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Application of pesticide simulation models to the Vredepeel dataset I. Water, solute and heat transport

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Abstract

The performance of 10 deterministic one-dimensional dynamic pesticide leaching models with different complexity was evaluated using data collected on a humic sandy soil with a shallow ground water table in the Netherlands. Both mechanistic models, based on the solution of the governing flow equations (the Richards equation for soil water and the convection dispersion equation for solute flow) and functional, more empirical models were considered in the analysis. Simulations were carried out by 18 modellers allowing the characterisation of model performance in terms of user specific model parameterisation. Both uncalibrated and calibrated results are presented which demonstrate the impact of model calibrations on modelling results. In this paper, the ability of the models to correctly represent the physical transport processes is evaluated, while in a subsequent paper (Tiktak, 2000. Agric. Water Manage. Vol. 44, pp 119–134), the potential of the models to represent pesticide fate correctly will be assessed.

Model calibration had a major impact on the simulation of water flow in soils. In general, after calibration, the Richards' type models were superior to the capacity type models. However, user-specific hydraulic parameter estimation procedures introduce considerable variability in model performance which sometimes overrules conceptual model differences (Richards'/capacity). The evaluation of the solute transport component of the models was inhibited by the lack of reliable tracer data. Heat transport modelling in the top soil was not felt as being a bottleneck in our modelling technology. A plea is made for developing good modelling practices in which guidelines for selecting robust parameter estimation methods are defined. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Pesticide leaching; Model validation; Parameter estimation

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1. Introduction

To protect the quality of the surface water and groundwater in Europe against the contaminant load from agrochemical products, uniform principles have recently been accepted by the EU to register agro-chemical products (Council of the European Union, 1997). It is agreed that in future only those products will be registered for which the contamination risk of the water bodies is below a given criterion. It is suggested that risk assessment should be based on model simulations, using 'validated' simulation models.

The fate of pesticides in soils is determined by a variety of physico-chemical soil processes and crop processes (Brown et al., 1995). Pesticide fate models are therefore holistic in nature: they encompass modules describing soil hydrology, solute transport, heat transport, pesticide sorption and degradation, and soil–crop interaction. The processes affecting pesticide fate are, however, poorly defined since they vary tremendously in space and time, and since the current measurement techniques give only a very limited view of what is happening with pesticide components in soil. As a result, the level of validation of pesticide fate models should be considered as low, and scope exists to improve the validation status of available pesticide fate models (Focus Leaching Modelling Workgroup, 1995).

A rigorous validation of a pesticide leaching model must consider, amongst other things, the validation of the physical modules constituting the model. The rationale is that a pesticide leaching flux will be inappropriately calculated if the soil water flux, solute flux and temperature are inappropriately described. Within this paper, the modelling of the physical flow phenomena in the context of pesticide leaching prediction will be evaluated. The performance of the water, solute and heat transport modules of 10 different pesticide leaching codes as used by 18 different model users will be analysed, using the experimental data collected at the Vredepeel field site (Boesten and van der Pas, 2000). The performance of the pesticide fate submodels is analysed in an accompanying paper (Tiktak, 2000). This evaluation is part of the integrated modelling validation exercise realised in the framework of COST66. The overall methodology and implementation structure of this validation exercise has been presented elsewhere (Vanclooster et al., 2000).

2. Materials and methods

2.1. The models

The list of the models used in this study is given in the heading of Table 1. The important characteristics of the models are given in Table 1 of Vanclooster et al. (2000) and the references therein. Six selected models belong to the category of the Richards' type of flow models, while four models are of the capacity type. The Richards' models explicitly solve the governing one-dimensional flow equation, the Richards' equation, which combines Darcy's law with the mass conservation principle. They are typically parameterised with the soil moisture retention and hydraulic conductivity relationship, and consider water flow to be driven by the total hydraulic potential encompassing

Table 1
Cross table model users-models

User_ID	GLEAMS	LEACHP	MACRO	PELMO	PESTLA	PESTRAS	PRZM	SIMULAT	VARLEACH	WAVE
U1					×					
U2			×							
U3							×			
U4								×		
U5	×									
U6	×									
U7				×			×			
U8					×					
U9	×									
U10			×							
U11		×								
U12	×									
U13		×		×						
U14						×				
U15		×							×	
U16										×
U17									×	
U18		×								

gravity and matrix forces. Models using the Richards' equation to model the water flow, typically solves the convection dispersion equation to model solute flow. With this solute flow concept, both convective and diffusive/dispersive solute transport is considered.

The capacity type of models adopts a more empirical description of the water flow process. With the capacity type of approach, downward water flow occurs at a maximal rate when field capacity is exceeded, and is reduced when the soil dries out. For the capacity type of models, only limited points of the moisture retention and hydraulic conductivity relationship (field capacity point, wilting point, saturated hydraulic conductivity) are needed. Solute transport in the capacity type models is considered to be driven by convection, while numerical dispersion is often considered to represent the phenomenon of physical solute dispersion.

Notwithstanding the fact that the Vredepeel dataset was collected on a sandy soil, preferential flow phenomena may occur. Given the high organic matter content in the humic layer, hydrophobicity may create unstable wetting fronts, provoking fingered flow (Ritsema et al., 1993). In addition, structural phenomena created by the presence of old root channels or the activity of the soil micro fauna, may enhance preferential flow. Preferential flow in structural macropores can be modelled with some of the selected available flow models (see Table 1 in Vanclooster et al. (2000)). However, preferential flow in structural homogeneous soils, which is likely to occur at the Vredepeel site, is not considered by any model of these models. We therefore conclude that the comparison of the considered preferential flow modules, using the data collected in the structural homogeneous soil, is inappropriate.

2.2. The model users

The user–model cross table is given in Table 1. Some of the models were used by different model users so characterising the impact of the model user on the modelling results. Model users belonged to both the academic and industrial community. In some cases (MACRO, PELMO, PESTLA, PESTRAS, SIMULAT, VARLEACH and WAVE) the model developer was included as model users. In all, 22 different user–model combinations simulated the Vredepeel dataset.

2.3. The evaluation method

The evaluation method presented by Vanclooster et al. (2000) was followed, in which. the water transport, solute transport and heat transport module of the models were separately evaluated. In order to qualify the impact of model calibration, both uncalibrated and calibrated simulation results are presented. All the simulations were performed for the Vredepeel dataset for which a summary description has been given elsewhere (Boesten and van der Pas, 2000). All the users, received the research report giving a detailed description of the dataset protocol (Boesten and van der Pas, 1998a) and the experimental data compiled in a standardised format.

Each model user was asked to transfer 10 standardised simulation output files to the authors. The files included (i) the simulated soil moisture profile at four different depths (0–30, 30–60, 60–90 and 90–120 cm) and three different dates (05 March 1991; 27

August 1991 and 10 March 1992) before and after calibration; (ii) the simulated bromide profiles at four different depths (0–30, 30–60, 60–90 and 90–120 cm) and three different dates (05 March 1991; 27 August 1991 and 10 March 1992); (iii) the calculated cumulative potential evaporation, actual evaporation, potential transpiration and actual transpiration at six different dates (23 November 1990, 02 March 1991, 10 June 1991, 18 September 1991, 27 December 1991 and 10 March 1991) before and after calibration; (iv) the daily calculated position of the groundwater table before and after calibration; and (v) the daily simulated temperature at 2.5 cm depth, before and after calibration. Unfortunately, not all model users compiled completely the 10 data files, which did not always allow to draw in depth conclusions.

The simulation results were processed by the authors, which encompassed the graphical comparison of the simulation results as compared to the field measured experimental data and the calculation of the root mean square error (RMSE), the coefficient of determination (CD), the model efficiency (EF) and the coefficient of residual mass (CRM), as defined by Vanclooster et al. (2000). Within this paper, in order to be synthetic, only the results with the summary statistics will be reported.

3. Results and discussion

3.1. Soil water flow

The statistical indices for the simulated soil moisture profiles are given in Tables 2 and 3. We note that the overall modelling efficiency is very low when no calibration is allowed. Seventeen of the 22 model–user combinations produced a modelling efficiency which is smaller than 0. The efficiency, however, increased considerably when calibration was allowed. In this case, 10 of the 16 model–user combinations produced positive model efficiency values. Calibration has therefore a considerable impact on model performance. The unsatisfying uncalibrated modelling results put a constraint on the use of leaching models in a regulatory context for which field data to calibrate the hydraulic functions will mostly not be available.

The water transport components of the leaching models are driven by the soil hydraulic parameters such as the soil moisture retention curve, the hydraulic conductivity curve, the wilting point and the field capacity. In most cases, calibration was performed on these hydraulic parameters. Laboratory measured values of the moisture retention curve, including the wetting and drying branch, and the hydraulic conductivity were given in the dataset report. However, given the spatio-temporal variability of the small scale hydraulic properties in the field, effective field scale hydraulic properties may be significantly different from the small scale laboratory values, which justifies the calibration of the laboratory values to simulate field behaviour.

During calibration, the difference between the field observed soil moisture profile and simulated profiles was used as object function. No user reported on the use of automatic statistical procedures to realise this task. Some model–user combinations considered equilibrium of the moisture profile with the groundwater level in the winter period to add some field scale points of the soil moisture retention characteristic.

Table 2
Statistical criteria for the uncalibrated simulated soil moisture profiles

User_ID	RMSE	CD	EF	CRM
U1_PESTLA	47.58	0.68	−0.48	−0.34
U8_PESTLA	71.77	0.30	−2.37	−0.67
U2_MACRO	30.60	1.63	0.39	0.07
U10_MACRO	19.11	4.19	0.76	0.07
U4_SIMULAT	33.45	1.37	0.27	0.13
U11_LEACHP	40.89	0.91	−0.09	0.13
U13_LEACHP	60.92	0.41	−1.43	0.48
U18_LEACHP	47.00	0.69	−0.44	−0.25
U14_PESTRAS	32.61	1.44	0.30	−0.12
U16_WAVE	18.06	0.75	0.49	−0.12
U3_PRZM	65.68	0.35	−1.82	0.51
U7_PRZM	63.53	0.38	−1.64	0.43
U15_PRZM	93.90	0.17	−4.77	0.26
U5_GLEAMS	56.17	0.48	−1.06	0.38
U6_GLEAMS	42.31	0.85	−0.17	0.28
U9_GLEAMS	41.76	0.88	−0.14	0.23
U12_GLEAMS	85.74	0.21	−3.81	−0.64
U7_PELMO	41.03	0.91	−0.10	−0.17
U13_PELMO	39.98	0.96	−0.05	−0.17
U15_VARLEACH	67.05	0.34	−1.94	−0.39
U17_VARLEACH	49.19	0.63	−0.58	−0.08
U18_VARLEACH	112.91	0.12	−7.34	−1.04

Notwithstanding the availability of detailed laboratory measurements of soil hydraulic properties, considerable differences are observed in the estimated hydraulic parameters. The variation in adopted hydraulic parameters is illustrated in Fig. 1, giving the values of the soil moisture content at field capacity ($h = -200$ hPa), before and after calibration, for a selection of model–user combinations. The variation of the adopted hydraulic parameters is explained by different parameter estimation strategies. Some of the users selected a range of the laboratory measured hydraulic properties and used curve fitting techniques to estimate the parameters. No users reported on how the wetting and the drying branches of the laboratory curves were considered within such an exercise. Other modellers used generic pedotransfer functions to estimate the hydraulic parameters from the measured soil texture and organic matter content.

It is observed that a difference exists in the model performance of the Richards' type of flow models and the more simple capacity models. The capacity type of flow models are not able to simulate appropriately upward water flow, and hence may be systematically biased in cases of prolonged evaporation or groundwater intrusion in the soil profile (Vereecken et al., 1991; Diekkrüger et al., 1995). Nevertheless, given the performance of the PRZM model after calibration, it can be argued that the modelling efficiency of a capacity type of model may situate in the range of the more mechanistic flow models. However, a cautionary note should be added. Capacity models assume that the soil moisture content will not exceed field capacity, so a groundwater table cannot exist in capacity models. Therefore, they cannot simulate the course with time of the level of the

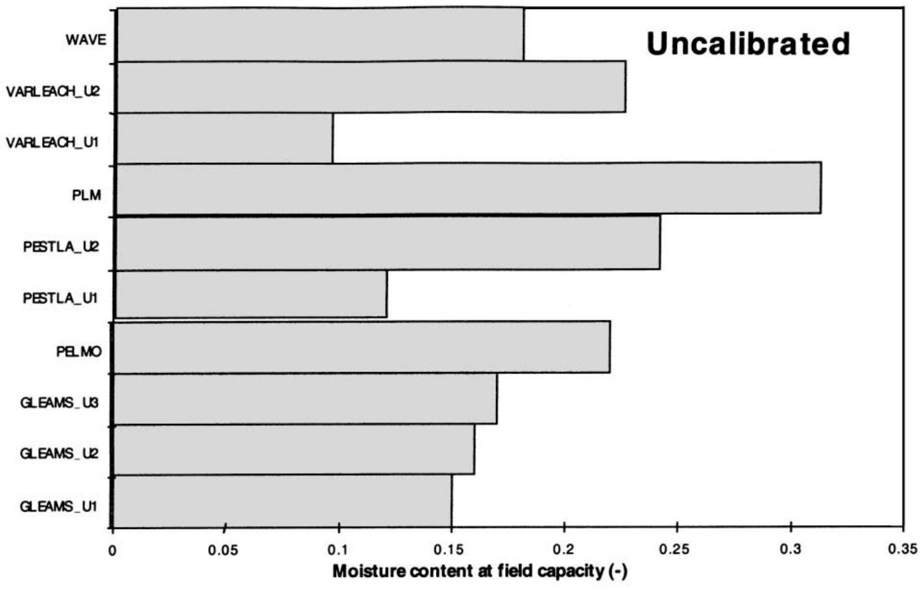
Table 3
Statistical criteria for the calibrated simulated soil moisture profiles

User_ID	RMSE	CD	EF	CRM
U1_PESTLA	16.72	5.47	0.82	−0.14
U8_PESTLA	16.04	5.95	0.83	−0.11
U2_MACRO	23.13	2.86	0.65	−0.02
U10_MACRO	22.93	2.91	0.66	0.11
U4_SIMULAT	9.80	15.93	0.94	−0.02
U11_LEACHP	16.98	5.30	0.81	−0.02
U13_LEACHP	NA	NA	NA	NA
U18_LEACHP	NA	NA	NA	NA
U14_PESTRAS	14.99	6.81	0.85	−0.04
U16_WAVE	15.11	6.70	0.85	−0.02
U3_PRZM	20.28	3.72	0.73	−0.05
U7_PRZM	NA	NA	NA	NA
U15_PRZM	93.90	0.17	−4.77	0.26
U5_GLEAMS	41.61	0.88	−0.13	0.06
U6_GLEAMS	44.97	0.76	−0.32	0.28
U9_GLEAMS	42.63	0.84	−0.19	0.24
U12_GLEAMS	NA	NA	NA	NA
U7_PELMO	32.51	1.45	0.31	0.03
U13_PELMO	NA	NA	NA	NA
U15_VARLEACH	70.07	0.31	−2.21	−0.28
U17_VARLEACH	52.85	0.55	−0.83	−0.14
U18_VARLEACH	NA	NA	NA	NA

groundwater table, which seems relevant for assessment of pesticide leaching to shallow groundwater. This was measured daily and fluctuated between 50 and 170 cm depth at the Vredepeel experimental field (Boesten and van der Pas, 1998a) and could not be modelled with the capacity models.

A considerable difference is further observed between different model users using the same model code. Before calibration, the model efficiencies are: for PESTLA between −0.48 and −2.47, for MACRO between 0.39 and 0.76, and for GLEAMS between −0.14 and −3.81. These variability ranges diminish after calibration (0.82 and 0.83 for PESTLA; 0.65 and 0.66 for MACRO; 0.13 and −0.32 for GLEAMS). This confirms the important impact of user specific interpretation of the dataset. The variability introduced by specific interpretation of the dataset by the user using a particular model may be as important as the variability between the models. A similar conclusion was drawn when considering the pesticide part of the model test (Boesten, 2000; Tiktak, 2000).

It is noted that the coefficient of variation of the estimated field capacity (33%) does not change before and after calibration (see Fig. 1). Given the improved simulation results after calibration, this indicates that different hydraulic parameters may result in apparent similar simulations of the moisture profiles. We further note that a comparison of the impact of different parameter estimation strategies on model performance did not allow the identification of the most appropriate strategy. Simulations performed with generic parameters were worse than those with parameters derived from the laboratory data for



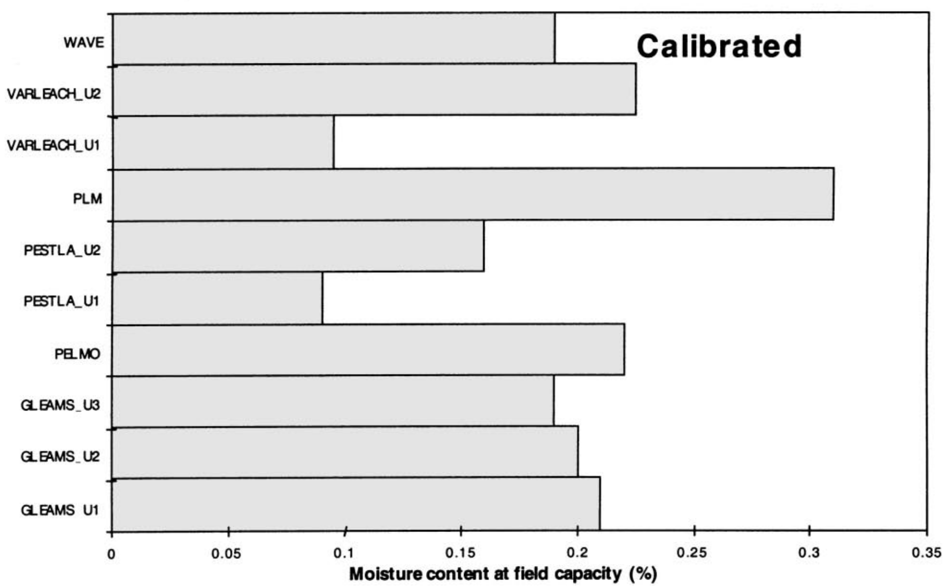


Fig. 1. Adopted field capacity for different models.

Table 4
Simulated cumulative actual evapotranspiration rates

User_ID	Uncalibrated	Calibrated
U1_PESTLA	482	471
U2_MACRO	409	452
U10_MACRO	377	404
U4_SIMULAT	370	398
U8_PESTLA	528	522
U11_LEACHP	419	549
U14_PESTRAS	434	433
U16_WAVE	532	544
U3_PRZM	362	404

PESTLA (Boesten and Gottesbüren, 2000), MACRO (Jarvis et al., 2000), and LEACHP (Dust et al., 2000), but better for PESTRAS (Tiktak, 1998).

The simulated cumulative actual evapotranspiration values after 474 days are given in Table 4. The variability between the simulated cumulative evapotranspiration rates may be as large as 170 mm for the whole period for the uncalibrated scenario and 146 mm for the calibrated scenario. In addition to the different ways to model water flow in the soil, this variability is due to different calculation procedures to estimate the reference evapotranspiration. Some authors used the Makkink reference evaporation rates supplied with the dataset (Boesten and van der Pas, 1998a), while others adopted alternative calculation procedures such as those proposed by Penman–Monteith. Other sources of variation are the different ways to convert reference evapotranspiration to potential transpiration, different methods to split evapotranspiration into evaporation and transpiration, and different alternatives to reduce the potential transpiration into the actual transpiration. It should be noted that confusion existed about the interception term. A MACRO user specified that 90 mm was considered by the model as interception. This quantity was not accounted for in the reported evaporation term, which may explain an underestimation of this term. The extreme variability of modelled actual evaporation will certainly have a considerable impact on the estimate of the drainage flux, and hence the predicted pesticide leaching flux. Unfortunately, the field data did not include measured water fluxes, and so it was not possible to comment on the accuracy of the various modelling approaches. We can only conclude that users should be aware of the fact that the 'reasonable' simulation of the soil moisture profiles in the soil does not necessarily imply the appropriate prediction of the soil water fluxes at the bottom of the soil profile.

3.2. Soil solute transport

Bromide was added to the soil surface and monitored in the soil, so providing a test of the solute transport component of the pesticide leaching models. The results of this analysis are shown in Tables 5 and 6. Compared to the modelling of the water flow, the overall modelling efficiency of the solute transport is lower. The impact of model calibration is further less pronounced, since there are fewer degrees of freedom permit to calibrate the solute transport submodule. Consequently, the difference between

Table 5
Statistical criteria for the uncalibrated simulated soil bromide profiles

User_ID	RMSE	CD	EF	CRM
U1_PESTLA	57.56	1.91	0.48	−0.12
U8_PESTLA	97.44	0.67	−0.50	0.25
U2_MACRO	53.35	2.23	0.55	−0.07
U10_MACRO	55.29	2.08	0.52	0.31
U4_SIMULAT	62.63	1.62	0.38	−0.26
U11_LEACHP	56.10	2.02	0.50	0.09
U13_LEACHP	103.93	0.59	−0.70	0.74
U18_LEACHP	126.14	0.40	−1.51	−0.42
U14_PESTRAS	44.71	3.18	0.69	0.29
U16_WAVE	65.17	1.50	0.33	0.16
U3_PRZM	109.55	0.53	−0.89	0.85
U7_PRZM	80.74	0.97	−0.03	0.50
U15_PRZM	125.89	0.40	−1.50	0.38
U5_GLEAMS	76.54	1.08	0.08	0.50
U6_GLEAMS	67.99	1.37	0.27	0.33
U9_GLEAMS	80.75	0.97	−0.03	0.38
U7_PELMO	118.70	0.45	−1.22	−0.05
U13_PELMO	77.78	1.05	0.05	0.49
U17_VARLEACH	126.48	0.40	−1.52	−0.34
U18_VARLEACH	237.36	0.11	−7.87	−1.06

Table 6
Statistical criteria for the calibrated simulated soil bromide profiles

User_ID	RMSE	CD	EF	CRM
U1_PESTLA	46.47	2.94	0.66	0.02
U8_PESTLA	54.65	2.13	0.53	0.40
U2_MACRO	52.78	2.28	0.56	0.13
U10_MACRO	52.35	2.32	0.57	0.41
U4_SIMULAT	44.78	3.17	0.68	0.02
U11_LEACHP	45.24	3.10	0.68	0.11
U13_LEACHP	NA	NA	NA	NA
U18_LEACHP	NA	NA	NA	NA
U14_PESTRAS	38.12	4.37	0.77	0.18
U16_WAVE	54.34	2.15	0.54	0.29
U3_PRZM	60.01	1.76	0.43	0.42
U7_PRZM	NA	NA	NA	NA
U15_PRZM	122.29	0.42	−1.36	0.43
U5_GLEAMS	59.50	1.79	0.44	−0.02
U6_GLEAMS	65.74	1.47	0.32	0.29
U9_GLEAMS	69.15	1.33	0.25	0.34
U7_PELMO	91.70	0.76	−0.32	0.18
U13_PELMO	NA	NA	NA	NA
U17_VARLEACH	98.08	0.66	−0.51	−0.08
U18_VARLEACH	NA	NA	NA	NA

capacity type and Richards' type of models is less evident. None of the reported simulations correctly reproduced the accumulation of the bromide in the surface layer of the top soil.

It should be noted that concerns were formulated about the appropriateness of the measured bromide profiles as a test of the pesticide transport components of the models. Being an anionic component, bromide can be taken up by the crop. van den Bosch and Boesten (1994) for instance estimated that about 50% of the dose of the 'tracer' could be assimilated by the crop. In addition, bromide was accumulated in the organic soil surface horizon, a phenomenon which was not observed when analysing the concentration profile of the 'mobile' bentazone. None of the available models could explain this accumulation of bromide at the soil surface, based on mass flow considerations. It is therefore concluded that other physico-chemical processes which are not considered in the pesticide transport component of the available models affected the fate of bromide in soils.

3.3. Soil temperature

The soil temperature was only measured at a depth of 2.5 cm. Having appropriate temperature data at shallow soil depths is important since most degradation of pesticides occurs in the surface horizon and since this degradation is controlled by the soil temperature. The calculated statistics of the uncalibrated model runs are given in Table 7. For most user–model combinations, model efficiency was acceptable even without calibration. Only User 11 reported deficiencies in the modelling of the soil temperature with the LEACHP model. He reported problems in the numerical discretisation of the soil profile when analysing temperatures at a depth of only 2.5 cm, problems in evaluating the time course of the temperature during the day and problems in defining correctly the

Table 7
Model efficiencies for simulated temperature

User_ID	Uncalibrated
U1_PESTLA	0.83
U2_MACRO	0.90
U10_MACRO	0.92
U4_SIMULAT	0.93
U11_LEACHP	0.44
U14_PESTRAS	0.92
U16_WAVE	0.86
U3_PRZM	0.89
U5_GLEAMS	0.80
U6_GLEAMS	0.77
U9_GLEAMS	0.79
U12_GLEAMS	0.76
U7_PELMO	0.91
U13_PELMO	0.93
U15_VARLEACH	0.51
U17_VARLEACH	0.51

initial conditions. In general however, the modelling of the temperature at the shallow soil depth was not felt as being a major bottleneck.

4. Conclusions

It is concluded that calibration has a major impact on the simulation of the soil moisture profiles at the Vredepeel dataset, as carried out by 18 modellers using 10 different leaching codes. The need for calibration puts a constraint on the use of a leaching model in a regulatory context. Performance differences are further observed which are due to the use of different modelling concepts and, in particular, to the use of different parameter estimation techniques. More attention should therefore be devoted to alternative robust parameter estimation methods for effective hydraulic parameters. In particular, attention could be paid to the use of generic soil hydraulic parameters such as those obtained from pedotransfer functions. It is further concluded that the Richards' type of flow models after calibration are superior to the capacity type of models, when simulating the moisture profiles at the Vredepeel site. The limited analysis, however, does not allow to generalise when the use of simplified modelling concepts, such as available in capacity type models, is still justified. A cautionary note is further added on the ability of the models to predict appropriately the fluxes at the site. Apparent acceptable simulated moisture profiles were presented unlike the variation in simulated actual evaporation. A proper simulation of the moisture profiles does therefore not necessarily imply the appropriate prediction of the drainage flux. Different users of the same model obtained distinctly different results, which emphasises the need for further developing good modelling practices and training.

The solute transport component of the pesticide leaching model could not be evaluated using the bromide data, since bromide did not behave as a perfect tracer. It is noted that the impact of the calibration on this part of the model is much less pronounced as compared to the water flow simulation. Heat flow modelling is finally not felt as being the major obstacle in the modelling of physical processes affecting pesticide fate in soil.

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