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The WAVE model and its application; Simulation of the substances water and agrochemicals in the soil, crop and vadose environment

Título: Aplicaciones del modelo WAVE: simulación del crecimiento del cultivo y del movimiento del agua y los agroquímicos en la zona no saturada del suelo

INTRODUCTION

EXPANSION OF HUMAN ACTIVITIES has a major impact on the environment in the broadest meaning. Worldwide climatologically changes, dispersion of pollutants (from industrial and agricultural activities) in the subsurface, struggle for water reserves, etc. are problems that will have to be countered. To assess the impact of changing activities, it would not be wise full to just wait and see what will happen. Therefore, existing groundwa-

ter, soil conservation and agricultural policies and strategies are reconsidered, while new are developed. To develop adequate and durable measures the analytic approach system 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 interaction of the different processes affecting the fate of nutrients, pollutants, and chemicals in the dynamic water-soil-crop environment. As a result, a tremendous interest in system studies, especially through mathematical modelling, has emerged the last decades. Mathematical modelling is an important part of many current environmental studies and it is believed that there is a lot of scope for model development as long as new insights in processes will emerge and computing facilities improve.

The WAVE model is, amongst many others, an example of such a mathematical tool. It describes the transport and transformations of matter and energy in the soil, crop and vadose environment. It is important to know that the WAVE model does not support processes that take place in groundwater, drains, rivers, etc. There exist other models to do so. Figure 1 shows the application area of the WAVE model related to hydrological cycle.

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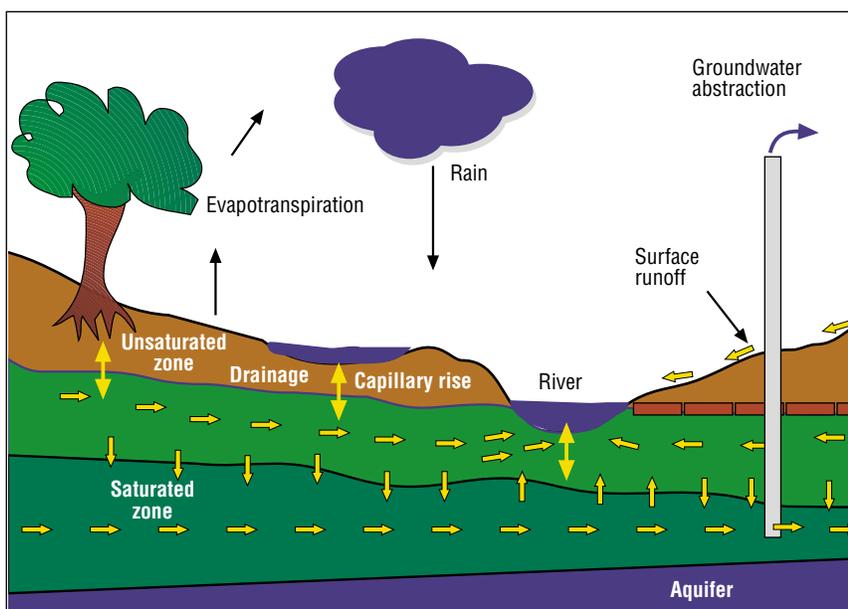


Figure 1. The hydrological cycle. Water flow processes incorporated in the WAVE model are described.

Characteristics of the WAVE model

The WAVE model is a one-dimensional or point model. It is thus assumed that the governing transport processes of matter and energy in the soil occur essentially in the vertical direction. This restriction has of course a large implication on the type of problems to be executed.

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 soil profile is therefore discretised into a number of equally sized compartments, and the total time period into discrete time steps of unequal lengths.

The model is deterministic, by which is meant that one set of input data always yields the same model output values.

The model is mainly process-based or mechanistic, since physical, chemical and biological laws were considered when developing the model.

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.

Finally, the model is an explanatory model because it helps to understand the different processes and process interactions governing for example chemicals in the soil. However, results from these explanatory studies can always be used in extrapolation or prediction studies for decision making. Hence, the model is one of the ad-hoc tools available to improve current management of the soil-crop environment. It is a unique tool for 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 fertilizers.

Different modules of the WAVE model

The WAVE model is structured in a modular way, enabling the user to use only those modules required to analyse each problem. To run certain problems, each module is feed by a specific set of input files. The precision of the input parameters has of course an enormous impact on the accuracy of the output. The more modules are used in the mo-

del, the more complex the problem becomes and the more input parameters are required.

In Table 1, the different modules of the WAVE model are briefly described, together with the main physical processes and some necessary parameters used in the module. It is always a tremendous job to gain proper parameters for each module in a way that the model execution does not fail during calculations and gives a realistic output. Recently, extra modules are written to tackle specific management problems (fertilizer applications, irrigation, pesticide problems, ...), but these are not discussed here since it

will be the aim to incorporate them in a new version of the WAVE model. The user is also free to add his own 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 become available. Expertise in reading and adapting computer codes (WAVE is written in Fortran) is however absolutely necessary if it's necessary to do this.

Figure 2 presents the different modules and the arrows indicate the 'uses-relationship' among them. It is clear that no module can be executed without the

Table 1. List of model concepts integrated in the WAVE model

Module	Model concept	Model parameters
Water	Richards equation, extraction equation for root uptake	Moisture retention curve, conductivity curve, crop coefficients, crop uptake factors, rooting depths and leaf area index
Solutes	Convection-dispersion equation, chemical diffusion, linear adsorption, decay (1st order)	Dispersion, diffusion and adsorption coefficients, decay constants
Heat	Fouriers heat flow equation	Thermal conductivity and heat capacity function
Nitrogen	Transformations (1st order nitrification, denitrification, hydrolyses), mineralization and immobilisation from organic pools (plus correction in function of temperature and moisture content)	Nitrogen transformation parameters, decay constants from organic carbon
Crop	Dry matter development, nitrogen uptake by plants, reduction in function of water and nitrogen	Specific crop parameters

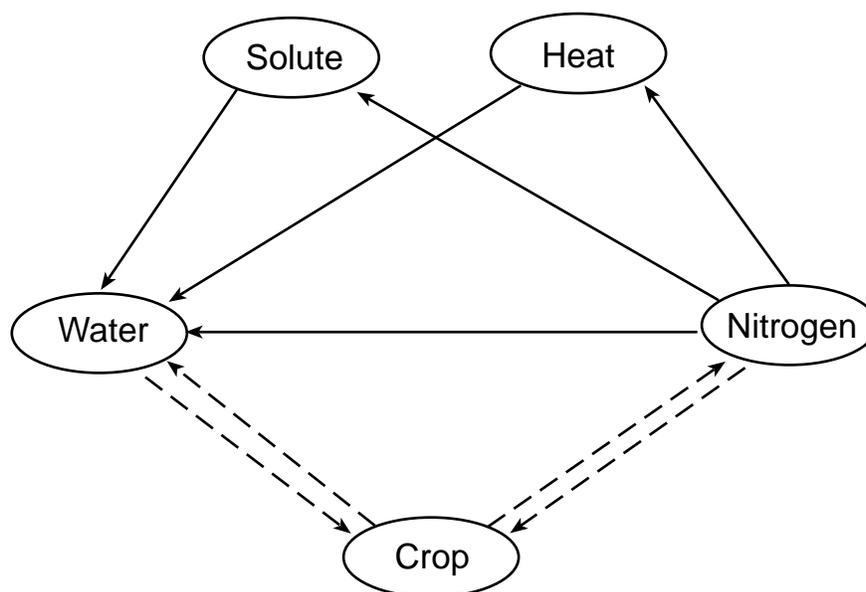


Figure 2. Schematic presentation of the modules in WAVE. Full line arrows represent obligatory 'uses-relationships', dashed lines are optional.

water module. 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. Therefore, a brief explanation of the water module and its mathematical sub-structure will be given inext without pursuing completeness. It is not possible to give a detailed description of all modules of the Wave model (these can be read in the user's manual. During the presentation, some basics concepts of some modules will be outlined.

Within the water module, the soil water flow equation is numerically solved to quantify the unknown terms of the water balance:

$$\Delta W = (P + I + U) - (R + ET + D)$$

Where ΔW is the change in water content (mm) in the soil 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), ET the actual evapotranspiration (mm) and D the percolation or drainage depth. Generally, P and I are known system inputs, while U , R , ET and D are unknown terms of the water balance and have to be calculated. Figure 3 illustrates the difference between a mathematical model and a simple field water balance model. In the WAVE model the Richards equation is used to describe the one-dimensional water flow in an infinitesimal small soil element (soil compartment):

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

Where θ is the volumetric water content, z is the vertical coordinate defined as positive upward, t is time, $K(h)$ the hydraulic conductivity and h the soil water pressure head.

In fact, the Richards equation combines the Darcian flow equation with the water mass conservation law (see concept of water balance in figure 2). This flow equation is solved numerically ($\delta h/\delta z$ becomes dh/dz , or within a small soil compartment and small time step, flow occurs under stationary conditions). To solve the flow equation, the moisture retention curve $\theta(h)$, and hydraulic conductivity curve $K(h)$, need to be specified. Parametric models exist to describe the shape of these curves. One of the

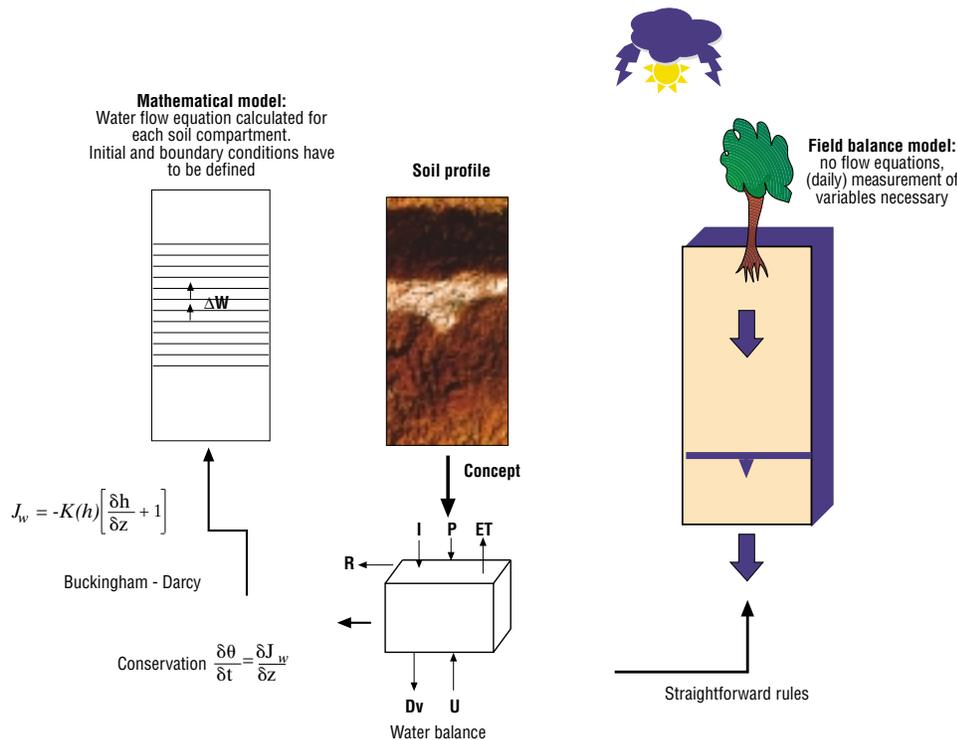


Figure 3: Difference between a mathematical model and field water balance model

most common parametric models is the van Genuchten-Mualem equation:

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

and

$$K(h) = K_s \frac{\left[1 - (\alpha|h|)^{mn} \left(1 + (\alpha|h|)^n\right)^{-m}\right]^2}{\left[1 + (\alpha|h|)^n\right]^{ml}}$$

With θ_s and θ_r [$L^3 L^{-3}$], the saturated and residual moisture content; α [L^{-1}] the inverse of the air entry value; n [-] and m [-], empirical shape parameters. Restricting $m = 1 - 1/n$ the conductivity model of Mualem can be described with the parameters of the moisture retention curve, $\theta(h)$. Herein l [-] is a tortuosity factor (in practice mostly 0.5), and K_s [LT^{-1}] the saturated hydraulic conductivity. These parameters are essential input parameters to run the WAVE (or other models), although other parametric model parameters can be used. They can be derived by direct measurements of moisture retention points and fitting the parametric model to this points or by pedotransferfunctions (indirect estimates of the parameters via easy meas-

urable variables such combinations of bulk density, carbon content, texture, ...). Hysteresis can also be implemented as input in the model.

To run the model, boundary conditions for the first (upper boundary) and last (bottom boundary) compartment have to be defined to solve the flow equations. Different types of boundary conditions can be chosen from the input files. Physical processes and model concepts for other modules can be found in the WAVE manual. It is however interesting to briefly discuss the crop growth module.

Crop growth in the WAVE model

When modeling 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 an 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 (necessary as input with other climatic data) with a crop specific coefficient which varies as a function of the crop development stage. 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. Nowadays, the WAVE model has standard parameters for five different crops that can be modeled (f.e., corn, wheat, potatoes, ...). One can always enlarge this list by looking for proper parameters for other crops.

Applicability of the WAVE model in time and space

Wave is essentially a one-dimensional 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 a arduous task. Hence, the model is conceived to describe flow only in 1-D systems, as in soil laboratory columns or field lysimeters. Nevertheless, 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) field parameters are used (Figure 4a). With 'effective' is meant that the variability present in a larger field is implied within the parameters.

In the vertical direction, the model considers the existence of heterogeneity in the form of soil layers within a soil profile (Figure 4b). 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

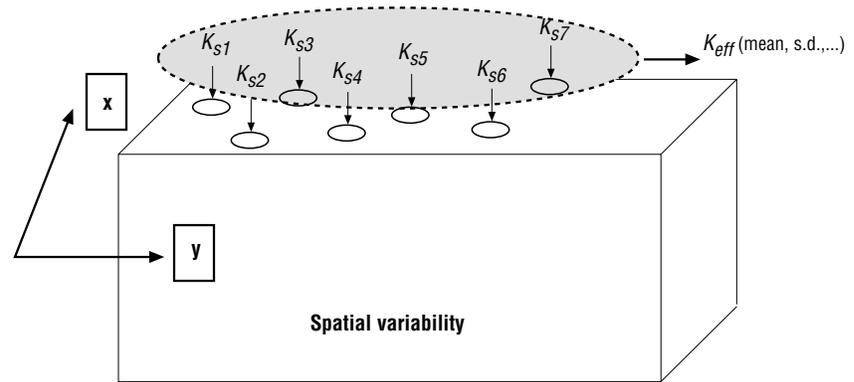


Figure 4a. Spatial variability can be implemented by using effective parameters representing variability measured from individually obtained parameters.

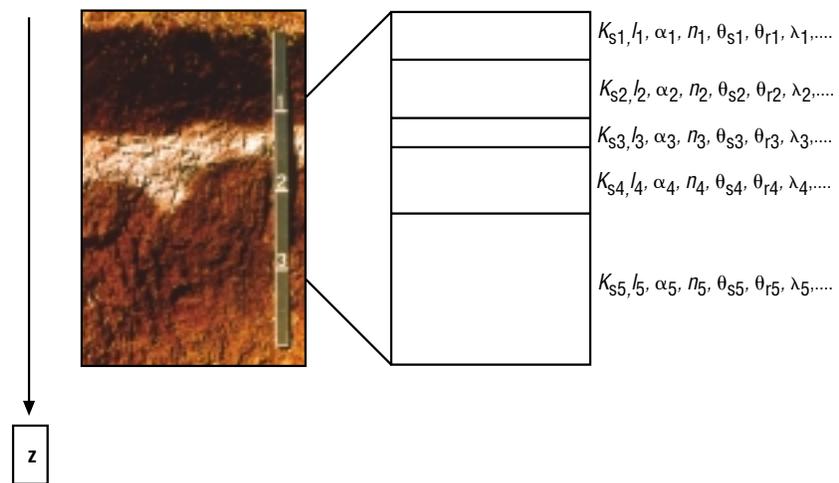


Figure 4b. Vertical variability can be implemented by dividing a soil profile into different layers and assigning different soil parameters to each layer.

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.

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. For processes that are strongly dynamic (water, heat solute transport), the model uses a time step smaller than a day to calculate the different system variables to limit mass balance errors induced by solving the water flow equation. For less dynamic processes (crop growth) a fixed daily time step is used. State variables are integrated after each day to yield daily output.

Overview of the model input and output of the WAVE model

Figure 5 shows the model input and output of the WAVE model. Nowadays, only text files are used. This makes that solving problems with WAVE is rather labour intensive. In the future, window input screens should solve the problem.

Some examples of the WAVE model

Before any mathematical model can be used in scenario analyses; it is absolutely necessary to be sure that the parameters used are proper parameters. This is tested in the calibration-validation procedure. Certain (sensitive) model parameters are adjusted in such a way that a satisfying match between model output and measured state variables is obtained (calibration). Thereafter, these parameters are validated.

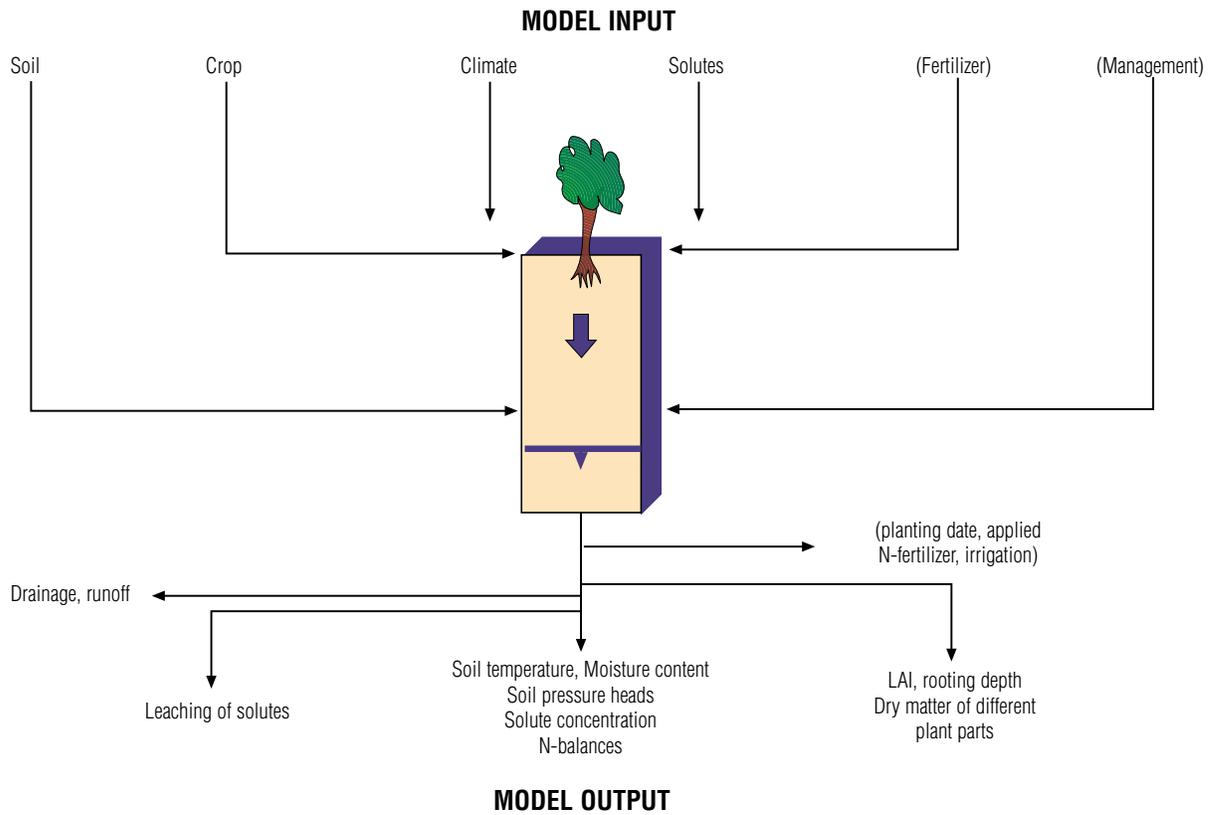


Figure 5. Model input and generated model output possible from the application of the WAVE model.

The model is then executed with calibrated parameters (no adjusting) and again model output is compared with another set of measured data. If the match is also satisfying, the obtained parameters can be used for scenario-analyse. Impact of changing climate, fertilizer application, groundwater table, etc., on ie. crop yield can then be investigated.

Figures 6a and 6b show some results between model output and measurements. The WAVE model is a software package developed by the Institute of 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 institutes. In the future a more user-friendly package will be available.

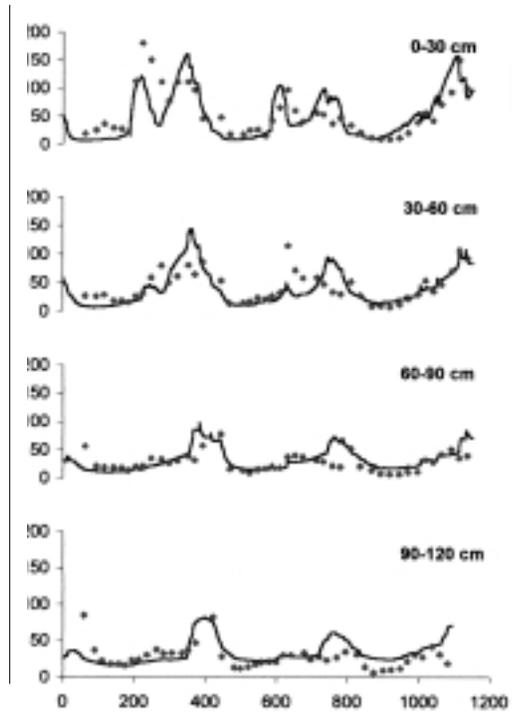


Figure 6a. NO₃ concentrations within the soil profile (bullets = measured, full line = WAVE).

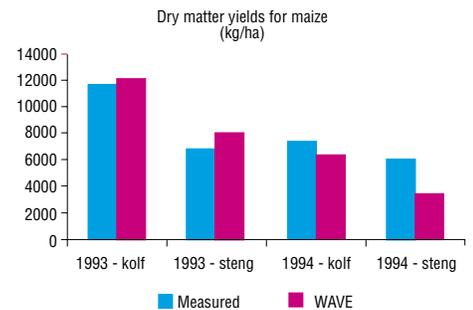


Figure 6. Comparison between measured and modelled dry matter yield on a unfertilised field.

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