Evaluation of the WAVE Model for Predicting Nitrate Leaching for Two Contrasted Soil and Climate Conditions

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ABSTRACT

The integrated soil–crop–atmosphere model Water and Agrochemicals in the Vadose Environment (WAVE) (Vanclooster et al., 1995) was evaluated for two contrasted sets of data. One was from the tropical climate and ferrallitic soil conditions that exist in Maré Island, in New Caledonia. The other was from a glacial terrace under the continental climate of La Côte Saint-André (Isère) in France. Water and NO_3 concentrations and fluxes were monitored during three consecutive years at instrumented sites with different surface covers (maize [*Zea mays* L.] or bare soil) or amount of applied fertilizer. The comprehensive set of measurements allowed us to evaluate the prediction capabilities of the WAVE model. Several parameters were determined independently, while others were adjusted on the basis of simulations for the wettest year at Maré and an average hydrological year at La Côte Saint-André. A stepwise approach was used to calibrate these parameters by sequentially integrating each individual model component. A screening sensitivity analysis was performed to address the most critical parameters. The predictive ability of the model was evaluated by comparing simulated and measured states variables and water and NO_3 fluxes using two different years of data obtained at the same sites. For both sites, the model gave the best results for wet conditions, which actually posed the most critical problems in terms of groundwater pollution under our specific conditions. However, the model was used beyond its capacity as both soils had specificities for which the model was not designed. Overall, WAVE gave quite good predictions, but further studies are needed to fully evaluate WAVE with its crop growth model, SUCROS.

One consequence of the dramatic change in the agricultural sector in the last several decades has been the intensive use of agrochemicals, which is not always in harmony with ecological constraints. Nitrogen is a key crop nutrient. Any shortage of N results directly in reduced crop growth and loss of income to farmers. Hence farmers often increase their use of fertilizer to maximize the growth of their crops. As a consequence, the mobility of some N compounds in the environment has become a crucial component to be studied. Any leaching of mobile NO_3 beyond the root zone can become an unwanted contaminant in drinking water.

The need for modeling N fate in the soil–crop–atmosphere system is now widely accepted. Many models of different types and for different applications (Addiscott and Wagenet, 1985; Wagenet and Hutson, 1989; Brusseau and Rao, 1990; Simunek and Suarez, 1993; Simunek et al., 1999, among many others) have been developed either to improve our understanding of transport processes in soils or to address the increasingly severe problems of pollution resulting from intensive agriculture. However, the modeling exercise is not a simple one because the fate of N is determined by many physical, chemical, and biological processes that can vary tremendously in time and space. Addiscott and Wagenet (1985) noted that the many N models also differ markedly, depending on the background and expertise of the developers, as well as the questions and problems the models are trying to solve. Only a few holistic models that describe each process in detail with the same level of complexity have been published. These holistic models, while being more complex, still face limitations in terms of parameterization and validation.

WAVE, developed by Vanclooster et al. (1994), is a model that is both mechanistic and deterministic. This model was initially developed and evaluated under temperate climate conditions (Vanclooster et al., 1995; Ducheyne and Feyen, 1999; Meiresonne et al., 1999; Ducheyne et al., 2001). Often, models are evaluated only by their developers at the site for which the model was developed. According to Thorsen et al. (1998), a model cannot generally be validated, but must be tested under all the conditions for which it will be used, that is, for different soil, climate, and crop conditions. We chose to evaluate WAVE using two comprehensive sets of data from very different field and climate situations. One was from the tropical climate and soil pedological conditions that exist in the Loyalty Islands of New Caledonia. The other was from the continental climate of La Côte Saint-André (Isère) in France, on a glacial terrace.

Following a description of the field experiments, we give a brief overview of the WAVE model and describe the calibration procedure used to determine suitable values for some of the unknown model parameters based on data from one specific year. The predictive capacity of WAVE is then evaluated against measurements acquired during two other years. The results of a sensitivity analysis of the main parameters are also presented.

MATERIALS AND METHODS

Field Experiments

Two intensive experiments were conducted during three consecutive years to study water and N transport in the soil unsaturated zone to establish a good fertilizer management practices that protect local groundwater resources from pollution. The studies took place between 1991 and 1993 (Kengni, 1993; Kengni et al., 1994; Normand, 1996; Normand et al., 1997) at La Côte Saint-André, near Grenoble, France, and between 1995 and 1997 (Duwig, 1998; Duwig et al., 1998, 2000) on Maré (Loyalty Islands), New Caledonia.

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Abbreviations: DAS, days after sowing; ETP, Penman–Monteith potential evapotranspiration; GMP, Good Modeling Practice code; WAVE, Water and Agrochemicals in the Vadose Environment model.

Table 1. Summary of agricultural practices at the Maré and La Côte Saint-André sites.

Crop	Year	Sowing date	Harvest date	Fertilization amount	Fertilization date	Rain between sowing and harvest	Number of irrigation applications and cumulated amounts	Total dry matter
				kg N ha^{-1}		mm		Mg ha^{-1}
					Maré			
Rainfed corn	1995	20 Jan.	20 Apr.	104	11 Jan.	434	–	10
	1996	18 Jan.	27 Apr.	104 (52 + 52)	15 Feb. + 14 Mar.	850	–	11
	1997	15 Jan.	No harvest	104 (52 + 52)	13 Feb. + 17 Mar.	300†	–	–
					La Côte Saint-André			
Irrigated corn	1991	22 Apr.	05 Oct.	260	22 Apr.	360	6–216.6 mm	24
	1992	23 Apr.	08 Oct.	160 (50 + 110)	23 Apr. + 16 June	516	4–106.4 mm	28
	1993	20 Apr.	20 Oct.	180 (22 + 158)	20 Apr. + 09 June	892	3–117.4 mm	24

† Until the 20 Apr. 1997.

Treatment and Measurement Protocols

Different treatments were considered: bare soil without and with fertilization, and corn crop with fertilization. Each plot on Maré was 400 m^2 and on La Côte Saint-André was 5000 m^2. Ammonium-nitrate in granular form was used as N fertilizer (61% NH_4–N and 39% NO_3–N on Maré, and 50 and 50%, respectively, on La Côte Saint-André). Corn was rainfed at Maré (cv. Hycorn 90) and irrigated at La Côte Saint-André (cv. Furio). Table 1 presents a summary of the agriculture practices at each site.

For both studies, similar measurement protocols were followed, which focused on obtaining estimates of water and NO_3 fluxes under bare soil and corn. The various terms of the water balance and N cycle were obtained from intensive monitoring of the root zone of the crop. At La Côte Saint-André, a set of five tensiometers (at 15, 30, 50, 70, and 90 cm depth), six replicates of suction cups (30, 50, and 80 cm), and a neutron moisture meter (measurements every 10 cm from 10 to 90 cm depth) were established in the soil to measure water pressures, NO_3 concentrations of the soil solution, and water contents, respectively. At Maré, two replicates of tensiometers (10, 20, 30, 40, and 50 cm) and six replicates of suction cups (10 and 40 cm) were utilized as well, whereas two replicates of horizontal time domain reflectometry probes (at 10, 20, 30, and 40 cm) were employed for water content measurement. Instrumentation for the water balance study was placed in 1 m^2 of each plot, whereas suction cup measurements were taken over the entire agricultural field. Climate variables were recorded at both sites. Some characteristics of the soil such as the hydraulic conductivity, solute dispersivity parameters, and N transformation rates were determined in situ or via complementary laboratory experiments. Other parameters were either taken from literature reviews or obtained by model calibration. Because the time series of the hydraulic head gradient and the water content were measured with high temporal resolution, drainage from the rooting zone could be inferred from the measured data using Darcy's Law. Actual evapotranspiration was calculated from the mass conservation equation. The NO_3–N storage in the root zone was derived from water contents and NO_3 concentrations in the soil solution sampled by the suction cups. Finally, NO_3–N leaching from the root zone was calculated by multiplying the drainage rate by the NO_3 concentrations measured at the considered depth, assuming pure convective transport. Details of the various measurements and calculations can be found in several previous papers (Kengni et al., 1994; Normand et al., 1997; Duwig et al., 1998, 2000).

Soils

The soil at Maré is an oxidic ferrallitic soil (Anionic Acrudox Oxisol), which primarily comprises Al and Fe oxides. Soil depths range from 0 to 1 m, with an average of 0.4 m across the experimental field (1 ha).

The soil at La Côte Saint-André is a heterogeneous, shallow, stony and sandy soil (Alfisol), representative of the glacial alluvial plain of La Bièvre, France. Its chemical and physical properties have been described in other studies (Kengni, 1993; Kengni et al., 1994; Angulo-Jaramillo et al., 1997; Netto et al., 1999; Sauboua, 2001). The soil upper layer (0–30 cm) is a loamy sand that consists of approximately 40% coarse material and is reasonably rich in organic matter (2–3%). An important point is the increase in percentage and size of gravel and stones with depth. As a result, the effective root zone is not much deeper than 0.8 m (Kengni et al., 1994). The main characteristics of both soils are presented in Table 2.

Climate

Maré island is situated at 21°30′ South and 168°3′ East in the South Pacific. The climate is semitropical with a hot, wet season between December and March, and a dry season between June and September. The average annual rainfall is 1641 mm. The average annual Penman–Monteith potential

Table 2. Selected properties of soils at the La Côte Saint-André and Maré sites.

Site	Horizon	Coarse†	Soil granulometry, % A	Lf	Lg	Sf	Sg	Organic matter	N	C/N
	cm	%						%	%	
Maré	0–15	0.0	35.9	36.2	4.3	8.9	1.9	13.1	6.06	13.0
	15–30	0.0	35.9	29.9	6.9	18.5	3.1	5.7	4.19	12.1
	30–50	0.0	46.8	32.9	5.8	9.3	2.3	3.3	1.36	12.2
La Côte Saint-André	0–30	40.0	17.5	23.3	17.7	16.6	24.9	2.6	1.25	10.3
	30–60	71.6	18.9	22.3	15.3	15.7	27.7	1.6	0.89	9.1
	60–90	69.3	13.9	17.7	8.6	13.8	46.1	0.7	0.46	7.4

† Coarse (>2 mm) expressed in percentage of the total (fine fraction + coarse material).
‡ In percentage in weight of fine fraction: A = clay (<0.002 mm); Lf = fine silt (0.002–0.005 mm); Lg = coarse silt (0.005–0.02 mm); Sf = fine sand (0.02–0.2 mm); Sg = coarse sand (0.2–2 mm).

evapotranspiration (ETP) is 1341 mm, and the monthly temperatures vary between 10 and 31°C.

The climate around La Côte Saint-André (45°24′ North, 5°15′ East) is of a continental type. The average annual rainfall is 907 mm, and the average annual ETP is 869 mm. The months of July and August are relatively dry, with a monthly rainfall rate below 70 mm. During those dry months, irrigation was applied (high pressure gun). Irrigation rates and the time of application were those used by farmers on conventional irrigation practices of the region; they are given in Table 1. Monthly average temperatures vary between −2 and 26°C.

MODELING

Model Description

The process-based WAVE model (Vanclooster et al., 1994) describes the one-dimensional transport and transformations of matter and energy in the soil, crop, and vadose zone environments. It combines the SWATNIT (Vereecken et al., 1991) and SUCROS models (Van Keulen et al., 1982; Spitters et al., 1988).

While a detailed description of the model was given by their developers (Vanclooster et al., 1994, 1995), we briefly review here the different modules, focusing on those relevant to this study (i.e., water, heat, solute, and N aspects of the model). Water, heat, and solute mass balance equations are solved for each soil compartment specified by the user, using finite difference techniques.

Water Flow

Water movement in the unsaturated soil is modeled using the Richards equation:

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

where h is the soil pressure head (L), θ is volumetric water content ($L^3\,L^{-3}$), z is depth (L) defined as positive downwards, t is time (T), and S (T^{-1}) is a sink term accounting for the crop water uptake. This formulation requires knowledge of the water retention $\theta(h)$ and hydraulic conductivity $K(\theta)$ ($L\,T^{-1}$) functions.

The van Genuchten (1980) $\theta(h)$ parametric expression is used in WAVE:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha_d|h|)^n]^m} \qquad [2]$$

where θ_r and θ_s are the residual and saturated water content, respectively; α_d (L^{-1}), m, and n are fitting parameters, and where the Burdine (1953) condition ($m = 1 - 2/n$) is used.

We considered the Brooks and Corey (1964) $K(\theta)$ expression among those available to model users:

$$K(\theta) = K_s\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{\frac{2}{\eta}+3} \qquad [3]$$

where K_s is the saturated hydraulic conductivity ($L\,T^{-1}$) and η is a shape factor. All of the above parameters are input data.

The crop water uptake rate S was modeled using the macroscopic sink model proposed by Hoogland et al. (1980). S is calculated from a maximum root water uptake rate as a function of depth $S_{max}(z)$ (T^{-1}), and a dimensionless reduction function $\alpha(h)$ that accounts for water stress by reducing the maximum extraction rate according to:

$$S(h,z) = \alpha(h)S_{max}(z) \qquad [4]$$

The actual transpiration rate, T_a ($L\,T^{-1}$), was calculated as the integral of the root water uptake term from the soil surface to some depth z less than or equal to the rooting depth L_r such that the integral becomes equal to the potential rate. If the integration over the complete rooting depth was insufficient to explain T_p, water stress was considered to occur and T_a is set equal to the integral of $S(h,z)$ over the entire rooting depth. This concept is written as follows:

$$T_a = \int_0^{z<L_r} S(h,z)dz \leq T_p \qquad [5]$$

where L_r is the rooting depth and T_p is the potential crop transpiration ($L\,T^{-1}$).

T_p as well as the potential soil evaporation rate E_p of a healthy crop are obtained by splitting the potential crop evapotranspiration rate ET_{crop} ($L\,T^{-1}$), using the leaf area index (LAI) as a division parameter:

$$E_p = \exp(-0.6\mathrm{LAI})\ ET_{crop} \qquad [6]$$

$$T_p = ET_{crop} - E_p - \mathrm{CanStor} \qquad [7]$$

$$\mathrm{CanStor}(j) = \min[\mathrm{Rainfall} + \mathrm{irrigation}, (\mathrm{CanStor}_{max} - \mathrm{CanStor}(j-1))] \qquad [8]$$

where CanStor is the amount of water that has been intercepted and is now released from the crop canopy ($L\,T^{-1}$) and j is the time step. ET_{crop} is calculated by multiplying the potential evapotranspiration rate (ET_o) of a reference surface with a crop coefficient K_c. LAI, K_c, ET_o, L_r, $\alpha(h)$, and $S_{max}(z)$ are model input parameters, as is the potential interception capacity $\mathrm{CanStor}_{max}$ ($L\,T^{-1}$).

A crop growth module, SUCROS, is available within WAVE, and, if it is used, LAI and L_r are calculated by the model depending on photosynthesis and water and nutrient availability. However, we did not use the SUCROS module, since our field experiments did not provide us the necessary parameters, and as such would have to rely on literature values for Dutch conditions (Vanclooster et al., 1994).

Heat Transport

Heat transport was modeled with the one-dimensional Fourier transport equation. The soil thermal properties (conductivity and volumetric heat capacity) were calculated as suggested by de Vries (1952).

Solute Transport

Solute transport was described by the convection–dispersion equation with a linear reversible adsorption isotherm for reactive solutes:

$$\frac{\partial(\theta C_r)}{\partial t} + \rho K_d\frac{\partial C_r}{\partial t} = \frac{\partial}{\partial z}\left(\theta D_s\frac{\partial C_r}{\partial z}\right) - \frac{\partial(qC_r)}{\partial z}\sum_i \varphi_i \qquad [9]$$

where C_r is the resident concentration ($M\,L^{-3}$) in the soil solution, ρ the soil dry bulk density ($M\,L^{-3}$), K_d the solute distribution coefficient ($L^3\,M^{-1}$), D_s the apparent dispersion coefficient ($L^2\,T^{-1}$), q the Darcian water flux ($L\,T^{-1}$), and $\Sigma_i\varphi_i$ a solute sink term ($M\,L^{-3}\,T^{-1}$) that includes crop uptake and transformations. Here we are mainly interested in nitrate and ammonium transport. Transformations refer to the N cycle.

Nitrogen uptake by the crop was described using a macroscopic model, and the uptake rate was restricted to a potential level. The potential uptake rate depends on a maximum N uptake rate, N_{max} ($M\,L^{-2}$), specified by the user, and is separated into a convective and diffusive fraction. The convective fraction is a function of water uptake and the total concentration of nitrate and ammonium. The diffusive fraction, calculated only

Table 3a. Summary of soil hydraulic and other parameters used in the WAVE model for the corn plot.

Site	Layers	ρ	θ_r	θ_s	α_d	*n*	K_s	η	λ
	cm	Mg m^{-3}	m^3 m^{-3}		cm^{-1}		cm d^{-1}		(mm)
Maré	0–14	0.68	0.02	0.65	0.115	2.16	720	0.16	30
	14–34	0.77	0.02	0.65	0.115	2.16	700	0.20	30
	34–52	0.88	0.02	0.65	0.115	2.16	600	0.20	30
	52–152†	0.80	0.0	0.03	0.030	2.50	90	0.50	30
La Côte Saint-André	0–40	1.38	0	0.30	0.16†	2.12†	35†	0.12	100
	40–60	1.34	0	0.30	0.05	2.17	12	0.17	100
	60–75	1.28	0	0.33	0.04	2.27	15	0.27	100
	75–150	1.30	0	0.33	0.15	2.22	15	0.22	100

† Calibrated value.

if the convective uptake rate is smaller than the potential level, is a function of the root density depth profile RDENS (z), the mean root radius RORAD (L), and the average distance between the soil solution and the root surface D0 (L).

The apparent dispersion coefficient D_s is calculated as:

$$D_s = \lambda\frac{q}{\theta} + D_e \quad [10]$$

where λ is the dispersivity (L) and D_e is the effective diffusion coefficient (L^2 T^{-1}) given by:

$$D_e = \frac{D_o\, a\exp(b\theta)}{\theta} \quad [11]$$

in which D_o is the molecular diffusion coefficient of the considered solute in pure water (L^2 T^{-1}) and *a* and *b* are empirical constants.

When solute is applied at the soil surface (during a fertilization or irrigation event), it is assumed to dissolve instantaneously in the mass of water entering the profile during the day of solute application (or the first day when infiltration occurs).

Nitrogen Cycle

The mineral N transformations (i.e., nitrification, denitrification, and volatilization) are described by means of first-order kinetics. The corresponding rate constants (K_{nit}, K_{denit}, and K_{vol}, respectively) are functions of soil temperature and water content as proposed by Johnsson et al. (1987) and Vereecken et al. (1990). Mineralization of the N from the organic matter is assumed to occur from three distinguishable soil organic matter fractions: litter, manure, and humus. The N demand for the internal cycling of C and N in the three pools is regulated by a constant C/N ratio identical for the soil biomass and the metabolization products. These three organic pools are characterized by degradation constants (T^{-1}) called K_{lit}, K_{man}, and K_{hum} respectively, which are also functions of soil temperature and water content. The turnover efficiency, f_e, determines which fraction is decomposed into CO_2, with the remainder being assimilated into another organic form. The humification constant f_h determines which fraction of the effectively turned-over C transfers to the humus pool.

Initial Conditions

The user has to specify an initial water content or pressure head value, as well as the initial concentration of solutes in each soil compartment. The initial concentrations of C and N in the different organic matter pools must also be entered by the user.

Model Parameters and Model Forcings

Soil Profiles

The soil profile was numerically discretized into compartments of 2 cm (in Maré) and 5 cm (in La Côte Saint-André) thickness and grouped into three and four pedological soil layers for the Maré and La Côte Saint-André sites, respectively, each having constant physical, chemical, and biological parameters (Table 2). We were interested in the quantities of water and NO_3 leaving the base of the root zone at 40 cm depth in Maré and at 80 cm depth in La Côte Saint-André.

Boundary Conditions

At Maré, a free drainage boundary condition at the very bottom of the soil profile was imposed by adding a fourth layer going down to 1.50 m. This deeper layer, which mimicked the underlying coral rock below the root zone, was described using hypothetical flow and transport properties. At La Côte Saint-André, the fourth existing layer was extended down to 1.50 m. The upper boundary condition was chosen to be a flux type with no ponding at the soil surface since the saturated hydraulic conductivity at both sites was higher than the rainfall and irrigation intensities.

The model used a variable time step, smaller than 1 d for strongly dynamic processes, such as the flow and transport processes and the solute transformations. Model input was specified on a daily basis, while the boundary conditions were assumed constant during a given day. This means, for example, that the daily precipitation is distributed equally over a day.

Water Flow

Water flow was first simulated for bare soil plots where only the hydrodynamic characteristics of each soil layer and the potential evaporation rate had to be estimated. For cultivated plots, more processes had to be considered: plant transpiration, function of leaf area development, water uptake by plant roots, and rainfall interception by the crop canopy. Hence, a number of parameters had to be determined by measurement or literature review.

The soil water retention curves were determined using the coupled measured water content and pressure heads at the same times and depths. The hydraulic conductivity was determined using the zero-flux plane method (Vachaud et al., 1978), and a tension disk infiltrometer (Ankeny et al., 1991; Angulo-Jaramillo et al., 1996) for values near saturation. Values of the fitting parameters of Eq. [2] and [3] are given in Table 3a (note that η of Eq. [3] was set equal to $n - 2$, except for the

Table 3b. Summary of some of the WAVE parameters under corn for the nitrogen cycle.

Site	Horizon	K_{nit}	K_{denit}	K_{hum}	K_{lit}
	cm	d^{-1}			
Maré	0–10	0.5	0.02	7×10^{-5}	8×10^{-3}
	10–30	0.5	0	7×10^{-6}	8×10^{-4}
	30–52	0	0	0	0
La Côte Saint-André	0–40	0.5	0	10^{-5}	8×10^{-3}
	40–85	0.5	0	7×10^{-8}	10^{-4}
	85–150	0	0	0	0

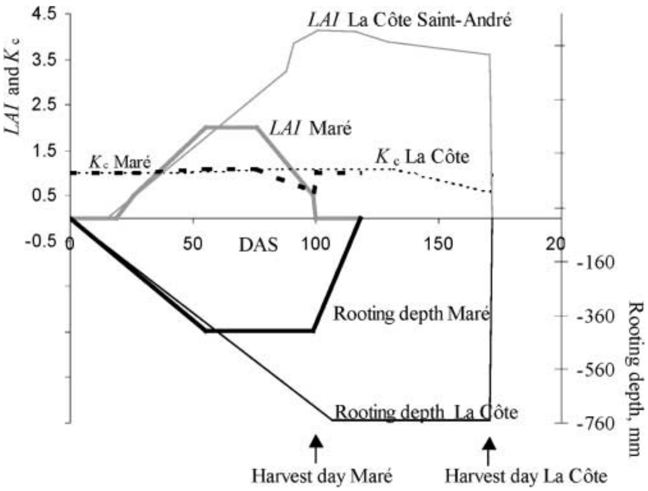

Fig. 1. Evolution in time (days after sowing, DAS) of LAI, K_c, and rooting depth at both sites.

subsoil layer at Maré). Those two functions were determined on bare soil and corn plots independently.

The potential evapotranspiration ET_o was calculated using the Penman–Monteith equation with daily values of wind speed, solar radiation, relative air humidity, and temperature measured at the field sites. K_c values were taken from Doorenbos and Pruitt (1977) with the dates of the different corn growth stages as observed in the field (Fig. 1). LAI were measured at La Côte Saint-André (Normand, 1996) and evaluated from values given in Eik and Hanway (1966) for Maré (Fig. 1). Since no values of $CanStor_{max}$ for corn were found in the literature, a value of 3 mm d^{-1} for small trees, as given by Rutter and Morton (1977), was used.

The relationship between the water stress reduction factor for root water uptake and the pressure head was considered hyperbolic. The critical wet-end pressure head above which water uptake is reduced was set equal to 100 cm, while the dry-end pressure head values were set equal to 1000 and 500 cm, for the Maré and La Côte Saint-André sites, respectively. The maximum root water uptake function $S_{max}(z)$ was determined using root length distribution observed in the field and taken from a literature review (Novak, 1987; Vanclooster et al., 1994). $S_{max}(z)$ was set to 0.02 d^{-1} at the surface of the Maré site, and assumed to decrease linearly to 0 at 40 cm depth. For La Côte Saint-André, $S_{max}(z)$ values were 0.01 d^{-1} in the upper layer (0–20 cm) and 0.001 d^{-1} from 20 to 75 cm depth.

Heat Transport

As mentioned above, parameters to describe heat transport, such as soil specific heat capacity and soil thermal conductivity, were calculated within the model depending on soil bulk dry density (ρ values given Table 2). The model assumes that the soil surface temperature is equal to air temperature at 2 m above the soil surface, which is calculated from the minimum and maximum temperature as specified by the user, while the temperature of the bottom boundary condition was fixed at 7°C. Since there were no soil temperature measurements for the Maré site, these conditions were kept constant. For La Côte Saint-André, available measurements of air and soil surface temperature showed a 4°C difference. Thus the upper boundary condition was defined as measured air temperature plus 4°C. For the bottom boundary condition, the soil profile being extended to 1.50 m, the temperature was fixed at a reasonable value of 7°C.

Solute Movement

The diffusion coefficient D_o and the empirical constants a and b in Eq. [11] were fixed at the following values: D_o = 120 mm^2 d^{-1}, a = 0.001 and b = 1.0 (Wagenet and Hutson, 1989). The dispersivity λ was set at 100 mm for La Côte Saint-André, estimated from breakthrough curves of inert solutes measured in a large undisturbed lysimeter near the experimental plot (Schoen et al., 1999), and at 30 mm for the Maré site after calibration.

The NO_3 was assumed to be more or less inert for the La Côte Saint-André soil ($K_d = 10^{-9}$ m^3 kg^{-1}), but shown to be reactive for the Maréan soil ($K_d = 10^{-4}$ at the surface and 4×10^{-4} m^3 kg^{-1} for the deeper layers) as determined on soil columns (Duwig et al., 1999; Duwig et al., 2003). Ammonium was assumed to be inert at Maré but reactive at La Côte Saint-André ($K_d = 1.5 \times 10^{-3}$ m^3 kg^{-1}, Vereecken et al., 1991).

Nitrogen Cycle and Nitrate Uptake by Plants

Some of the N turnover parameters were selected from literature values given in the user's manual of WAVE. The C turnover efficiency f_e was fixed at 0.6 for Maré, as advised by McGill et al. (1981) for a well-aerated soil. For La Côte Saint-André, f_e was set equal to 0.3, which is the middle point of the range [0.05; 0.6] advised by Vanclooster et al. (1994). The humification constant f_h is usually fixed at 0.2 for rapid recycling (Johnsson et al., 1987 in Vanclooster et al., 1994). The total soil organic matter was distributed across the litter (5% for Maré and 2% for La Côte Saint-André, C/N ratio = 30) and the humus pool (C/N ratio = 10). The C/N ratio of the metabolized products and the soil biomass was measured to be 11 for Maré. For La Côte Saint-André, it was calculated as the average of the C/N value for biomass in arable soils given in Bradbury et al. (1993) (C/N = 6.7) and the measured value of the organic matter at the soil surface (C/N = 10.3 for La Côte Saint-André; see Table 2).

The decomposition rate of the humus pool K_{hum} was initially set at 7×10^{-5} d^{-1} for the entire soil profiles of both sites, but later calibrated since the simulated NO_3 leaching was overestimated. The best fit for Maré was found to be 7×10^{-5} d^{-1} between 0 and 15 cm and 7×10^{-6} d^{-1} below 15 cm. These values are relatively small compared with those given by Desjardins et al. (1994) for an Ultisol in Brazil. However, the biodegradation of organic matter decreases significantly when it is complexed by Al and Fe oxides (Boudot et al., 1989). For La Côte Saint-André, K_{hum} was 10^{-5} d^{-1} between 0 and 30 cm and 7×0^{-8} d^{-1} between 30 and 75 cm. The decomposition rate of the litter pool K_{lit} was calibrated to 8×10^{-3} d^{-1} in the surface layer and to a smaller value in the deeper layer (8×10^{-4} d^{-1} for Maré and 10^{-4} d^{-1} for La Côte Saint-André). No manure was applied at either site.

Nitrification of mineral N at both sites was described by a nitrification constant of K_{nit} = 0.5 d^{-1} since ammonium was found to disappear rapidly from the soil solution. The denitrification constant K_{denit} was taken to be 0.02 d^{-1} for Maré, as given by Jabro et al. (1995). The denitrification activity of the soil from La Côte Saint-André was studied in the laboratory and found to be relatively low compared with others soils, from 0.07 to 0.13 μg N g^{-1} h^{-1}. Tables 3a and 3b summarize all the values of the parameters that were used in the model for the corn plot.

Considering N content measured in mature plants, the maximum N root uptake (N_{max}) was fixed at 70 kg N ha^{-1} for Maré and 300 kg N ha^{-1} for La Côte Saint-André. Information about root density were found in Durieux et al. (1994); densities at the soil surface were fixed at 3000 and 3400 cm m^{-1} for Maré and La Côte Saint-André, respectively. The model constrains the root density to decrease exponentially with depth, and the corresponding decay coefficient was fixed at 0.0016 and 0.002 mm^{-1} for Maré and La Côte Saint-André, respectively. D0 was set to 0.10 mm for Maré as suggested in the user's manual of WAVE. For La Côte Saint-André, a much smaller value of 0.001 provided the best model fit.

Modeling Approach

The model was calibrated step by step because of the interactions among many of the N fate and transport processes involved (Normand, 1996). Nitrogen transformation parameters were calibrated using bare-soil plot data without fertilizer amendment. Addition of fertilizer to the bare soil plot allowed us to calibrate the convective and dispersive parameters for solute transport. Below we present only results for the bare soil plots with fertilizer. Finally, data from the cultivated plots were used to determine the remaining parameters related to N uptake by plant roots. This calibration procedure relies on the assumption that the transport and transformation parameters do not vary from plot to plot. A trial and error method was adopted, using statistical and graphical criteria for evaluating model performance. An intermediate sensitivity analysis was performed to address the critical parameters in the system. This calibration procedure was followed using 1992 measurements for La Côte Saint-André since the annual rainfall was close to the average rainfall from 1952 to 1998 (953 vs. 907 mm). For Maré, we used 1996 for calibration since that year had the most data. The prediction capability of the model was subsequently evaluated on the two remaining years, 1995 and 1997, for Maré, and 1991 and 1993 for La Côte Saint-André.

To express differences between the simulated and observed values in terms of statistical quantities, we used the modeling efficiency EF, the root mean square error RMSE, as defined by Loague and Green (1991), as well as the bias B, as follows:

$$\mathrm{EF} = \frac{\sum_{i=1}^{n}(O_\mathrm{i} - \overline{O})^2 - \sum_{i=1}^{n}(P_\mathrm{i} - O_\mathrm{i})^2}{\sum_{i=1}^{n}(O_\mathrm{i} - \overline{O})^2} \qquad [12a]$$

$$\mathrm{RMSE} = \frac{100}{\overline{O}}\sqrt{\frac{\sum_{i=1}^{n}(P_\mathrm{i} - O_\mathrm{i})^2}{n}} \qquad [12b]$$

$$B = \frac{\sum_{i=1}^{n}(P_\mathrm{i} - O_\mathrm{i})}{n} \qquad [12c]$$

where P_i and O_i are the model calculated and observed values respectively, n is the number of samples, and $\overline{O}$ is the mean of the observed data. These statistical quantities were calculated on unsorted data, observed and predicted values being compared directly. EF, RMSE and B should be as close as possible of 1, 0, and 0 respectively. A negative value of EF indicates that the model-predicted values are worse than simply using the observed mean.

RESULTS AND DISCUSSION

Since the WAVE model is a mechanistic model, we found it important to not only compare fluxes across the boundaries of the soil profile (drainage and leaching rates at the bottom and actual evapotranspiration at the top), but to look also at internal state variables, such as soil water contents, water pressure heads, and NO_3 concentrations at selected depths.

Water Flow

At a depth corresponding to the base of the corn root zone (40 cm at Maré and 80 cm at La Côte Saint-André), simulated and measured state variables (θ and h for the bare soil with fertilizer and the corn plots) and fluxes (drainage and actual evapotranspiration rates for the bare and corn plots) for both the calibration and the prediction periods are presented in Fig. 2a (Maré) and 2b (La Côte Saint-André). The statistical values (Eq. [12]) are given in Table 4.

Step 1: Model Calibration

For Maré, the only parameters related to water flow that were not measured were the hydraulic functions of the coral rock layer below the root zone (between 50 and 150 cm). A sensitivity analysis (Duwig, 1998) revealed that these parameters did not have a large influence on cumulative drainage model output at 40 cm depth.

For La Côte Saint-André, water retention and hydraulic conductivity parameters were calibrated, since the experimental curves did not give much information at the lower water contents. The calibration was performed in a trial and error approach defining as objective functions both the measured time series of soil moisture and pressure head and the measured cumulative fluxes at the boundaries. Parameters of the top layer were found to be the most important (Normand, 1996). Among those, the scale parameter α_d (Eq. [2]) was the most sensitive to annual cumulative drainage at the base of the soil profile and evapotranspiration (respectively, +5/−30% and −13/+77% for a change of ±80% on the bare soil). Shape parameters (m, n, and η) were sensitive to time series of the pressure head, especially to the lowest values obtained during the crop season. The saturated hydraulic conductivity measured using a monodisk tension infiltrometer (around 1.3 cm d^{-1} at a saturated water content of 0.3 $cm^3\ cm^{-3}$) produced almost 190 mm of runoff, whereas no ponding water at all was observed at the soil surface during the experiment. K_s was thus calibrated so that no runoff occurred (see Table 3).

For the bare soil plots of both sites, water contents and drainage at depths corresponding to the base of the corn root zone (40 cm at Maré and 80 cm at La Côte Saint-André) were well simulated (Fig. 2a and 2b). For both water content and pressure head, agreement between measurements and simulations was also fair (EF values larger than 0.4, RMSE values lower than 50%, and B close to 0; see Table 4). However, at La Côte Saint-André, simulations were not so good in the top layer. The model overestimated water contents at 10 cm depth, leading to a negative EF value. Measurements with a neutron probe are less accurate close to the soil surface (between 0 and 15 cm depth). At 15 cm depth, pressure head showed larger differences than those for deeper depths, as shown by the larger RMSE value.

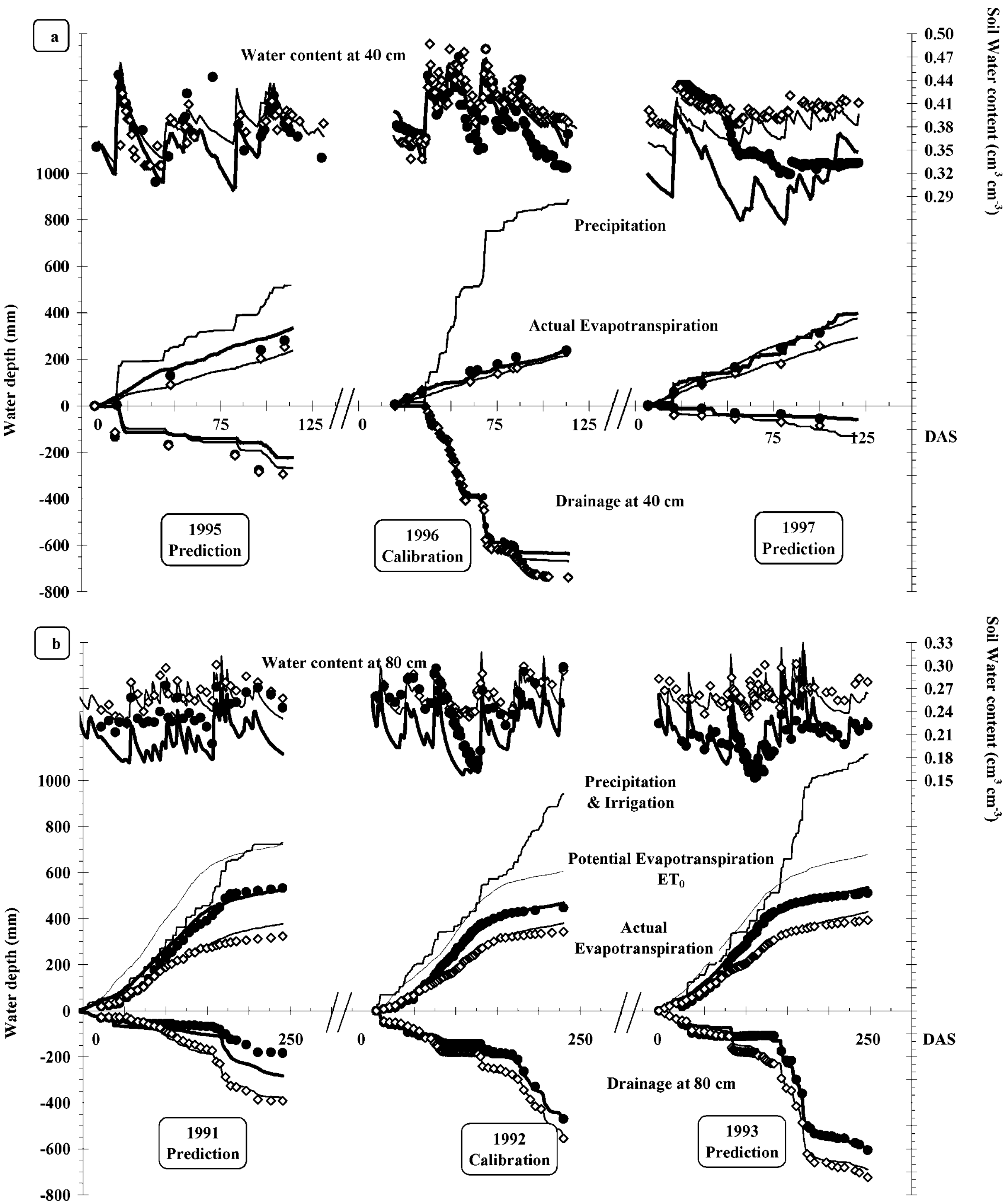

Fig. 2. Components of the soil water balance at (a) Maré and (b) La Côte Saint-André: measurements on bare soil with fertilizer (◇) and on corn plots (●); simulation on bare soil (thin line) and on corn plots (thicker line). DAS is days after sowing.

As explained above, some parameters describing evaporation and plant water uptake on the corn plot had to be taken from the literature. Water contents on Maré were simulated satisfactorily, except at the end of the cycle when soil dries out quicker than was simulated (Fig. 2a). The model stopped all root uptake at the

Table 4. Values of EF, RMSE, and *B* (Eq. 12) between observed and simulated values of *h*, θ, and *C* for the bare soil and corn plots at different depths. *B* is given in centimeters for the pressure head, in cubic centimeters per cubic centimeter for the water content, and in milligrams NO_3–N per liter for the concentrations. *n* is the number of observations.

	Bare soil			Corn		
EF, RMSE, *B*	1995‡	1996†	1997‡	1995‡	1996†	1997‡
			Maré			
h (cm)	*n* = 25	*n* = 59	*n* = 69	*n* = 56	*n* = 56	*n* = 53
10 cm	0.7, 23, −16.7	0.8, 35, 30.6	0.5, 35, 46.0	0.6, 34, 13.2	0.3, 48, 68.9	<0, 356, −1083
20 cm	0.5, 23, −18.3	0.8, 29, 4.2	0.4, 30, −17.9	0.2, 44, 48.3	0.5, 41, 85.7	<0, 216, −753
30 cm	0.9, 10, −0.2	0.9, 16, 12.7	0.2, 30, 27.4	0.5, 48, 63.3	0.5, 35, 59.8	<0, 208, −768
40 cm	0.7, 15, 3.7	0.8, 22, 25.7	0.1, 27, 29.7	0.5, 49, 53.5	0.3, 32, 35.3	<0, 225, −799
50 cm	0.0, 19, 27.7	0.8, 21, 22.7	<0, 28, 47.2	0.4, 43, 66.0	0.3, 33, 46.9	<0, 229, −797
θ (cm^3 cm^{-3})	*n* = 29	*n* = 72	*n* = 68	*n* = 31	*n* = 68	*n* = 61
10 cm	0.1, 13, 0.02	0.7, 11, −0.02	<0, 18, −0.05	0.7, 11, 0.02	0.2, 18, 0.04	0.5, 11, 0.00
20 cm	0.3, 9, 0.01	0.7, 8, 0.009	<0, 11, −0.03	0.8, 7, −0.01	0.5, 9, −0.01	0.4, 15, 0.02
30 cm	0.3, 11, 0.00	0.7, 6, −0.005	<0, 13, −0.05	0.7, 9, 0.008	0.4, 9, 0.02	0.1, 13, 0.02
40 cm	<0, 11, 0.02	0.4, 5, −0.002	<0, 6, −0.02	0.8, 7, 0.01	0.2, 8, 0.02	<0, 17, 0.05
C (mg N L^{-1})	*n* = 6	*n* = 25	–	*n* = 6	*n* = 25	–
10 cm	<0, 92, 27.4	<0, 98, 7.3	–	<0, 78, −4.8	<0, 78, −7.9	–
40 cm	<0, 82, 16.8	<0, 64, 4.4	–	<0, 75, 9.8	0.4, 57, 1.1	–
			La Côte Saint-André			
EF, RMSE, *B*	1991‡	1992†	1993‡	1991‡	1992†	1993‡
h (cm)	*n* = 109	*n* = 133	*n* = 158	*n* = 109	*n* = 134	*n* = 156
15 cm	0.8, 34, −4.4	0.5, 71, 19.1	0.4, 95, 22.8	0.4, 78, −28.5	<0, 322, −117	<0, 141, −103
30 cm	0.8, 29, 0.5	0.7, 49, −3.4	0.6, 57, −12.1	0.3, 83, 85.0	0.7, 72, −11.4	0.8, 49, 5.2
50 cm	0.4, 26, 12.3	0.6, 26, 6.2	0.5, 24, −2.8	0.0, 91, 70.8	0.7, 55, 14.8	0.5, 61, 25.2
70 cm	0.0, 28, 13.1	0.5, 24, 6.5	0.3, 21, −0.7	0.0, 44, 4.1	0.7, 43, 10.0	0.6, 36, 3.3
90 cm	<0, 28, 9.6	0.5, 21, 0.2	0.0, 30, −4.8	<0, 40, 2.9	0.6, 52, 19.5	0.6, 35, 4.4
θ (cm^3 cm^{-3})	*n* = 31	*n* = 54	*n* = 65	*n* = 31	*n* = 51	*n* = 62
10 cm	<0, 13, −0.03	<0, 15, 0.03	<0, 37, 0.06	<0, 19, −0.04	<0, 14, 0.01	<0, 15, −0.03
30 cm	<0, 18, −0.05	0.6, 5, 0.00	0.5, 5, 0.00	<0, 19, −0.05	0.5, 14, −0.01	0.5, 10, −0.01
50 cm	<0, 7, 0.01	0.4, 4, 0.00	<0, 5, 0.00	<0, 6, −0.01	0.8, 8, 0.00	0.5, 8, −0.01
70 cm	<0, 7, 0.01	0.5, 5, 0.01	<0, 7, 0.00	<0, 9, −0.01	0.7, 8, 0.00	<0, 15, 0.03
80 cm	0.3, 6, −0.01	0.8, 3, 0.00	0.0, 6, −0.01	<0, 16, −0.03	<0, 17, −0.04	0.1, 10, 0.01
C (mg N L^{-1})	*n* = 28	*n* = 29	*n* = 34	*n* = 29	*n* = 26	*n* = 29
30 cm	0.5, 62, −22.1	0.4, 54, 2.3	0.1, 84, 10.5	0.5, 52, 14.4	<0, 76, 0.2	0.3, 111, −27
50 cm	0.6, 33, −8.7	0.5, 30, 1.9	0.4, 64, 4.6	0.7, 29, 3.8	0.2, 70, 3.2	0.4, 39, −8.5
80 cm	0.5, 44, −2.9	<0, 49, 3.3	<0, 56, 1.8	<0, 103, 31.1	0.6, 35, 0.5	<0, 56, −4.6

† Model calibration.
‡ Model prediction.

harvest date (Table 1). However, the corn plants were left uncut during more than 1 mo after grain harvest. These plants plus the weeds that colonized the plots must have continued to consume water. This may explain why the EF values were lower and RMSE and *B* were higher than those calculated for the bare soil plot (Table 4). Indeed, parameters describing crop water uptake were determined with less precision than those describing water flow, thus leading to more imprecise simulations of state variables and cumulated drainage.

For La Côte Saint-André, the maximum root water uptake rate, S_{max} (Eq. [4]), was calibrated by trial and error. Both the cumulative drainage at the base of the root zone and the actual evapotranspiration were accurately simulated (Fig. 2b). Nevertheless, internal state variables were not so well reproduced. In particular, from 100 to 130 days after sowing (DAS), calculated pressure heads at depths deeper than 30 cm did not reach the very low observed values (−400 cm at 50 cm depth and −300 cm at 70 cm depth), whereas the model also systematically underestimated water content at the base of the root zone (80 cm), leading to negative EF and *B* values (Fig. 2b and Table 4). As observed for the bare soil plot, pressure heads at 15 depth were badly reproduced, with all three statistical indicators far from the ideal values. At lower depths, the correlation between measurements and simulations was better, as indicated by much larger EF values (0.6–0.7), even though a large deviation persisted (RMSE > 43%).

A sensitivity analysis of drainage for the unmeasured parameters K_c, LAI, S_{max}, and $CanStor_{max}$ for Maré is presented in Fig. 3. The cumulative drainage was not very sensitive to the root water uptake parameters. This is

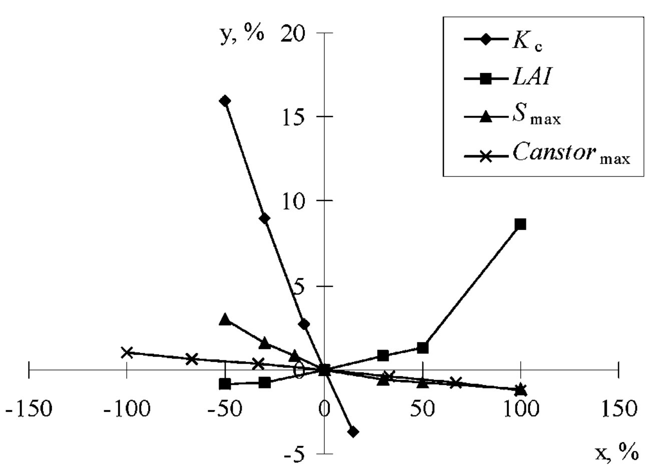

Fig. 3. Sensitivity of cumulative drainage (*y*-axis) toward parameters defining interception and root extraction of water by corn (*x*-axis), in 1996 for Maré.

partly due to the fact that 1996 was a very wet season and water uptake by plant was low compared with other components of the water balance. The most sensitive parameter was K_c, which was also among the most difficult parameters to determine. Curiously, increasing LAI produced larger drainage rates. In fact, when increasing the *LAI* and leaving all other parameters constant, soil evaporation decreased more than the added increase of interception by canopy and plant transpiration. This situation appears impossible because for a larger LAI, $CanStor_{max}$ as well as S_{max} should also be larger and drainage would then decrease. Similar results were obtained for La Côte Saint-André (results not shown). This sensitivity analysis highlights the uncertainty in model outputs when estimating parameters within a range of values.

Step 2: Model Prediction

The calibrated parameters were used to simulate the state variables and fluxes in 1995 and 1997 (Maré) and 1991 and 1993 (La Côte Saint-André) with the appropriate climatic inputs.

For Maré, the 1995 and 1997 cropping seasons were much drier than in 1996 (see Table 1). In 1995 at both plots, the predicted pressure heads (not shown here) and water fluxes were very close to the measured values (Fig. 2a), giving good values for the statistical indicators for the pressure head (Table 4). However, EF values for the water content of the bare soil were less satisfying. This may be explained by spatial variation in the retention curve $h(\theta)$ due to the fact that the instruments were removed at the end of each corn cycle before soil tillage. A similar change would explain the poor simulation of the water content of the bare soil plot in 1997. Indeed, EF values were negative. However, notice that RMSE values are in the same range as those obtained for the calibration year. This shows that the correlation between measurements and simulation is strong but with a systematic bias. Thus, a unique statistical indicator may not to be sufficient to evaluate the model simulations. For the 1997 corn plot, water contents were well simulated, whereas pressure heads were severely underestimated (pressure heads being negative) by the model. It did not rain for nearly 1 mo from DAS 30 to DAS 60. The soil then became very dry under the corn, and the tensiometers stopped functioning properly for pressures lower than −700 cm. Furthermore, the parameters describing crop growth were left unchanged from 1996 to 1997. In 1997, since the climate was much drier, plants must have been under water stress.

For La Côte Saint-André (Fig. 2b), the 1993 season was wetter than the calibrated one (1992) and the predicted water content and terms of the water balance were once again very close to the measured values for both plots. For the corn plot, the annual cumulative drainage and evapotranspiration rates were well predicted, except from DAS 15 to DAS 80.

The 1991 season was drier (see Table 1). For the bare soil, simulations of evapotranspiration and drainage were still very close to the observed values, whereas the state variables were poorly predicted, as reflected by the EF values shown in Table 4. At 50 and 70 cm depth, the small RMSE and *B* values showed a strong correlation between measurements and the simulation, but far from the one-to-one line. For the corn plot, the model overestimated drainage during summer, while the evapotranspiration rate was simulated very well, thus reflecting a poor prediction of the change in soil water storage. At every depth, the EF values were either negative for the water content or very low for the pressure head. Those poor results were expected, since the calibrated water retention curve determined in 1992 did not fit the measured sets of pressure heads and water contents in 1991. This may have been due to a temporal change in soil hydraulic properties. This explanation is consistent with findings by Angulo-Jaramillo et al. (1997), who showed that during the corn growing season the structure of the fine fraction of soils at La Côte Saint-André changed from a well-interconnected microporous network to a poorly connected one. Furthermore, due to tillage operations performed in spring a few weeks before sowing, and to winter freezing, all the measurement devices were removed from the soil in December and reinstalled after tillage, but not exactly at the same place.

The way we used WAVE for prediction purposes faced several difficulties:

1. There was no correlation between plant development and water and nutrient availability.
2. Soil hydraulic properties varied from one year to another, and also spatially since the measurement devices had to be removed every year before each tillage.

Nitrate Movement

The measured NO_3 collected with the solution samplers at the base of the corn root zone (40 cm in Maré, and 80 cm in La Côte Saint-André), the total amount of NO_3 present in the root zone (expressed in kg N ha^{-1}), and cumulative mass leaching are compared with the model simulations (Fig. 4a and 4b). Statistical indicators were calculated for NO_3 concentration at various depths (Table 4). Nitrate storage and leaching were not measured in 1997 at Maré because there were very few dates when soil solution could be sampled in suction cups because of very severe drought conditions.

Step 1: Model Calibration

The first step in our calibration was to estimate some of the parameters involved in the N cycle using measurements made on the bare soil plot without fertilization, especially those describing the soil production capacity (nitrification rate constant and humus mineralization rate; results not shown). The same parameters were then used to simulate the concentrations and leaching from the fertilized bare soil plot.

Figure 4a shows concentration, storage, and cumulative leaching values vs. time for the Maré site in 1996. For the bare soil, all variables were well simulated, except for the concentrations after the second fertilizer input. However, cumulative leaching was correctly sim-

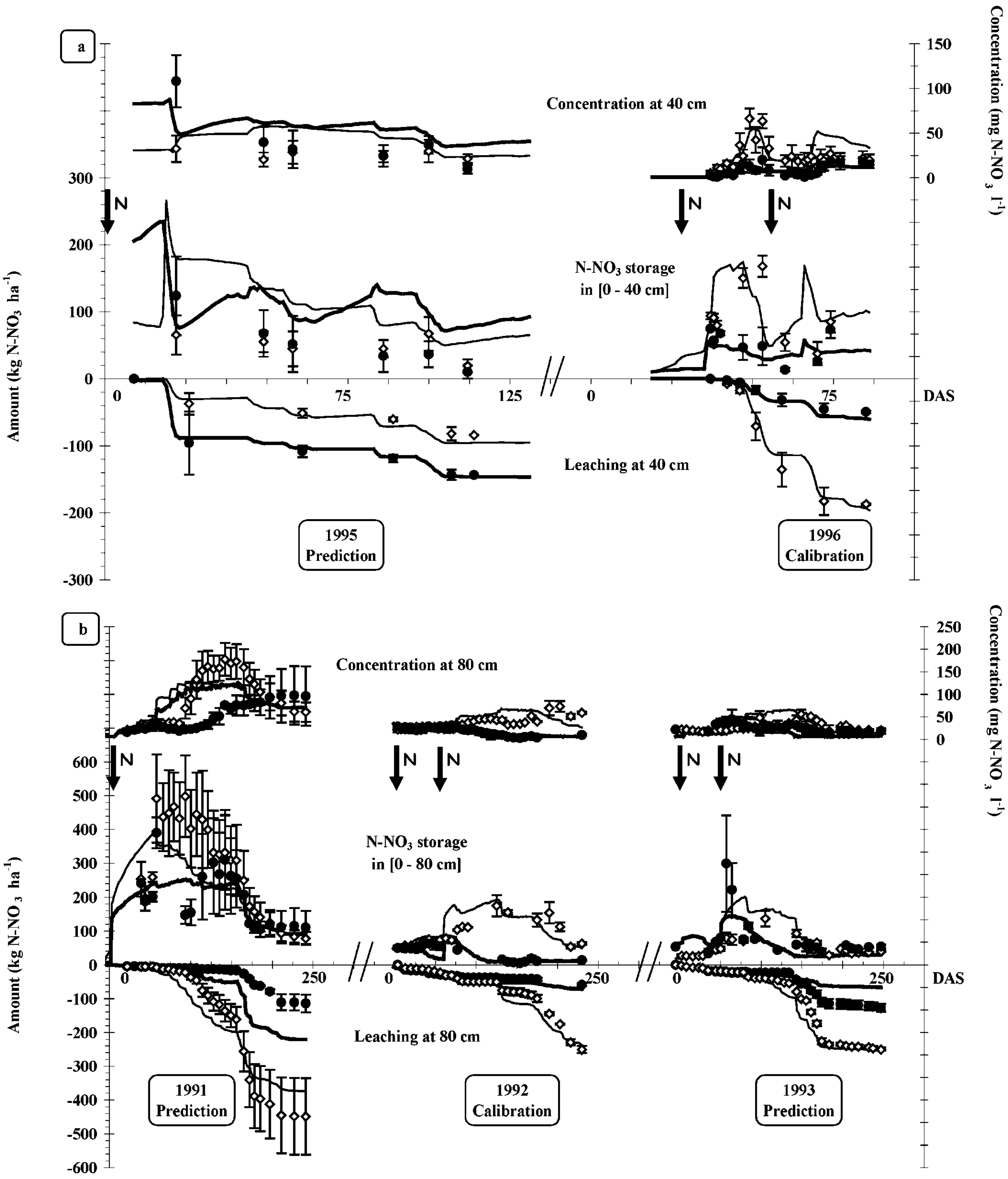

Fig. 4. Components of the soil NO_3–N balance at (a) Maré and (b) La Côte Saint-André: measurements on bare soil with fertilizer (◇) and on corn plots (●); simulation on bare soil (thin line) and on corn plots (thicker line). DAS is days after sowing. Error bars are estimates of standard deviations between six replicates of soil NO_3–N concentration. Arrows indicate the time of fertilizer inputs.

ulated. The fertilizer was given just 10 d before a cyclone that produced 238 mm of rain in 4 d. The model assumed that the fertilizer instantaneously dissolved in the soil solution and thus infiltrated with the water. In reality, this may not have been the case because of the time-dependent dissolution of solid fertilizer and adsorption of NO_3 on soil particles. This adsorption is nonlinear (Duwig et al., 2003) and depends on NO_3 concentration, two features that were not considered by the model. The measured NO_3 peak was thus lower and more dispersed. EF values were lower than 0, and RMSE values were quite large. The use of suction cups for measuring soil solution NO_3 concentrations leads to very dispersed data. Furthermore, the discrepancy between the second simulated and measured peaks also produced poor EF values.

For the bare soil at La Côte Saint-André (Fig. 4b), calibration was performed to best fit the beginning of the concentration time series. Sensitive parameters were initial contents in NH_3 and NO_3, nitrification, humus and litter mineralization rates. Those rates drastically decreased in the deeper part of the profile (depths >30 cm), reflecting the fact that microbial activity was not very effective due to a lack of available nutrients and/or C. However, no parameter set could be found to accurately fit the data around DAS 60 where part of the fertilizer input was not observed in the field. From DAS 53 to DAS 78, the model overestimated the observed NO_3 in the top of the soil profile by nearly 100 kg N ha^{-1} (Fig. 4b). The apparent disappearance of the NO_3 after fertilization, and the associated slow release in early spring, could be interpreted as an artifact caused by heterogeneous flow in the soil and difficulty producing representative soil water samples with the solution samplers in the heterogeneous flow domain. The remaining time series were quite well reproduced by the model (positive EF values and small *B* values), especially the soil NO_3 content remaining at corn harvest (DAS 168) and at the end of November (DAS 216) after autumn rainfall. Leaching was only influenced by the concentration at 80 cm and the water percolation rate, while the cumulative value was simulated quite accurately. However, time series at 80 cm were less well predicted, as reflected in the negative *EF* values for the concentration (Table 4).

To simulate NO_3 behavior in the crop plots, the last step was to take into account NO_3 root uptake. Parameters describing crop NO_3 uptake (both convective and diffusive parts) were calibrated and initial concentrations of total N and C were modified relative to those

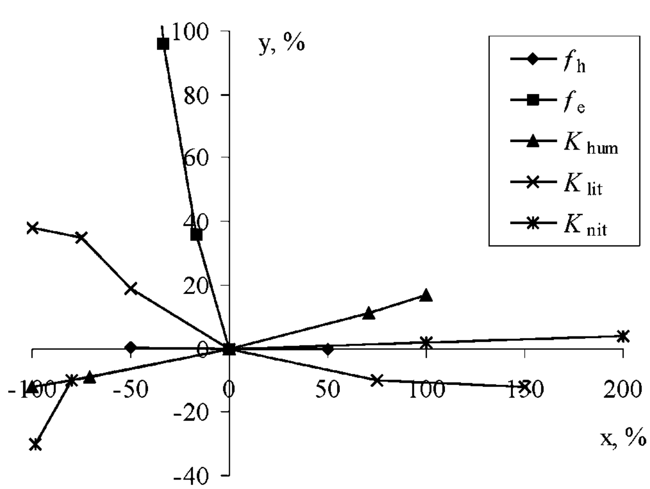

Fig. 5. Sensitivity of cumulative NO_3 leaching (*y*-axis) toward organic matter transformation parameters (*x*-axis), in 1996 for Maré.

for bare soil, since harvest residues were incorporated into the soil. Measured and simulated concentrations and NO_3 leaching at the base of the root zone are presented on Fig. 4a and 4b for Maré and La Côte Saint-André, respectively.

Concentrations peaks for the Maré corn plot (Fig. 4a) were well predicted, suggesting the dispersivities were reasonable. Plant uptake (as measured by analysis of total N in plant samples; data not shown) and cumulative leaching were simulated quite well (<10 kg ha^{-1} difference) considering the variability in measurements with suction cups and in analyses of plant materials. However, simulated mineralization (35 kg N ha^{-1}) and net nitrification (40 kg N ha^{-1}) were somewhat lower for the relatively hot and humid climate conditions. We decided not to modify parameters related to these transformations since there were already too many unknowns. The statistical indicators at 10 cm depth were quite poor, presumably, as explained above, because soil solution NO_3 contents measured with suction cups are highly variable, especially near the soil surface. However, all three statistical indicators values at 40 cm depth were acceptable, which is quite satisfying.

For the La Côte Saint-André corn plots (Fig. 4b), in the upper part of the profile (0–50 cm), the model underestimated concentrations between the two fertilizer applications, resulting in less NO_3 storage, as shown in Fig. 4b. During this period, measured concentrations remained almost constant, which may be explained by a balance between crop uptake and production due to mineralization. Conversely, the decrease in NO_3 storage after the second fertilizer application was well reproduced. During the growing season, the model generated higher plant uptake and higher soil NO_3 production rates, which were not in phase with the observed rates. On the water balance graph (Fig. 2b), it has already been observed that the final cumulative evapotranspiration value was well reproduced, whereas the simulated time series did not always match the observed ones. In any case, the model accurately reproduced the low amount of NO_3 remaining in the soil at harvest resulting from a reduction of NO_3 fertilization. As the soil remained bare after corn harvest, this is an important point to consider when trying to limit groundwater pollution. Simulated concentrations at 80 cm depth were very close to the measurements as shown by the statistical indicators in Table 4, whereas leaching (both time evolution and final cumulative value) also was simulated accurately.

The calibration was completed by performing a sensitivity analysis. Figure 5 shows the sensitivity of the cumulative NO_3 leaching to parameters defining the turnover of organic matter at Maré. The C turnover efficiency, f_e, was by far the most sensitive parameter. It was calibrated to its maximum possible value of 0.6, but a 30 % decrease in its value increased the leaching by nearly 100%. The degradation rate of the litter pool, K_{lit}, appears also to be a significant parameter. Increasing this rate led to a decrease in NO_3 leaching. In fact, the release of excess mineral N because of more rapid degradation of the litter pool led to its immobilization. When K_{lit} is increased by 150%, the immobilization during the corn growth season is 140 kg ha^{-1}, whereas it is zero when K_{lit} is decreased by 99%. The same trend was observed for La Côte Saint-André.

Step 2: Model Prediction

For the 1995 Maré NO_3 concentration simulations, the 1996 parameters were kept the same, except for the litter pool C/N ratio, which was increased from 20 to 30, considering that there would have been more plant residues because this plot was cultivated for the first time in 1995. One can notice that in 1995, NO_3 leaching was more pronounced under corn than under bare soil. The initial pool of NO_3 was much larger under corn than under bare soil because of different previous agricultural practices (Duwig et al., 2000). Thus, the initial concentration under corn in the model was set larger than under bare soil. For both plots, simulated NO_3 concentrations at 40 cm and NO_3 storage in the root zone overestimated the measurements (Fig. 4a), as shown by the negative EF values and the large RMSE values. There are several explanations for this discrepancy:

1. The model is very sensitive to initial N concentration, which was not measured in 1995.
2. The model is even more sensitive to crop parameters, like the crop coefficient (K_c) or the decomposition rate of the litter pool (K_{lit}), which were not determined in the field, and probably did not extrapolate well from a wet to a drier year.

However, cumulative NO_3 leaching was well simulated. Overestimation of NO_3 concentration in the root zone is thus balanced by other N transformations, which leads to a good representation of leaching.

For the 1991 and 1993 La Côte Saint-André simulations (Fig. 4b), the 1992 parameters were also kept the same, except the initial contents in NH_3 and NO_3. These contents had not been measured directly in the field and hence were adjusted to best fit the beginning of the concentration time series. In 1993, for both plots, EF values calculated for the concentrations at 30 and 50 cm depth were satisfying. For the bare soil, as was observed for the calibration year, simulated concentrations were overestimated immediately after fertilizer application (DAS 50). But from mid September (>148 DAS), simulations were very close to measurements at every depth. Because drainage was very low during the summer (Fig. 2b), the underestimation had only a small impact on the simulated leaching, which appears to be accurately predicted. On the other hand, the model significantly underestimated the concentrations at all depths of the corn plot when the heavy rainfall events started (>140 DAS). This period was crucial for water percolation, and thus the model largely underestimated NO_3 leaching. The year before the experiments, large quantities of manure were added. Unfortunately not enough information was available from the farmer to quantify those applications and initialize the different organic matter pools. Hence, the 1991 crop season was characterized by a particularly large contribution of soil N to N plant nutrition (readily observable by the total dry matter yield of the unfertilized corn, which reached 80% of the fertilized one, as compared with 50% for the two other years) and large amounts of NO_3–N observed in the bare soil (Fig. 4b). To best reproduce those large amounts of NO_3–N stored in the soil during the 1991 corn cycle, the initial amount of NH_3 in the first 50 cm of soil was set equal to 168 kg N ha^{-1} (instead of 5 kg N ha^{-1} in 1992). Calibration of the initial NH_4 content in the soil was relatively easy using a trial and error approach since it has a direct effect on NO_3 content. However, NH_3 nitrification rate was probably too high, and we probably also should have increased the stable organic N pool (humus and litter) to better predict the beginning of the increase in concentration. The resulting simulated cumulative leaching appeared to be quite good considering the large variability in NO_3 concentration observed for that plot (error bars in Fig. 4b). Conversely, for the corn plot, a much lower amount of NO_3 stored in the soil was measured the same year. Even with a very low initial content of both NH_3 and NO_3, the simulations could not accurately fit the measured data at 80 cm depth from DAS 60 to 120 where the concentrations remain constant at a low level. As discussed for Maré, this discrepancy is probably linked to difficulties in estimating the parameters dealing with crop development. Cumulative NO_3 leaching was thus overpredicted.

CONCLUSIONS

Comprehensive data sets collected during three consecutive years and for two contrasted field situations were used to evaluate the performance of the WAVE model under very different environmental conditions. The stepwise calibration approach used was found to be a valuable tool for evaluating the performance of the different model components. At both sites, the model gave the best results for the wettest years (1992 and 1993 for La Côte Saint-André, 1996 for Maré), which actually posed the biggest problems in terms of groundwater pollution. The soil at both sites being very permeable, their hydraulic conductivities were found not to be a very sensitive parameter. Under such wet conditions and soil types, fluxes seemed to be mostly a function of climate. For dry years, predictions of NO_3 concentrations and fluxes were generally less accurate. Parameters related to the N cycle and plant NO_3 uptake were more difficult to estimate directly in the field, while some had to be either determined through independent laboratory experiments or estimated from literature reviews. Furthermore, the crop growth module SUCROS was not used, since we did not have the necessary parameters. Thus, the prediction capability of WAVE was limited due to the lack of interactions between crop growth, climate, fertilization, and soil variables.

The model was used beyond its capacity in that WAVE was initially designed for European soil and climatic conditions. The soil physical and chemical characteristics at Maré are quite unique. The soil is very porous with a low bulk density, and the NO_3 retention varies with pH and concentrations. These features are not considered in WAVE. The soil at La Côte Saint-

André is also somewhat unusual. It is very stony (with porous stones), having hydraulic properties that cannot be described using the parameterization in WAVE. Consequently, the calibrated parameters should be viewed as effective parameters, rather than as representing in situ processes, rendering the model semiempirical. Nevertheless, the calibrated model gave quite good results overall.

The evaluation of such a holistic model requires several measured sets of time series, to implement the calibration and then proceed with predictions. Using the same parameters to simulate several years of data may be inaccurate because of temporal variability. For example, several parameters evolve from one crop cycle to the other, such as hydraulic properties that can vary with soil plowing or water and nutrient uptake by plants that depend on water and nutrient availability in the soil. Furthermore, measurements were not always obtained exactly at the same place. The devices had to be removed each year because of plowing or freezing periods (i.e., at La Côte Saint-André). Comparisons between simulations and measurements may then be problematic.

WAVE was found to be a useful research tool for better understanding the various processes involved in NO_3 leaching. The model was found to be robust enough to work for conditions for which it was not designed. Calibration of the model, especially the N cycle, could have been facilitated by using data recorded specially for this purpose. Also, additional field studies are needed to fully validate the SUCROS crop growth module of WAVE. Along with the model, Vanclooster et al. (2000) proposed a code of Good Modeling Practice (GMP) whose main objective is to provide full transparency of all steps used in the modeling process. This GMP should be used to improve both the quality of data sets and the description of NO_3 leaching processes in models.

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