_i + \beta_3 \cdot DB_i) + \alpha^* (C_{m_i}^j - C_{m_i}^{j+1})
\end{aligned}$$

Equation (87) is easily derived for each node except for the top and bottom node. Two similar equations are derived when expanding the top and bottom boundary transport equation. For the top node, the following expression holds:

$$BL_1 \cdot C_{m_1}^{j+1} + CL_1 \cdot C_{m_2}^{j+1} = DL_1 \tag{3.26}$$

while for the bottom node the equation yields:

$$AL_n \cdot C_{m_{n-1}}^{j+1} + BL_n \cdot C_{m_n}^{j+1} = DL_n \tag{3.27}$$

So, for n equations with n unknowns, it is possible to obtain the concentration for each node on the $j+1$ -th time step. The unknown vector is found by solving Eqs. (87, 89, 90) simultaneously using the Thomas algorithm (Remson et al., 1978). Writing Eqs. (87, 89, 90) in matrix format yields:

$$(3.28) \quad \begin{pmatrix} BL_1 & CL_1 & & & \\ AL_2 & BL_2 & CL_2 & & \\ & AL_3 & BL_3 & CL_3 & \\ & & & & AL_{n-1} & BL_{n-1} & CL_{n-1} \\ & & & & & AL_n & BL_n \end{pmatrix} \cdot \begin{pmatrix} C_{m_1}^{j+1} \\ C_{m_2}^{j+1} \\ C_{m_3}^{j+1} \\ \\ C_{m_{n-1}}^{j+1} \\ C_{m_n}^{j+1} \end{pmatrix} = \begin{pmatrix} DL_1 \\ DL_2 \\ DL_3 \\ \\ DL_{n-1} \\ DL_n \end{pmatrix}$$

The coefficient matrix is tri-diagonal. Hence, the unknown vector $(C_{m_1}^{j+1}, C_{m_2}^{j+1}, \dots, C_{m_n}^{j+1})$ can be obtained, using the Thomas algorithm.

In addition to the solution of the transport equation in the mobile soil region, the mass balance equation in the immobile soil region Eq.(80) is solved explicitly. Defining g as:

$$g = \theta_{im} + (1 - f) \cdot \rho \cdot k_d \quad (3.29)$$

and substituting, reduces Eq.(80) to:

$$\frac{\partial(g \cdot C_{im})}{\partial t} = -\alpha^* (C_m - C_{im}) \quad (3.30)$$

Expanding the left-hand side of Eq.(93) in a Taylor series and ignoring the higher order terms yields:

$$\frac{\partial(g \cdot C_{im})}{\partial t} = \frac{g \cdot C_{im_i}^{j+1} - g \cdot C_{im_i}^j}{\Delta t} - \frac{\Delta t \cdot \partial^2(g \cdot C_{im})}{2 \cdot \partial t^2} \quad (3.31)$$

The expansion of the second order term in Eq.(94) yields:

$$\frac{\partial(g \cdot C_{im})}{\partial t} = \frac{\partial}{\partial t}(-\alpha^* (C_m - C_{im})) = \frac{-\alpha^* \cdot C_{m_i}^{j+1} + \alpha^* \cdot C_{m_i}^j}{\Delta t} + \frac{\alpha^* \cdot C_{im_i}^{j+1} - \alpha^* \cdot C_{im_i}^j}{\Delta t} \quad (3.32)$$

Substituting Eq. (95) into (94) and (93) and rearranging, the mass balance equation for the immobile soil region becomes:

$$AG_i \cdot C_{im_i}^{j+1} = BG_i \cdot C_{im_i}^j + \frac{\alpha^* \cdot C_{m_i}^{j+1}}{2} + \frac{\alpha^* \cdot C_{m_i}^j}{2} \quad (3.33)$$

where:

$$AG_i = \frac{\theta_{im_i}^{j+1}}{\Delta t} + \frac{(1 - f_i) \cdot \rho_i \cdot k_{di}}{\Delta t} + \frac{\alpha_i^*}{2} \quad (3.34)$$

$$BG_i = \frac{\theta_{im_i}^j}{\Delta t} + \frac{(1 - f_i) \cdot \rho_i \cdot k_{di}}{\Delta t} + \frac{\alpha_i^*}{2} \quad (3.35)$$

Notwithstanding the use of an implicit numerical scheme and keeping second order terms in the finite difference analogue, numerical dispersion influences model calculations. Numerical dispersion increases when the compartment size increases. To quantify the impact of numerical dispersion, the development of a solute plume was calculated with the numerical model, given a pulse type top boundary condition and a steady-state water flow condition. Solute resident concentrations predicted by the model were used to fit an analytical solution of the transport equations through it. The solution proposed by van Genuchten and Alves (1982) was used. The optimised apparent diffusion coefficient was compared with the model input dispersivity times the simulated pore water velocity. This comparison yielded a linear relationship, with a slope close to one and intercept equal to 0.13 times the compartment size. This intercept is a measure of the induced numerical dispersion. A standard correction on the apparent dispersion constant in the WAVE-model has been made according to these results.

3.3.2 Definition of the Upper boundary condition

To solve the solute transport equation, an additional numerical equation, similar to Eq.(86), needs to be defined for the top node. A flux type boundary condition is used to define the top boundary in the WAVE-model.

$$\begin{aligned} \text{infiltration : } q_w < 0 : J_s &= C_f \cdot q_w \\ \text{evaporation : } q_w > 0 : J_s &= 0 \end{aligned} \quad (3.36)$$

where C_f equals the solute flux concentration (kg m-3) and J_s the solute mass flux (kg m-2 s-1). To define C_f , an artificial solute mass reservoir is assumed to exist outside the soil profile. When solute is applied (with a fertilisation or irrigation event), it dissolves in the mass of water entering the profile during the day of solute application (or the first day when infiltration occurs). Hence, the solute mass flux J_s is determined by the water flow across the soil surface, filling or depleting the hypothetical reservoir. During infiltration, solute mass enters only the mobile soil region. Assuming zero dispersion in the hypothetical reservoir, the solute concentration at the soil surface is set equal to $C_f = J_s/q_w = C_s$. In case of evaporation, the solute concentration at the soil surface equals zero ($C_f = C_s = 0$). Taking into account above considerations, the finite difference equation for the soil mobile region at the top becomes:

$$\begin{aligned}
C_{m_1}^{j+1} & \left(\frac{\theta_{m_1}^{j+1}}{\Delta t} + AB_1 + BB_1 + \frac{f_1 \cdot \rho_1 \cdot k_{d1}}{\Delta t} - \beta_2 \cdot DB_1 + \beta_4 \cdot CB_1 \right) \\
& + C_{m_2}^{j+1}(-BB_1 - \beta_3 \cdot DB_1) = \\
& C_s^j(AB_1 - \beta_1 \cdot CB_1) - C_s^{j+1}(AB_1 + \beta_1 \cdot CB_1) \quad (3.37) \\
C_{m_1}^j & \left(\frac{\theta_{m_1}^{j+1}}{\Delta t} - AB_1 - BB_1 + \frac{f_1 \cdot \rho_1 \cdot k_{d1}}{\Delta t} + \beta_2 \cdot DB_1 - \beta_4 \cdot CB_1 \right) \\
& + C_{m_2}^j(BB_1 + \beta_3 \cdot DB_1)
\end{aligned}$$

with

$$\begin{aligned}
AB_1 &= \frac{\Delta t \cdot V_{m_1}^{j+1/2} \cdot q_{w1-1/2}^{j+1/2} \cdot (\theta_{m_1}^{j+1} - \theta_{m_1}^j)}{16\Delta x^2} \quad (3.38) \\
BB_1 &= \frac{\Delta t \cdot V_{m_1}^j \cdot V_{m_1+1/2}^{j+1/2} \cdot (\theta_{m_1}^{j+1} - \theta_{m_1}^j)}{16\Delta x^2} \\
CB_1 &= \frac{q_{w1-1/2}^{j+1/2}}{2\Delta x} \\
DB_1 &= \frac{q_{w1+1/2}^{j+1/2}}{2\Delta x} \quad (3.39)
\end{aligned}$$

and which can be rearranged to:

$$BL_1 \cdot C_{m_1}^{j+1} + CL_1 \cdot C_{m_2}^{j+1} = DL_1 \quad (3.40)$$

3.3.3 Definition of the lower boundary condition

In the WAVE-model, a zero concentration gradient at the bottom of the flow domain is considered:

$$\left. \frac{\partial C_m}{\partial x} \right|_{x=L} = 0 \quad (3.41)$$

In discretised form, the bottom boundary condition definition is defined as:

$$C_{m_{n+1}}^{j+1} = C_{m_n}^{j+1} \quad (3.42)$$

Using Eq.(103) the finite difference scheme for the lower boundary node becomes:

$$\begin{aligned}
C_{m_n}^{j+1} & \left(\frac{\theta_{m_n}^{j+1}}{\Delta t} + AB_n + BB_n + \frac{f_n \cdot \rho_n \cdot k_{dn}}{\Delta t} - \beta_2 \cdot DB_n + \beta_4 \cdot CB_n \right) \\
& + C_{m_{n-1}}^{j+1}(-AB_n - \beta_2 \cdot CB_n) = \\
C_{m_n}^j & \left(\frac{\theta_{m_n}^{j+1}}{\Delta t} - AB_n - BB_n + \frac{f_n \cdot \rho_n \cdot k_{dn}}{\Delta t} + (\beta_2 + \beta_3) \cdot DB_n - \beta_4 \cdot CB_n \right) \\
& + C_{m_{n-1}}^j(AB_n - \beta_1 \cdot CB_n) \quad (3.43)
\end{aligned}$$

with

$$\begin{aligned}
 AB_n &= \frac{D_{m_{n-1/2}}^{j+1/2} \cdot \theta_{m_{n-1/2}}^{j+1/2}}{2\Delta x^2} + \frac{\Delta t \cdot V_{m_n}^{j+1/2} \cdot V_{m_{n-1/2}}^{j+1/2} \cdot (\theta_{m_n}^{j+1} - \theta_{m_n}^j)}{16\Delta x^2} \\
 BB_n &= \frac{\Delta t \cdot V_{m_n}^{j+1/2} \cdot V_{m_{n+1/2}}^{j+1/2} \cdot (\theta_{m_n}^{j+1} - \theta_{m_n}^j)}{16\Delta x^2} \\
 CB_n &= \frac{q_{w_{n-1/2}}^{j+1/2}}{2\Delta x} \\
 DB_n &= \frac{q_{w_{n+1/2}}^{j+1/2}}{2\Delta x}
 \end{aligned} \tag{3.45}$$

3.4 References

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Chapter 4

The heat transport module

4.1 Introduction

Most soil biological and bio-chemical processes are influenced by soil temperature. Processes like nitrogen mineralisation e.g., occur at an optimal rate in optimal temperature conditions. The correct assessment of these processes therefore involves a correct description of the soil temperature. Heat flow in the WAVE-model is simulated one-dimensionally. The heat flow module is similar to the model of Tillotson et al. (1980) and Wagenet and Hutson (1989). The calculation of the soil thermal properties is based on work of de Vries (1952), as adopted by Wierenga et al. (1969) and Wagenet and Hutson (1990).

4.2 The soil heat flow equation

To model the transport of heat in porous media, the one-dimensional heat flow equation is used:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\lambda(\theta)}{\rho C_p} \cdot \frac{\partial T}{\partial x} \right) \quad (4.1)$$

where T is the soil temperature ($^{\circ}\text{C}$); $\lambda(\theta)$ is the thermal conductivity ($\text{J m}^{-1} \text{s}^{-1} \text{C}^{-1}$); ρ is the wet bulk density (kg m^{-3}); and C_p is the specific heat capacity of the soil ($\text{J kg}^{-1} \text{C}^{-1}$). Neglecting the heat capacity of the soil gaseous phase, the volumetric heat capacity of the soil is governed by the heat capacity of the soil solid and water phase or:

$$\rho \cdot C_p = \rho_s \cdot C_s + \theta \cdot \rho_w \cdot C_w \quad (4.2)$$

where ρ_s is the bulk density of the soil solid phase; ρ_w the density of water; C_s is the specific gravimetric heat capacity of the soil solids ($840 \text{ J kg}^{-1} \text{C}^{-1}$); C_w is the specific gravimetric heat capacity of water ($4.2 \text{ kJ kg}^{-1} \text{C}^{-1}$). The thermal conductivity is calculated in the WAVE-model as reported by Wierenga et al.

(1969). Considering soil as a continuous medium of either water or air and solids dispersed in it, then the thermal conductivity can be approximated as:

$$\lambda = c \cdot \frac{\sum_{i=0}^n k_i \cdot X_i \cdot \lambda_i}{\sum_{i=0}^n k_i \cdot X_i} \quad (4.3)$$

where n is the number of different components, X_i is the volume fraction of the i -th component (-), λ_i is the thermal conductivity of the i -th component (J m⁻¹ s⁻¹ C⁻¹), and c is an empirical correction factor (-). The volume fraction of quartz, organic matter and other solids is default set equal to 0.54, 0.045 and 0.015 respectively, while the value of c equals 1.65, for $\theta < 0.22$, and 0.0 for $\theta > 0.22$ (Skaggs and Smith, 1967). The subscript zero refers to the continuum medium, e.g. air for dry soil or water for moist soil, with $k_0 = 1$. Other values of k_i may be calculated from:

$$k_i = \frac{1}{3} \cdot \sum_{j=0}^3 \left(1 + \left(\frac{\lambda_i}{\lambda_0} - 1 \right) \cdot g_j \right)^{-1} \quad (4.4)$$

where g_j is a dimensionless factor depending on the particle shape of the i -th component, with $g_1 + g_2 + g_3 = 1$. The values of λ_i for quartz, organic matter, other solids and air at 20 C are default equal to 20.4, 0.6, 0.7 and 0.0615 mCal cm⁻¹ sec⁻¹ C⁻¹. The apparent thermal conductivity of the air filled pores is taken to be $\lambda_a + \lambda_v$, where λ_a is the thermal conductivity of the air and λ_v accounts for the heat movement by vapour across the gas-filled pore. For water contents above 0.20, the air in the soil water pores is considered to be saturated and a value of 0.176 mCal cm⁻¹ sec⁻¹ C⁻¹ is used for λ_v . It is assumed that the value of λ_v decreases linearly from 0.176 mCal cm⁻¹ sec⁻¹ C⁻¹ at a moisture content of 0.2 to 0. at oven-dryness. For quartz and solid particles, g_j is set equal to 0.125, 0.125, 0.750 respectively. For organic matter $g_1 = g_2 = 0.5$, while $g_3 = 0.0$. Values of g_1 and g_2 for the air particles were assumed to decrease linearly from 0.333 in water saturated soil to 0.105 at a soil water content of 0.2. Below this water content, g_1 and g_2 were assumed to decrease linearly to a value of 0.015 at oven dryness.

4.3 Numerical solution of the heat flow equation

4.3.1 The solution procedure

The right hand term of Eq.(106) is expanded as a Taylor series and rearranged in an implicit central difference scheme:

$$\frac{\partial}{\partial x} \left(\frac{\lambda(\theta)}{\rho C_p} \cdot \frac{\partial T}{\partial x} \right) = \frac{1}{x_{i+1} - x_{i-1}} \left(\frac{\lambda_{i-1/2}^{j-1/2} (T_{i-1}^{j-1} + T_{i-1}^j + T_i^{j-1} + T_i^j)}{2 \cdot \rho_{i-1/2} \cdot C_p^{j-1/2} \cdot (x_i - x_{i-1})} \right) - \left(\frac{\lambda_{i+1/2}^{j-1/2} (T_i^{j-1} + T_i^j + T_{i+1}^{j-1} + T_{i+1}^j)}{2 \cdot \rho_{i+1/2} \cdot C_p^{j-1/2} \cdot (x_{i+1} - x_i)} \right) \quad (4.5)$$

Equation (110) is formulated for each node. The rearranged system of linear equations has a tri-diagonal form and can be solved using the Thomas algorithm (Remson et al., 1978).

4.3.2 Definition of the upper boundary condition

The upper boundary condition for the soil temperature is defined using the method of Kirkham and Powers (1972). The method considers the daily variation of soil temperature at the surface as a result of the fluctuation of the daily solar radiation. The foregoing is described using a sine function:

$$T = T_a + \gamma \cdot \sin\left(\frac{2\pi t}{p}\right) \quad (4.6)$$

where T is the actual soil surface temperature ($^{\circ}C$), T_a is the daily average soil surface temperature ($^{\circ}C$), γ is the amplitude of the soil surface temperature ($^{\circ}C$) (usually taken equal to the difference between maximum and minimum temperature), p is the period for completing one cycle (usually one day) and t the time (day).

4.3.3 Definition of the lower boundary condition

For the lower boundary condition, a constant soil temperature (default fixed at $7^{\circ}C$) is assumed.

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Chapter 5

The crop growth module

Chapter 6

The nitrogen fate module

6.1 Introduction

The fate of nitrogen in the soil is determined by different processes (Fig.16). Nitrogen can enter the soil environment through atmospheric deposition (rainfall and dry deposition), fertilizer application, organic matter addition or through nitrogen fixation by rhizobia. Nitrogen can leave the soil environment through nitrogen denitrification, volatilization, plant uptake or leaching. Mineralisation from organic into mineral nitrogen, immobilisation from mineral nitrogen in organic matter, nitrification from ammonia to nitrate and denitrification change the form, and so, the properties of nitrogen in the soil. Each of these processes has been the subject of intensive studies. Simulation models have been used for the description of the different subprocesses (Van Veen, 1977; Rachhpal-Singh and Nye, 1988; Verbruggen, 1985; De Willigen and Noordwijk, 1987, amongst others). However, to be of use for policy makers and to be able to solve a number of problems, an integrated model of the nitrogen cycle is required.

Fig.16 : Schematic flow chart of the nitrogen cycle.

Different levels of complexity exist for describing the nitrogen transfer and transformation processes. The complexity level of a selected model will strongly depend on the desired level of explanation. A simple, first order decay model for the mineralisation of the organic nitrogen might give a good description of the mineralisation processes shortly after an organic matter addition. However such a model might fail to describe the long term mineralisation process involving the decomposition of the organic matter fractions. A detailed model description, on the other hand reduces the model applicability for extrapolative purposes. Parameters describing the transformation processes of nitrogen for a wide set of soil and management scenarios are still lacking at this moment.

The nitrogen module used in the WAVE-model, was originally developed by Vereecken et al. (1990, 1991) and named SWATNIT (Simulating WATer and NITrogen). The nitrogen module describes the transformation processes for the

organic and inorganic nitrogen in the soil. Also, the uptake of nitrogen by the plants is described by means of a sink term added to the transport equation. The potential transformation rates, which are model input, are reduced for temperature and moisture content in the soil profile. The model comprises research findings with field results. For the processes which are believed to be better understood and for which relevant data are available a more complex approach is used. Other processes, such as soil denitrification or volatilization, are described using simple kinetics.

6.2 Modelling of nitrogen transformations in soils

6.2.1 Mineralisation of the soil organic nitrogen

Organic nitrogen transformations and resulting mineralization of organic carbon and nitrogen are described using a three pool concept as reported by Johnsson et al. (1987) and shown in Fig.17. These authors distinguish a fast cycling pool of organic matter/microbial bio-mass complex (soil litter pool), receiving fresh organic matter and a slow cycling pool of stabilized decomposed products (soil humus pool). Because of the different properties of the applied slurry or manure, a third pool (soil manure pool) is distinguished. The soil biomass, which constitutes 1 to 5 % of the soil organic matter, though being the eye of the needle where all the organic material at least once passes through (Jenkinson and Ladd, 1981; Dendooven, 1990), is not modelled explicitly. However, it is assumed that the nitrogen demand for the internal cycling of carbon and nitrogen in the three pools, which is modelled explicitly, is regulated by a constant C/N ratio of the soil biomass, which is model input. In addition, it is assumed that the C/N ratio of the turn-over metabolites equals the C/N ratio of the soil bio-mass. Consequently, this C/N ratio controls the soil mineral nitrogen release from the three organic matter pools.

Fig.17: Organic matter turnover concept as applied in the nitrogen fate module (Johnsson et al., 1987)

The turnover of the carbon in the litter pool is represented by the upper loop in Fig. 17. The fraction of C in the litter pool which is turned over per unit time equals k_{lit} . The turn-over efficiency f_e (-) determines which fraction is effectively transformed into new organic matter through the biomass and which fraction is decomposed. The humification constant f_h determines next which fraction of the effectively turned-over C goes to the humus pool. Hence, the net increase of C in the litter pool is written as:

$$\frac{\partial C_{lit}}{\partial t} = IN - OUT = ((1 - f_h)f_e - 1) k_{lit} C_{lit} \quad (6.1)$$

where C_{lit} is the carbon content of the litter pool (kg C m⁻³ soil); f_h is the dimensionless humification constant (-); f_e is the dimensionless turn-over effi-

ciency (-); k_{lit} is the decomposition rate of the litter (day-1).

During the turn-over of the litter-C, N-immobilization or N-mineralization can occur, depending on the C/N ratio's of the litter (C_{lit}/N_{lit}) and the biomass (ρ). From Eq. () it follows that the net increase of the N-content in the litter pool is written as:

$$\frac{\partial N_{lit}}{\partial t} = \left((1 - f_h)f_e \frac{1}{\rho} - \frac{N_{lit}}{C_{lit}} \right) k_{lit} C_{lit} \quad (6.2)$$

where N_{lit} is the N-content of the litter pool (kg N m-3 soil) and ρ is the biomass C/N ratio. In Eq. (154) it is assumed that the turn-over metabolites have the same C/N ratio as the biomass (ρ).

For the manure pool, a similar turn-over loop is represented in the Fig. 17. Equation similar to Eqs. (153) and (154) can be written as follows:

$$\frac{\partial C_{man}}{\partial t} = ((1 - f_h)f_e - 1) k_{man} C_{man} \quad (6.3)$$

$$\frac{\partial N_{man}}{\partial t} = \left((1 - f_h)f_e \frac{1}{\rho} - \frac{N_{man}}{C_{man}} \right) k_{man} C_{man} \quad (6.4)$$

where C_{man} and N_{man} are respectively the C content (kg C m-3 soil) and N-content (kg N m-3 soil) in the manure pool; and k_{man} is the decomposition rate of the manure pool (day-1). It is assumed that the same f_e and f_h constants apply for the litter and manure pools. From Fig.17 it can be seen that the net increase rate of C and N in the humus pool is written as:

$$\begin{aligned} \frac{\partial C_{hum}}{\partial t} &= f_e f_h (k_{lit} C_{lit} + k_{man} C_{man}) - k_{hum} C_{hum} \\ \frac{\partial N_{hum}}{\partial t} &= \frac{f_e f_h}{\rho} (k_{lit} C_{lit} + k_{man} C_{man}) - k_{hum} N_{hum} \end{aligned} \quad (6.5)$$

where C_{hum} and N_{hum} are respectively the C content (kg C m-3 soil) and N content (kg N m-3 soil) in the humus pool; and k_{hum} is the decomposition rate of the humus pool (day-1). All C/N turn-over reactions represented in Fig. 17 can result in a net production or consumption of ammonium, depending on the C/N ratio's of the biomass and the three pools. As the increase of NH_4^+-N , due to mineralisation is equal to the decrease of organic N in the three organic matter pools, we obtain from the Eqs. (154), (156) and (157):

$$\frac{\partial N_{NH_4^+}}{\partial t} = \left(\frac{N_{lit}}{C_{lit}} - \frac{f_e}{\rho} \right) k_{lit} C_{lit} + \left(\frac{N_{man}}{C_{man}} - \frac{f_e}{\rho} \right) k_{man} C_{man} + k_{hum} N_{hum} \quad (6.7)$$

Eq.(158) determines whether mineralisation (right hand side of the equation is positive) or immobilisation (right hand side is negative) is occurring. In case

no ammonium is available for immobilisation, nitrate is used as given by the following equation:

$$\frac{\partial N_{NO_3^-}}{\partial t} = -\frac{f_e}{\rho}(k_{lit}C_{lit} - k_{man}C_{man}) \quad (6.8)$$

Equations (153) to (159) are integrated numerically using the Euler integration method. The resulting mineralisation/immobilisation rates enter the sink term of the solute transport equation.

In order to account for soil water and temperature effects on the organic matter turn-over, the potential rate constants, k_{lit} , k_{man} and k_{hum} are reduced. It is assumed that between a low ($pF=3$) and high ($pF=2$) critical moisture content no reduction occurs. In non-optimal conditions a reduction factor is derived by linear interpolation between 1 and 0 in the moisture content interval ($\theta(pF = 3) - \theta(ovendryness)$), and between 0 and 1 in the moisture content interval ($\theta(saturation) - \theta(pF = 2)$). The effect of soil temperature is considered through a default Q10 ($Q_{10}=3$) reduction function.

$$REDTEMP = 3^{\frac{T-16}{10}} \quad (6.9)$$

where T is the soil temperature ($^{\circ}C$).

A compilation of literature data on the bio-mass C/N ratio r_o , is listed in Table 32.

Table 32: C/N ratio's of soil bio-mass as reported in literature (Dendooven, 1990).

For solving the mineralisation equations the organic matter pools need to be initialised. The distribution of the organic matter in both the nitrogen and carbon fraction of the three pools is model input. Paul and Juma (1981) stated that 92 % of the organic matter in the soil can be situated in the stable humic pool. This figure can be used to initialise the humus pool. The remaining soil organic matter can then be distributed equally over the litter and manure pool. In practice, a warm-up period of several years to equilibrate the nitrogen and carbon content in the different pools is recommended.

The turn-over of the organic matter is further controlled by the carbon turn-over efficiency. The carbon turn-over efficiency equals the fraction of the mineralised carbon which turns over in the organic matter immediately and hence is not lost as carbon dioxide. This fraction governs the amount of immobilised or mineralised nitrogen through the given constant C/N ratio of bio-mass and metabolism products. Carbon turn-over efficiency values range between 10 and 60% depending on the kind of substrate or decomposing micro-organisms. Compiled literature data (Dendooven, 1990) for this parameter are given in Table 33. A part of the soil organic carbon which turns over is incorporated in the humus pool of the soil. This fraction is controlled by the humification coefficient which can be set equal to e.g. 0.2 (Johnson et al., 1987). The carbon turn-over efficiency constant and humification coefficient are model input. (6.9)

Table 33: Efficiency constants of the carbon assimilation as reported in literature (Source: Dendooven, 1990) fe Description

The mineralisation or immobilisation of soil organic matter from the different pools is governed by the potential decomposition rates. Literature values of possible decomposition rates, for the different organic matter fractions, are given in the Tables 34, 35, and 36. (6.10)

Table 34: Decomposition rate of soil litter as reported in literature (Source: Dendooven, 1990) (6.11)

Table 35: Decomposition rate of soil manure as reported in literature (6.12)

kman (day-1) Reference

Table 36: Decomposition rate of soil humus as reported in literature (6.13)

khum (day-1) Reference

6.2.2 Denitrification

Due to the anaerobic respiration of soil bacteria, soil nitrate-nitrogen is reduced to gaseous nitrogen forms such as N₂O and N₂. The soil pH, the texture, the organic carbon supply, the amount of crop residues, the soil temperature, the soil mineral nitrate availability, the soil aeration and moisture status, among others, are factors controlling the denitrification in field conditions. In the nitrogen module of WAVE, a first order kinetic approach is used to assess the soil denitrification. The anaerobic respiration is not linked to turn-over model for the organic matter. The following equations are used:

$$\frac{\partial[NO_3^-]}{\partial t} = k_{denit}[NO_3^-] \quad (6.15)$$

where NO_3^- is the nitrate concentration in the soil water and k_{denit} is a first order denitrification constant (day-1).

Few studies are available yielding potential denitrification rates for a range of soil types. Breeuwsma et al. (1991) report on potential soil denitrification rates, based on the soil texture, carbon content and mean groundwater level. The following relations are suggested for sandy and clay soils under Dutch conditions:

The potential denitrification rate is reduced using the Q10 temperature reduction function (Eq.(160)). The effect of the soil moisture status on denitrification is assessed through the use of the soil water reduction factor for denitrification, R_w (Johnsson et al.1987; Aulakh et al., 1992):

$$\begin{aligned} \text{Sandy : } k_{denit} &= 0.41 \cdot \text{Carbon}(\%) - 0.35 \cdot \text{meangroundwaterlevel}(\%) \\ \text{Clay : } k_{denit} &= 0.61 - 0.51 \cdot \text{Clay}(\%) + 0.20 \cdot \text{Carbon}(\%) \\ S_e > 0.8 : R_w &= \left(\frac{\theta - \theta_d}{\theta_s - \theta_d} \right)^d \\ S_e < 0.8 : R_w &= 0 \end{aligned}$$

where θ_d is a critical threshold value, corresponding to a saturation degree of 0.80, and d an empirical constant, set equal to 2.

6.2.3 Volatilisation

In the soil environment ammonia might be present in gaseous form. If conditions are favourable ($pH > 7.5$) and the partial pressure head gradient between NH_3 in the soil and the atmosphere is sufficiently large, ammonia gas can volatilise. Ammonia volatilisation in WAVE is simulated using a first order kinetic approach.

6.2.4 Nitrification

Nitrification, which transforms ammonia-N to nitrate-N and which is ruled by heterotrophic soil organisms, is modelled using a first order kinetic equation. Since soil nitrification is controlled by the soil bio-mass, the former defined temperature and water reduction (see section 6.2.1) mechanisms are applied.

6.2.5 Hydrolysis of urea

The hydrolysis of urea, which is a basic constituent of many inorganic and organic fertilizers, is modelled using a first order kinetic approach. Again, temperature and water stress reduction mechanisms are considered (see section 6.2.1).

6.2.6 Uptake of ammonia and nitrate

The nitrogen uptake by plants is described using a macroscopic uptake model as proposed by Mc Isaac et al. (1985) and adapted by Huwe and van der Ploeg (1988). The macroscopic uptake component restricts the nitrogen uptake rate to a potential level.

If crop growth is not modelled, the potential uptake rate $(\partial N/\partial t)_p$ is calculated as:

$$\begin{aligned} t < G : \left. \frac{\partial N}{\partial t} \right|_p &= A \cdot t \cdot (G - t) \\ t \geq G : \left. \frac{\partial N}{\partial t} \right|_p &= 0 \end{aligned} \quad (6.17)$$

where G the time when the plant N uptake stops (day), A a parameter to assure that in non-stressed conditions the maximum N uptake is reached ($\text{mg m}^{-2} \text{ day}^{-3}$). Integrating Eq. 166 yields $N = AGt^2/2 - At^3/3$ which in optimal conditions ($t=0, N=0; t=G, N=N_{\max}$) enables to calculate A as $A = N_{\max}/(G^3/2 - G^3/3)$. The user has to specify a value for G and for the maximum N uptake (mg m^{-2}). To simplify the input, G is input as a fraction of the total growing season. Hence, its value must range between 0 and 1.

If crop growth is modelled the potential uptake rate is simulated as:

$$\left. \frac{\partial N}{\partial t} \right|_p = \left. \frac{\partial N}{\partial t} \right|_{\text{leaves}} + \left. \frac{\partial N}{\partial t} \right|_{\text{stems}} + \left. \frac{\partial N}{\partial t} \right|_{\text{roots}} \quad (6.18)$$

where the right hand terms of Eq.(167) refer to the nitrogen demand of the leaves, stems and roots, respectively. The potential uptake rates for leaves, stems and roots is modelled with:

$$\begin{aligned}\frac{\partial N}{\partial t}\bigg|_{p,leaves} &= WL V \cdot XNCLE - N_{leaves} \\ \frac{\partial N}{\partial t}\bigg|_{p,stems} &= WST \cdot XNCST - N_{stems} \\ \frac{\partial N}{\partial t}\bigg|_{p,roots} &= WRT \cdot XNCRT - N_{roots}\end{aligned}\quad (6.19)$$

where WL V, WST, WRT is the accumulated dry matter (kg ha-1); XNCLE, XNCST, XNCRT the potential fraction of nitrogen N in the crop dry matter (kg N kg-1 DM); and Nstems, Nleaves and Nroots is the nitrogen N accumulated in the leaves, the stems and the storage organs. The fraction of the nitrogen N in the leaves, XNCLE, is input as a function of crop development stage. The fraction of nitrogen N in the stems and roots is assumed to be 50 % of the fraction in the leaves. (6.19)

The potential nitrogen uptake rate is further divided in a convective and diffusive fraction. The potential convective nitrogen uptake rate (mg m-2 day-1) is defined as:

$$\frac{\partial N}{\partial t}\bigg|_{conv} = \int_0^{zmax} S_w \cdot C_m \cdot dx \quad (6.21)$$

where zmax is the rooting depth at time t (mm), C_m is the concentration of either nitrate or ammonia in the soil water (mg l-1), and S_w is the convective root water uptake rate (day-1). The convective root water uptake is calculated in the water flow module of WAVE. The convective uptake rate is limited to the potential uptake rate. If the convective uptake rate is smaller then the potential, a potential diffusive nitrogen uptake rate is calculated:

$$\frac{\partial N}{\partial t}\bigg|_{difp} = \frac{\partial N}{\partial t}\bigg|_p - \frac{\partial N}{\partial t}\bigg|_{conv} \quad (6.22)$$

The maximum diffusive nitrogen uptake rate, for both nitrate and ammonia, is calculated as:

$$\frac{\partial N}{\partial t}\bigg|_{difmax} = \int_0^{zmax} \frac{2 \cdot \pi \cdot RDENSI \cdot RORAD \cdot Dif(\theta) \cdot C_{mi} \cdot \theta}{10^5 \cdot D0} dx \quad (6.23)$$

where RDENSi is the root density (cm l-1); RORAD the mean root radius (mm); $Dif(\theta)$ is the chemical diffusion coefficient in a soil (mm² day-1); $1/D0$ the travel distance resistance between the bulk soil solution and the root (1/mm); C_{mi} the concentration of either nitrate or ammonia in the soil solution (mg l-1) and dx the depth increment (mm). The maximum diffusive uptake rate is limited to the potential diffusive uptake rate. If the SUCROS-model is used, RDENSi is directly obtained from the crop growth module (1000* RLDFL (cm cm-3) = RDENSi (cm l-1)). If no crop growth model is used, the root density function is simulated with an exponential decreasing function :

$$RDENS = RDENS_0 \cdot e^{-\alpha_{r,dens} \cdot x} \quad (6.24)$$

where $RDENS_0$ (cm l⁻¹), the root density at the soil surface and $\alpha_{r,dens}$ (-) are model input. Both parameters can be derived from Table 31.

The total actual uptake rate is calculated as the sum of the actual convective and the diffusive uptake rate or:

$$\left. \frac{\partial N}{\partial t} \right|_{act} = \left. \frac{\partial N}{\partial t} \right|_{conv} + \left. \frac{\partial N}{\partial t} \right|_{dif} \quad (6.25)$$

If crop growth is modelled, the actual uptake rate in the different crop components is modelled according to:

$$\left. \frac{\partial N}{\partial t} \right|_{act}^{leaves} = \left. \frac{\partial N}{\partial t} \right|_{pot}^{leaves} \cdot \left(\frac{\frac{\partial N}{\partial t}}{\frac{\partial N}{\partial t}} \right) - \left. \frac{\partial N}{\partial t} \right|_{pot}^{storageorgans} \cdot \left(\frac{WLV}{WLV + WST} \right) \quad (6.26)$$

$$\left. \frac{\partial N}{\partial t} \right|_{act}^{stems} = \left. \frac{\partial N}{\partial t} \right|_{pot}^{stems} \cdot \left(\frac{\frac{\partial N}{\partial t}}{\frac{\partial N}{\partial t}} \right) - \left. \frac{\partial N}{\partial t} \right|_{pot}^{storageorgans} \cdot \left(\frac{WST}{WLV + WST} \right) \quad (6.27)$$

$$\left. \frac{\partial N}{\partial t} \right|_{act}^{roots} = \left. \frac{\partial N}{\partial t} \right|_{pot}^{roots} \cdot \left(\frac{\frac{\partial N}{\partial t}}{\frac{\partial N}{\partial t}} \right) \quad (6.28)$$

$$\left. \frac{\partial N}{\partial t} \right|_{act}^{storage,organs} = \left. \frac{\partial N}{\partial t} \right|_{pot}^{storage,organs} = (WSO \cdot XBCSO - N_{storage,organs}) \cdot REDFACT \quad (6.29)$$

The reduction factor is calculated using:

$$\begin{aligned} REDFACT &= 1 - \sqrt{1 - NITRED} \\ 0 &\leq NITRED &= \left(\frac{ANCL - RLNCL}{RMNCL - RLNCL} \right) &\leq 1 \end{aligned} \quad (6.30)$$

where ANCL is the actual nitrogen fraction in the leaves, RMNCL the leaf nitrogen threshold concentration for unrestricted growth assumed to be 0.5*XNCLE and RLNCL the leaf nitrogen threshold concentration below which there is no growth anymore, assumed to be equal to 0.005 kg N kg⁻¹ D.M. The potential fraction of nitrogen N of the storage organs, XNCSO (kg N kg⁻¹ D.M), is set default equal to 0.0125 kg N kg⁻¹ D.M for winter and spring wheat, 0.025 kg N kg⁻¹ D.M for potatoes and maize and 0.075 kg N kg⁻¹ D.M for sugar beet. This uptake model of the different crop components is based on the PAPRAN model (Seligman and van Keulen, 1981).

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Chapter 7

Description of model input and output

Chapter 8

Description of the computer programme