

# A review of available pesticide leaching models: Selection of models for simulation of herbicide fate in Finnish sugar beet cultivation

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The quality of simulation results depends on the model structure and its parameterisation. The aim of this study was to find the best available models for herbicide fate simulation for Finnish conditions. Subjective model selection criteria were developed for the simulation domain: pesticide fate in Finnish sugar beet cultivation. An inventory was made of available models and a number of different pesticide and solute transport models were identified. Thirteen one-dimensional deterministic models (CRACK-NP, EPIC, GLEAMS, LEACHP, MACRO, OPUS, PELMO, PEARL, PESTLA, PLM, PRZM, RZWQM and SIMULAT) were compared and evaluated for their characteristics. The comparison showed that none of these models fulfilled all of the desired criteria. Finally, MACRO 4.1 and GLEAMS 3.0 were selected for herbicide fate simulations. The other high regarded models were RZWQM, PEARL and PELMO.

## Introduction

Herbicides are man-made organic compounds used as crop protection chemicals in intensive farming. These organic compounds, besides being very toxic to weeds, can be harmful to human health and the environment if sensitive receptors are affected at elevated concentrations. Even low concentrations of leached agricultural pesticides or herbicides can cause environmental risks in fresh waters.

Intensive pesticide monitoring programs have been carried out in North America and Europe. In a Swedish monitoring program, pesticides were detected in stream water samples and from mobile sediments and bed sediments of

streams (Kreuger *et al.* 1999). In Finland, pesticides are not routinely monitored in the environment. However, over 3000 tonnes of agricultural pesticides and herbicides were sold in 1998 in Finland (Hynninen and Blomqvist 1999), corresponding to 226 pesticide products differing in leaching potential and toxicological properties.

Using data from the Finnish leaching field experiments, Laitinen *et al.* (1996) estimated that 0.01%–1.0% of applied pesticide mass is usually lost to surface and subsurface drainage waters. This is inline with Flury's (1996) review of experimental studies of pesticide leaching. In most of the reviewed studies, pesticide losses below root zone was < 0.1%–1% reaching up to 4% of applied mass in worst case conditions.

Surface losses represented 7%–93% of total pesticide losses (< 0.005 to 5.43% of applied mass) in the studies, where both surface and subsurface losses were identified (Flury 1996). However, a storm soon after pesticide application may cause very high pesticide losses (up to 17% of applied atrazine mass) to surface waters (Wauchope 1978).

Sampling and chemical analyses of pesticides are expensive. Therefore, other tools for assessing the fate and concentration in the environment have been developed. Mathematical models provide a quick and inexpensive method for estimating losses that are difficult to measure under field conditions. In addition, models allow the assessment of various management practices. Different scenarios and the effect of soil, weather and management practices can also be simulated. Pesticide leaching models are increasingly used in pesticide registration within the European Union since the 1990s. A model is a mathematical description and approximation of true natural phenomena. The model structure defines which processes are included and how they are described. There are numerous different pesticide leaching models available. Therefore, model selection is an important part of the simulation process. To be able to choose the most suitable model, one has to know the system to be simulated. In this particular study, model selection criteria should be based on the knowledge of both solute transport phenomena and of sugar beet cultivation practices in Finland.

Sugar beet cultivation is limited to south-west Finland, where the soil is frozen about five months every year and snow affects the hydrology to a great extent annually. The fields consist of both clay soils (55%) and coarser (silt and fine sand) soils (42%). Almost all sugar beet fields are equipped with subsurface drainage systems and the distance between tiles is normally 3–5 m shorter than in cereal fields (Erjala and Raininko 1994). Compared to other Finnish field crops, the use of fertilisers and crop protection chemicals in sugar beet fields is high. In 1998, on average, 0.34 g m<sup>-2</sup> pesticides were used for sugar beet fields, of which 90% were herbicides. The most used herbicides were metatritron (66% of herbicide use), phenmedipham (17% of herbicide use) and ethofumesate (14% of herbicide use).

The whole cultivation area is normally sprayed 2–4 times during May and June with these three herbicides. Because crop rotation is minimal, the same herbicides have been applied on the same fields year after year. Cultivation of genetically modified herbicide resistant sugar beet varieties would increase either the use of glyphosate or glufosinate-ammonium, depending on variety, and decrease the use of the conventional herbicides: metatritron, ethofumesate and phenmedipham. The five herbicides (metatritron, ethofumesate, phenmedipham, glyphosate and glufosinate-ammonium) are water-soluble, and none of them are easily volatile. Their sorption properties vary, and they do not adsorb solely to soil organic matter (Behrendt *et al.* 1990, Cox *et al.* 1997, de Jonge *et al.* 2001).

The purpose of this review study was to find the most suitable model(s) to simulate pesticide losses from sugar beet cultivation in Finland. Simulation results will assist in comparison of the environmental risks of herbicide tolerant, genetically modified sugar beet cultivation to traditional sugar beet cultivation. In section 'material and methods' the criteria for model screening and the available models are described. In section 'model comparison' the processes, applicability and performance of models that were not rejected in preliminary screening of the previous sections are described and compared. In section 'conclusions' the above are evaluated against the predefined criteria.

## Material and methods

### Selection criteria

The desired model design for a particular purpose depends on the scope and the spatial and temporal scales of the application, and on the available data. The subjective criteria developed for model selection for our purposes are listed in Table 1.

### Available models

To inventory available pesticide fate models, a search was carried out from two model data-

bases: REM (REM (Register of Ecological Models) 2000) and CAMASE (CAMASE 1995). In addition, all of the models recommended by FOCUS (FORum for the Co-ordination of pesticide fate models and their Use) working groups (e.g. FOCUS 1996), and the models, studied within the COST66 programme 'Pesticides and the environment' (Vanclouster *et al.* 2000a), were taken into consideration. Altogether 82 solute transport and pesticide models were identified. In the model evaluation, the found models were classified into three groups: unsuitable models, models that would have needed major modifications or were too complex, and finally models that were selected for further consideration.

### Unsuitable or too complex models

At first, out of the found 82 models 28 were rejected because the purpose of the models differed from the scope of the present study. Most of these rejected models were solute transport models, which did not include pesticide processes. These models are not shown or documented in the paper. The reasons for rejection of the 41 models, which included pesticide processes, are presented in Table 2. These included reasons such as (1) the main media was not vadoze zone soil, (2) the rejected model did not calculate a quantitative estimation of pesticide losses, (3) the rejected model was too simple for the simulation purpose or (4) too complex compared to the available input data.

### The considered models

The remaining 13 models are deterministic one-dimensional models, which simulate pesticide persistence and losses from agricultural fields. The models are presented in Table 3, and compared later in detail.

GLEAMS and EPIC are American management type models, developed for agricultural advisors. GLEAMS is an extension to CREAMS (Knisel 1980), which originally did not calculate percolation and leaching. GLEAMS estimates erosion and agrochemical losses at the edge of the field and at the bottom of the root zone. EPIC calculates the loading of nutrients and pesticides in a very similar way to GLEAMS. Moreover, EPIC simulates the effects of different management practices on yields and farm economy (Mitchell *et al.* 1997). PRZM was developed for pesticide registration in Georgia, U.S. The first version of the German pesticide registration model PELMO was a modification of an early PRZM version.

LEACHM, OPUS and RZWQM are mechanistic research models from USA. Development of these models started already in the late 1980s. LEACHM was the first of these three. It estimates vertical transport of water and chemicals in soil. It consists of four submodels, LEACHW for water, LEACHN for nitrogen, LEACHP for pesticides and LEACHC for salinity. OPUS simulates the movements of nonpoint source pollutants within and from a field or small catchment. It is a mechanistic management model,

**Table 1.** Selection criteria.

1	For the hydrology and pesticide processes, priority was given to deterministic models where hydrology and pesticide processes are explicitly described.
2	Preference was given to models, which considered winter hydrology including snow accumulation and melting, soil freezing and thawing, and the effects of temperature on pesticide processes.
3	Description of preferential pathways, like macropores or cracks, was regarded as an advantage for a model.
4	The ability to simulate sugar beet cultivation practices was required from the model.
5	Only one-dimensional models were taken into account. Two- and three-dimensional models require spatial data, which was not available.
6	Additional criteria for selecting a model were the quality of model documentation and version control. Because the number of found models was high, only easily accessible, low-cost and well-documented models were taken into account.
7	Performance in model comparison tests was an extra criterion. Published performance tests, which included at least two models and observed values, were reviewed and models were ranked according to performance.

**Table 2.** Unsuitable and too complex models.

Acronym	Name/comment	Reason for disqualification
BIOPLUME3 (Rafai <i>et al.</i> 1998)	2D model for attenuation of organic contaminants in groundwater (advection, dispersion, sorption, and biodegradation)	For groundwater, no vadose zone processes
BIOSCREEN (Newell <i>et al.</i> 1996)	Natural Attenuation Decision Support System	For groundwater, no vadose zone processes
HST3D (Kipp 1997)	Heat- and Solute-Transport in 3-Dimensions	For groundwater, no vadose zone processes
MOC3D (Konikow <i>et al.</i> 1996, Goode 1999)	Method Of Characteristics solute transport	For groundwater, no vadose zone processes
MT3D (Zheng 1990)	Modular Transport in 3-Dimensions	For groundwater, no vadose zone processes
WASP (Ambrose <i>et al.</i> 1993)	Water Quality Analysis Simulation Program	For lake, no soil processes
SWAP (Kroes <i>et al.</i> 1999)	Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment	Incorporated into pesticide leaching model PESTLA
VADOFT (Carsel <i>et al.</i> 1998)	The Vadose Zone Flow and Transport Model	Incorporated into pesticide leaching model PRZM-3
FINDER_CL (REM 1997f)	Model finds the best chemical for specific crop protection problem	Crop protection model, no estimation of losses
RBWHIMS (REM 1997k)	Rule Based Wholistic Insect Management System	Crop protection model, no estimation of losses
TPE-Uncon (REM 1997o)	UNCertainty analysis applied to supervised CONtrol of aphids and brown rust in winter wheat	Crop protection model, no estimation of losses
WCA_TX (REM 1997s)	Weed control advisor	Crop protection model, no estimation of losses
SOLTRANS (REM 1997n)	SOLute TRANsport Simulator	Focus in plant physiology, not in soil science
RICEWQ (REM 1998d)	Pesticide Runoff Model for Rice Crops	For rice cultivation only
VEGIGRO (REM 1997r)	Winter wheat crop growth (+ environmental factors of cultivation practices)	No quantitative estimation of losses
PATRIOT (REM 1997j)	Pesticide Assessment Tool for Rating Investigations of Transport	Management tool and user interface for PRZM2
PIRANHA (REM 1998b)	Pesticide and Industrial Chemical Risk Analyses and Hazard Assessment	Risk assessment tool, uses PRZM and EXAMS
PRE-AP (REM 1998c)	Pesticide Registration and Environmental Application Program	Pre- and post processor for GLEAMS model
EXAMS (REM 1997e)	Exposure Analysis Modeling System	Only for rapid evaluations, no quantitative estimation of pesticide losses
SURFEST (REM 1998e)	Surface Water Pesticide Exposure Estimation	Only for screening, no quantitative estimation of pesticide losses
E4CHEM (REM 1996a)	Exposure Estimation for potentially Ecotoxic Environmental CHEMicals	Designed for chemical ranking and evaluation of the need of further studies
ECOFATE (REM 1997c)	An environmental risk assessment software package for MS Windows	Risk assessment tool, no quantitative estimation of pesticide losses
CEMOS_CHAIN (REM 1997a)	Food chain model for chemicals (concentrations in producer, 1-level and 2-level consumers)	Focus is not in persistence and losses of chemicals, no quantitative estimation of pesticide losses from a field

Continued

Table 2. Continued.

Acronym	Name/comment	Reason for disqualification
CEMOS_LEVEL2 (REM 1997b)	Fugacity model, chemical concentrations in different ecosystem compartments (e.g. air, soil, water, fish)	Model bases on partitioning coefficients, focus is not in persistence and losses of chemicals, no quantitative estimation of pesticide losses from a field
CARRY (Knabner <i>et al.</i> 1996, Totsche <i>et al.</i> 1996)	Carrier-influenced transport of chemicals	For forest soils
2PAR_DEGRADE (Liu and Zhang 1987)	The model with two parameters for microbial degradation of pesticides	no hydrology -> no estimation of losses
HERBSIM (UFIS model database 1996)	Herbicide degradation simulation	no hydrology -> no estimation of losses
TRANSOL23 (REM 1997p)	Transport of a Solute	Hydrology must be supplied
CMLS (REM 1997c 1998)	Chemical movement in layered soils	Too simple, no surface processes included
VARLEACH (Trevisan <i>et al.</i> 2000b)	A British pesticide leaching model	Too simple, no crop
MIKE SHE (Jørgensen <i>et al.</i> 1998)	A Danish model originally only for hydrology	Too complex
SWMS_2D (Simunek <i>et al.</i> 1994, REM 1997i)	Simulating water and solute movement in 2D-variably saturated media	Too complex
SWMS_3D (REM 1997i)	Simulating water and solute movement in 3D variably saturated media	Too complex
CHAIN2D (REM 1998a)	Movement of Water, Heat, and Multiple Solutes	Too complex
2DSOIL (REM 1997i)	Modular Simulator of Soil and Root Processes	Too complex
HYDRUS-2D (REM 1997h)	Simulating water and solute movement in two-dimensional variably saturated media	Too complex
FEHM (REM 1997g)	Finite Element Heat and Mass Transfer Code	Too complex
SWRRBWQ (General Science corporation 2000)	Simulator for Water Resources in Rural Basins-Water Quality	Watershed scale, simple pesticide part, only surface losses
CREAMS (Knisel 1980)	Chemicals, Runoff and Erosion from Agricultural Management Systems (Simulation model Network)	Simple pesticide part, only surface losses
SNAPS (Behrendt and Brueggemann 1993, Behrendt <i>et al.</i> 1995, REM 1997m)	Atmosphere-Plant Soil A German physically based research model for pesticide fate in unsaturated soil zone	No manual, not enough data to evaluate the ability to simulate cultivation practices
WAVE (REM 1997q, Vanclooster <i>et al.</i> 2000b)	A Belgium modular software to simulate transport in agricultural soils	Modular structure, a user may choose the process descriptions => no specific process descriptions for evaluation

used as a research tool in many surface loss studies. The development of RZWQM started in the late 1980s by evaluating the USA models available at that time (CREAMS, GLEAMS, PRZM and OPUS). RZWQM simulates water quality and the effects of management practices on crop growth, hydrology, nutrient cycling,

organic matter and chemical losses. Crop growth is linked to environmental factors, like available water and nutrients, both in OPUS and in RZWQM. Originally LEACHM, OPUS and RZWQM required detailed rainfall data, but the later versions of OPUS accept also daily-based climate data as input.



Table 3. An overview of the models selected for more detailed evaluation.

Acronym	Name	References	Origin	Originally purpose	Version history	Assistance <sup>1</sup>
CRACK-NP	CRACK-NP (A British model for cracking clay soils)	Armstrong <i>et al.</i> 1996, Armstrong <i>et al.</i> 2000b	Great Britain	Research	Ver. 1.1 in 1996	D, M
EPIC	Erosion-Productivity Impact Calculator/Environmental Policy Integrated Climate Groundwater Loading Effects of Agricultural Management Practices	Mitchell <i>et al.</i> 1997	Texas, USA	Management model for farms	Published in 1983, the latest version in 1997	D, M, S, W (www.brc.tamus.edu/epic/)
GLEAMS	Groundwater Loading Effects of Agricultural Management Practices	Leonard <i>et al.</i> 1987, Knisel 1993, Knisel and Davis 2000	Georgia, USA	Management model for agricultural advisors	Published in 1987, ver. 2.10 in 1993, ver. 3.0 in 2000	D, M, S, W (sacs.cpes.peachnet.edu/ sewrl/models)
LEACHM	Leaching Estimation and Chemistry Model	Wagenet & Hutson 1989, Dust <i>et al.</i> 2000	New York, USA	Research (mechanistic model for vertical transport)	Ver. 1 in 1987, ver. 2 in 1989 and ver. 3 in 1992 Ver. 3.1 in 1994, ver. 4.1 in 1998, ver. 4.3b in 2002	D, M, S
MACRO	MACRO (Pesticide fate in macroporous soil)	Jarvis & Larsson 1998	Sweden	Research	Ver. 3.1 in 1994, ver. 4.1 in 1998, ver. 4.3b in 2002	D, W (www.rmv.slu.se/bgf/ Macrohtm/macro.htm)
OPUS	OPUS (Fate of non point pollutants in field)	Ma <i>et al.</i> 1999	Colorado, USA	Research—management	First version in 1990, ver. 1.62 in 1995	D, M
PELMO	PEsticide Leaching Model	Klein 1995, Jene 1998, Klein <i>et al.</i> 2000	Germany	Pesticide registration	Ver. 1.0 in 1991, ver. 2.01 in 1995, ver. 3.2 in 1999	D, M (arno.ei.jrc.it:8181/focus/ models/PELMO/)
PEARL	Pesticide Emission Assessment at Regional and Local scales	Leistra <i>et al.</i> 2000, Tiktak <i>et al.</i> 2000	The Netherlands	Pesticide registration (after PESTLA)	Ver. 1.1 in 2000, ver. 2.2.2 in 2002	M, D, W, S (www.alterra.nl/models/ pearl/home.htm)
PESTLA	PESTicide Leaching and Accumulation	Van den Berg & Boesten 1998, Boesten & Gottesbüren 2000	The Netherlands	Pesticide registration	Ver. 1.1 in 1989, 3.4 in 1998 (replaced by PEARL in 2000)	D, M, D
PLM	Pesticide Leaching Model	Nicholls <i>et al.</i> 2000, Nicholls & Hall 1995	Great Britain	Research (empirical model for lysimeters)	Documentation in 1993, ver. 3 used in 2000	D
PRZM	Pesticide Root Zone Model	Carsel <i>et al.</i> 1998	Georgia, USA	Pesticide registration	First publication in 1984, ver. 1.00 in 1992, 2.01 in 1995, 3.12 in 1998	D, M, W, S (www.epa.gov/ceampubl/ przm3.htm)
RZWQM	Root Zone Water Quality Model	Singh <i>et al.</i> 1996, Kumar <i>et al.</i> 1998, Ahuja <i>et al.</i> 1999	Colorado, USA	Research—management	Ver. 1 in 1992, the latest version in 2000	D, M, W (gpsr.ars.usda.gov/ products/rzwqm.htm)
SIMULAT	SIMULAT (Pesticide fate in soil)	REM 1996b, Aden & Dieckruger 2000,	German	Research	Ver. 2.2 in 1993	D, M,

D = documentation, M = manual, S = source code available, W = home page on the internet (homepage address).

CRACK-NP and PLM are British research models. CRACK-NP simulates preferential flow of water, nitrate and pesticides in cracking clay soils. PLM is an empirical model, which takes into account quick preferential flow of pesticides. CRACK-NP and Swedish MACRO model have common roots. In addition to preferential flow, MACRO can simulate matrix flow, and therefore it is suitable for sandy soils as well. MACRO-DB (Jarvis *et al.* 1997) is a combination of the MACRO model, a Windows user interface and databases, which minimise the number of user-specified parameters. The soil databases originate from Britain and Sweden.

PESTLA has been used in pesticide registration in the Netherlands. It uses the output of a Dutch hydrology model SWAP (Van Dam *et al.* 1997) as input for the pesticide chemistry and transport model. The first PESTLA version was released in 1989 and the last, version 3.4 in 1999. PESTLA and another Dutch pesticide fate model were combined and a new model, called PEARL, was released in 2000. SIMULAT is a German research model for pesticide fate simulations. It uses the same equations for pesticide degradation and sorption processes as HERBSIM (UFIS model database 1996). In addition, SIMULAT calculates transport of water, solutes and heat in soils.

All of the compared models can be executed on PC's either in DOS or Windows operating systems. The run times vary depending on the model complexity. Model development history and the existence of documentation, manuals, source code and Internet home pages are presented in Table 3. The FOCUS groundwater group (FOCUS 2000a) selected PELMO, PRZM-2, MACRO and PESTLA to be used in pesticide registration in the European Union. Later, PESTLA was replaced by PEARL (FOCUS 2000b). The official FOCUS versions and guidance for their use are available on the Internet (FOCUS 2000b).

## Model comparison

### Hydrology process descriptions of the selected models

Losses of non-volatile pesticides are generated in two ways. Dissolved pesticides are trans-

ported with water and adsorbed pesticides are transported with eroded sediment, which in turn is affected by water flow. Therefore, a proper description of hydrology is important.

### Soil moisture and water flow

The models were divided into two categories according to the description of soil moisture and water transport in soil: (a) capacity models and (b) models using Richard's equation. This categorisation is indicated for each model in Table 4.

In capacity models, water flow is driven by water storage rather than water potentials. It is often assumed that the downward water flow occurs at maximal rate when field capacity is exceeded. This simple concept does not require many input parameters (Vanclooster *et al.* 2000a): soil moisture at field capacity and at wilting point, and the total porosity or maximal pore volume. In addition, the maximal rate of water flow is needed. In most of the capacity models, it is given as saturated hydraulic conductivity of each soil layer.

Richard's equation is a physically based differential equation for the calculations of the changes in soil moisture content. In Richard's type models, soil hydraulic potentials determine the direction of water flow in soil, and the hydraulic gradient and moisture dependent hydraulic conductivity determines the rate of water flow. Soil hydraulic properties, like the relations between volumetric water content, pressure head and hydraulic conductivity are approximated with physico-empirical functions (e.g. the Brooks-Corey/Mualem model is used in MACRO and Van Genuchten model in SWAP, which is the hydrological model of PEARL and PESTLA.)

Most of the models can be divided into one or other of these two categories. However, PRZM-3 uses a capacity approach in the root zone and Richard's type flow in deeper soil layers (Carsel *et al.* 1998). The British CRACK-NP model assumes that water flows only in cracks and macropores (Armstrong *et al.* 2000b). It suits well to the simulations of heavy clay soils, where water flows mainly via preferential pathways rather than in the soil matrix.

## Evaporation and transpiration

Evaporation and transpiration are significant water outflows from the soil system during the summer period in Finland. Some models require daily potential evaporation as input. Many models calculate the potential maximum evapotranspiration using equations which associate other climatic variables to evaporation. The most used equations are the Penman-Monteith, Priestly-Taylor, Ritchie, Hamon, and Haude equations. In some models, the user may specify which equation is used. The needed input for these equations varies; the most demanding approaches require temperature, solar radiation, air humidity, and wind speed. The method used for calculation of potential evapotranspiration

for each model is presented in Table 4. The leaf area, rooting depth, and root density distribution play a significant role in transpiration.

## Drainage water

In the models, tile flow is described as a sink term in specified soil layer. Hooghoudt's equation (Skaggs 1978) is used, with some modifications, in PEARL, PESTLA, OPUS, MACRO, RZWQM, and in a specific version of SIMULAT (Armstrong *et al.* 2000a) to mimic two-dimensional effects of tile drainage. A simpler approach is used in PELMO and PLM. The drainage options (yes, simple and no) included in each model are presented in Table 4.

**Table 4.** Hydrology processes of the models.

Model	Water flow	Surface runoff	Erosion	Evapo-transpiration	Subsurface drainage	Preferential flow	Winter hydrology
GLEAMS	Capacity	SCS	Yes	2 calculation options	No	No	Snow +(1)
EPIC	Capacity	SCS	Yes	2 calculation options	No	No	Snow +(2)
PELMO	Capacity	SCS	Yes	As input/2 calculation options	Simple	No	Snow
PLM	Capacity	No	No	Calculation method not provided	Simple	Simple	No
PRZM3	Capacity/ (Richards)'	SCS	Yes	As input/Hamon's equation	No	No	Snow
CRACK-NP	Capacity/ cracks only	Simple	No	As input	Yes	Yes	No
LEACHM	Richard's	No	No	As input	No	No	No
MACRO	Richard's	Simple	No	As input/ Penman's equation	Yes	Yes	Snow
OPUS	Richard's	Yes	Yes	Ritchie's equation	Yes	No	Snow
PEARL	Richard's	Simple	No	As input/Penman-Monteith equation	Yes	No	No
PESTLA	Richard's	Simple	No	As input/Penman-Monteith equation	Yes	No	No
RZWQM	Richard's	Yes	No (3)	Modified Penman-Monteith equation	Yes	Yes	Snow
SIMULAT	Richard's	No	No	Penman-Monteith equation	Yes(4)	Simple	No

1) Soil water storage capacity is decreased for those days when calculated soil temperature is  $< 0$  °C (Knisel and Turtola 2000).

2) Water can flow into a frozen soil layer but is not allowed to percolate from the layer, if soil temperature is below 0 °C (Mitchell *et al.* 1997).

3) Feature not included in the current version, but the calculation method is already documented in manual (Ahuja *et al.* 1999).

4) In a specific version (Aden and Diekkruger 2000).



## Surface runoff and overland flow

There are two main approaches used to calculate the surface runoff. The empirical SCS-curve-number method (Mocus 1972) is based on numerous rainfall and runoff measurements in USA. The other, infiltration based, approach calculates runoff as the part of the rainfall that exceeds soil infiltration capacity. The infiltration capacity may be exceeded because the intensity of rainfall is higher than the water conductivity of soil surface or because the water table has risen to the soil surface. To approximate the runoff volumes from the edge of the field the latter method must be followed by an overland flow description. If this option is lacking, the surface runoff option of a model is called simple in Table 4. The available meteorological data defines whether OPUS uses the SCS method or the infiltration based method, which requires detailed rainfall data (Ma *et al.* 1999).

## Erosion

Models, which estimate erosion losses, are addressed in Table 4. As indicated in the table, the models that calculate surface runoff or overland flow using SCS method also take into account erosion. In these models, the erosion calculation is based on a modification of the Universal Soil Loss Equation (USLE) (Wischmeier and Smith 1978). USLE is a conceptual approach to estimate annual sediment losses from annual rainfall and from factors describing field, soil, crop, and management practices. The modified versions of USLE (e.g. MUSLE, Onstad-Foster USLE, MUSS) utilises runoff parameters and allows the estimation of sediment losses of a single storm event (Renard *et al.* 1997)

## Preferential pathways

Preferential pathways have an essential role in water and solute leaching especially in clay soils (Beven and German 1982, Flury 1996, Djodjic *et al.* 1999) but also in coarser soils (Bergström and Jarvis 1994, Elliott *et al.* 2000). CRACK-NP,

MACRO, PLM and a few modified versions of other pesticide leaching models consider preferential pathways (Table 4). The models use different approaches.

A simple way to handle preferential pathways is presented in PLM. It divides soil water into immobile, slow and fast mobile phases. This fast phase represents the flow in macropores and cracks. The PLM user specifies how many soil layers can slow phase solution and fast phase solution pass during a given time step. CRACK-NP assumes that water flows via cracks and fissures. It does not take into account matrix flow. The user specifies the hydraulic conductivity of cracks and crack volume at different moisture conditions. Lateral infiltration (depending on soil hydraulic properties) decreases the water flowing in cracks. In the CRACK model, preferential flow is connected to surface runoff and subsurface drainage flow. MACRO divides the simulation system into micropore and macropore systems. The driving force for macropore flow is gravity. Moreover, MACRO considers pesticide sorption and degradation separately in micropore and macropore systems. The two systems are linked together by source/sink terms for water and pesticide exchange by convection and diffusion.

A preferential flow option has been added into RZWQM (Kumar *et al.* 1998), SIMULAT (Armstrong *et al.* 2000a), GLEAMS (Morari and Knisel 1997) and LEACHM (Ma *et al.* 2000). These models are, however, usually run without preferential flow calculation. The preferential flow submodel of RZWQM was tested by Kumar *et al.* (1998). The use of the macropore option slightly improved simulation results.

## Winter hydrology

Snow accumulation and melting processes are incorporated into half of the models (Table 4). Most of the models calculate soil temperature in order to correct degradation rates (Table 5). Nevertheless, temperature affects soil hydrology currently only in GLEAMS and in EPIC. In GLEAMS version 3.0, soil water storage capacity decreased, if the calculated soil temperature

Table 5. Chemical part of the models, the information referring to the newest available versions is used.

Models	Plant		Sorption			Degradation			Transport Equation <sup>f</sup>
	Foliar application	Uptake	Dynamics <sup>a</sup>	Isotherm <sup>b</sup>	In deeper soil layers <sup>c</sup>	Kinetics <sup>d</sup>	Rate affected by <sup>e</sup>	Metabolites	
CRAC-NP	-	-	E	L, (F)	As input	X	M, T	No	C
EPIC	+	-	E	L	Same	X	-	No	C
GLEAMS	+	+	E	L	OC	X	M, T, D	Yes	C
LEACHP	-	+	E + N	L/F	As input	X	M, T, D	No	C + d
MACRO	+	+	E	F	As input (micro/macropores)	4X	M, T, D	Yes	C + d
OPUS	+	+	E + (N)	L	OC	X	M, T, D	No	C + d
PELMO	+	+	E + N	F	OC/pH dependence	X	M, T, D	Yes	C
PEARL	+	+	E + N	F	OC/pH/user specified	X	M, T, D	Yes	C + d
PESTLA	-	+	E + N	F	OC	X	M, T, D	Yes	C + d
PLM	-	-	E + N	L	As input	X	M, T, D	No	C
PRZM-3	+	+	E	L	Same	2X (m&cm)	T	Yes	C
RZWQM	+	+	E + N	L/F	OC/pH dependence	PX	M, T, D	Yes	C + d
SIMULAT	-	-	E + N	L/F/Lag	Same	X/MM/m&cm	M, T	Yes	C + d

a) Dynamics: E = constant equilibrium sorption kinetics, N = non-equilibrium or time dependent sorption.

b) Isotherm: L = linear sorption isotherm, F = Freundlich sorption isotherm, Lag = Langmuir isotherm.

c) In deeper soil layers: as input = separate sorption parameters are given into each soil horizon, OC = model calculates sorption parameters in deeper soil layers from Koc and organic carbon content of soil layers, same = same sorption parameters are used for all layers in the whole simulation profile.

d) Degradation kinetics: X = lumped first order kinetics, 4X = separate first order functions in four phases, 2X = separate first order functions in two phases, PX = pseudo first order kinetics, m&cm = metabolic and co-metabolic degradation, MM = Michaelis-Menten kinetics.

e) Degradation rate affected by: M = soil moisture, T = soil temperature, D = soil depth.

f) Transport equation: C = convection, d = dispersion and diffusion.

was below 0 °C. In EPIC, water can flow into a frozen layer but is not allowed to percolate from the layer. The snow and soil freezing routines, taken from the SHAW model, have been incorporated into RZWQM98 model (Flerchinger *et al.* 2000). However, this modified version is not yet available.

## Chemical process descriptions in the models

Pesticide degradation and sorption are considered the most important chemical processes affecting the fate of pesticides. Pesticide adsorption results from different chemical and physical bonds between pesticide and soil particles. It decreases the pesticide concentration in the solute phase, and therefore, the toxicity and leaching risk are decreased. However, the adsorbed pesticides may desorb back into solution. Degradation means the transformation of a pesticide into another chemical compound or compounds, and is mainly a microbiological process for most compounds. Strongly adsorbed pesticides are not available for microbes and form soil bound residues (Gevao *et al.* 2000). A proper model takes also into account the effect of plants. The five herbicides to be simulated are not volatile. Therefore, the descriptions of pesticide volatilisation or vapour phase processes in soil are not considered here.

### The effects of plants on pesticide fate

In post-emergence pesticide applications, part of applied pesticides end up on foliage. Dissipation from foliage may differ from that in soil. Rain may wash off pesticides from canopy to soil. This is considered in eight of the 13 models (Table 5). Moreover, plants may take up pesticides from the soil solution. This uptake may be active or passive depending on the crop and the pesticide. Uptake is taken into account in nine models (Table 5).

### Sorption

The simplest way to handle sorption is to divide the pesticide mass into adsorbed and solute

phases according to a linear partitioning coefficient ( $K_d$ ). The linear adsorption coefficient ( $K_d$ ) does not take into account the fact that the number of available sorption sites decreases when the concentration of a given chemical increases. Instead of using the  $K_d$ -value, half of the 13 models use the non-linear Freundlich isotherm (Table 5). The user has to define the Freundlich exponent ( $1/n$ ) in addition to the Freundlich adsorption coefficient ( $K_f$ ). A PELMO user has to define a minimum concentration of the chemical in question, in which the Freundlich isotherm is still valid. When pesticide concentration in soil solute is below the limit, the model uses the linear sorption isotherm. SIMULAT users may choose between the linear, Freundlich and Langmuir isotherms.

In MACRO, sorption sites are divided between micropores and macropores and separate sorption values are given for both phases. Up to three different sorption sites are used in SIMULAT. Most of the models assume constant equilibrium sorption. However, sorption is partly an irreversible process and adsorption increases with time (Leake and Gatzweiler 1995, Craven 2000). SIMULAT, PELMO and VARLEACH take into account time-dependent sorption. The user may specify a separate desorption coefficient in PESTLA and PEARL.

A model may use the same sorption parameters in all layers, allow the user to give parameters separately for each layer or calculate internally different sorption parameters for layers based on soil properties (Table 5). Many non-polar chemicals adsorb mainly on soil organic matter. Instead of  $K_d$  or  $K_f$ , many models use a sorption coefficient in proportion to soil organic carbon content ( $K_{oc}$  or  $K_{foc}$ ) as an input parameter. The model then calculates the corresponding  $K_d$  or  $K_f$  values for each simulation layer. If pesticides are not adsorbed to organic carbon, like e.g. glufosinate-ammonium and glyphosate, this 'user friendly' option is useless and may result erroneous sorption parameters in deeper soil layers.

It has been shown that temperature may have a significant role in sorption process (Spurlock 1995, Brücher and Bergström 1997). This is not considered by any of the considered models.

## Degradation

For the relevant herbicides, the main processes in transformation path are microbiological. In addition, hydrolysis and photochemical reactions may be important. The dominant process varies with a given chemical, available microbes and environmental conditions, and is seldom known. Though observed patterns of transformation seldom follow lumped first order kinetics (Vancloster *et al.* 2000a), only five of the 13 models use degradation approaches, which differ from this assumption (Table 5). Multiple first order kinetics are used in PRZM (Trevisan *et al.* 2000a) and MACRO. Users of these models may give separate degradation rates for pesticides in different phases. In PRZM these phases are adsorbed, dissolved and gas, and in MACRO adsorbed and dissolved in micropores and macropores. RZWQM uses pseudo-first-order functions, where separate transformation rates are given into separate processes like hydrolysis, anaerobic and aerobic biodegradation. The model calculates the sum of the process rates for each time step. PELMO model has additional option for calculating kinetics that differ from the first order kinetics. This option is however not included in the Windows version (Klein 1995). In addition, GLEAMS 3.0 has two research options for degradation kinetics (Truman *et al.* 1998, Knisel and Davis 2000).

Temperature affects pesticide degradation in 12 of the 13 models (Table 5). The Arrhenius equation, or its simplified modification, is the most used temperature correction function. PELMO and optionally SIMULAT use O'Neills temperature correction function for degradation rate. This is an optimum curve where the user has to specify optimum and maximum temperatures for degradation, and, in addition, a value that describes the slope of the curve (Aden and Dieckrüger 2000). In a simple approach, e.g. GLEAMS version 2.10, degradation stops if soil temperature falls below a limit value. The calculation method of temperature effect on degradation was not specified for PRZM-3 (Carsel *et al.* 1998) nor for PLM (Nicholls *et al.* 2000). Soil moisture affect pesticide degradation in 11 of the 13 models (Table 5). Degradation is

slower in dry soil than at field capacity. The most used correction function is Walker's power law (e.g. Aden and Dieckrüger 2000). An optimum curve, in which the degradation rate decreases whenever soil moisture is above or below the given optimum moisture, is used in SIMULAT, PELMO and GLEAMS version 3.0. The optimum moisture may be an input parameter or internally set like in GLEAMS 3.0.

Soil microbiological activity usually decreases with depth. Therefore, the rate constant of biodegradation may be given separately for each soil layer, or depth factors, related to soil properties like organic carbon content, are used to correct the rate constant (Table 5).

Pesticide degradation products are called metabolites. Half of the considered models can simulate the fate of metabolites (Table 5).

## Pesticide transport equations

Convection is assumed to be the driving force for pesticide transport in soil in all studied models. In addition, mechanistic models take into account also hydrodynamic dispersion and diffusion. The most used input parameters are dispersion length for hydrodynamic dispersion and tortuosity factor for diffusion. In practice, capacity type models do not take into account dispersion whereas Richard's type models do (Table 5).

The descriptions of pesticide losses into surface waters are based on pesticide concentrations in an active mixing layer and on hydrological variables. The mixing layer is a thin soil layer near the soil surface (e.g. 10 mm). The pesticide concentration in the soil solution in the mixing layer, or in runoff water, does not remain constant during a runoff event. The calculation time step of the models is usually even longer: the most common time step among the models, which estimate surface losses, is a day. Therefore, the product of a daily runoff volume and pesticide concentration of soil solute in mixing layer gives an erroneous estimate of pesticide losses into surface waters. PELMO uses a correction term for the product (Klein 1995). GLEAMS, EPIC, MACRO and OPUS use estimates, in which the

pesticide partitioning coefficient ( $K_d$ ), extraction coefficient ( $B$ ) and several hydrological properties of the soil active mixing layer specify the pesticide losses into surface runoff (Leonard *et al.* 1987).

Methods to calculate (initial) pesticide concentrations in macropore flow are similar to those methods used for pesticide concentration calculations in surface runoff water. Estimations of pesticide losses in eroded sediment are based on pesticide concentrations in the adsorbed phase in top soil and sediment detachment. The latter is calculated as a component of erosion. Adsorbed pesticides may be carried by suspended colloidal particles into subsurface drainage water (Sprague *et al.* 2000). This is not considered in any of the models.

### Ability to simulate sugar beet cultivation practices

The ability to simulate at least a 10-year period and to consider multiple pesticide applications per summer was required from the model. EPIC, GLEAMS, LEACHM, MACRO, OPUS, PELMO, PEARL, PESTLA, PRZM and RZWQM fulfilled both criteria, but CRACK-NP, PLM and SIMULAT did not. SIMULAT has been designed for a vegetation period only and it can not simulate a 10-year period. The temporal scale was not specified for CRACK-NP and PLM. CRACK-NP simulates pesticide fate based on the initial concentration profile and no pesticide can be applied to the system.

Tillage practices (ploughing, cultivation, harrowing and beet harvesting) mix the soil and affect pesticide distribution in the soil. PESTLA, PEARL and RZWQM consider this phenomena in pesticide fate simulations. GLEAMS has a soil-mixing submodel for nutrients but not for pesticides. No data about this phenomenon was found for OPUS or PELMO. In addition, tillage affects soil hydrology and reduces herbicide leaching via preferential pathways (Elliott *et al.* 2000). EPIC, GLEAMS, MACRO, PRZM and RZWQM98 allow the user to change parameters, related to field hydrology or erosion, at specified time points during the simulation.

### Performance in validation and model comparison tests

We reviewed model studies, which compared simulation results of several models to experimental data, to elucidate performance of the selected models. In addition to the models selected by us, some model comparison studies included additional models. The results are summarised in Table 6. The factors, which were assumed to have affected the result in each model comparison study, are included in the table. These are e.g. model version and the experimental data used. No study was carried on in conditions similar to those of our application: sugar beet cultivation in northern climate. Vancløoster and Boesten (2000) observed that similar soil moisture contents were simulated with different parameter sets, which in turn produced remarkably different predictions of drainage fluxes. Malone *et al.* (2000) noted that, because of the occurrence of preferential flow, the use of pesticide concentration in soil as an indicator of pesticide movement through soil is questionable (Malone *et al.* 2000). Therefore, our review of published model comparison studies is divided into two parts: (1) studies that focus on state variables, like soil moisture and pesticide concentration in soil and (2) studies that focus on losses.

As a summary of the six reviewed model comparison studies focusing on state variables (Table 6), the ranking order of models depended on soil (Trevisan *et al.* 1995) and on pesticide (Zacharias *et al.* 1999, Tiktak 2000). In addition, it was concluded that the effect of model user on simulation results was remarkable and that the choice of parameters may override model differences in predicting state variables (Gottesbüren *et al.* 2000, Tiktak 2000, Vancløoster and Boesten 2000). Moreover, Vancløoster and Boesten (2000) found out that the ranking order of models, based on model performance in validation tests, depends on the statistical criteria used. In general, the Richard's type models were superior to the capacity type models in predicting soil moisture content, but calibration was needed (Vancløoster and Boesten 2000). Nevertheless, Richard's type models did not estimate pesticide concentration profiles any better than



**Table 6.** Summary of reviewed performance tests, s refers to model comparison studies focusing on state variables and l focusing on leaching losses.

L/S	Study	Order (from the worst to the best)	Data
S	(Trevisan <i>et al.</i> 1995)	PESTLA 2.3 < (PRZM-2 1.02, LEACHP 3.1 or VARLEACH 2.0) depending on soil => none of the models good enough	Three Italian fields: pesticide mass and concentration profiles.
S	(Zacharias <i>et al.</i> 1999)	OPUS ~ GLEAMS	A field: Soil moisture and pesticide degradation.
S	A study by Borah & Kalita (Ma <i>et al.</i> 2000)	MLEACHM ~ RZWQM (in clay soil); LEACHM < RZWQM (in sandy soil)	Fields (sandy and clay soil): pesticide concentration in suction lysimeters
S	(Vanclooster and Boesten 2000)	Moisture profile: (PRZM-2, VARLEACH, GLEAMS, PELMO) < (MACRO, LEACHP, MACRO, PESTLA, WAVE, PESTRAS, SIMULAT); none of the models good enough for tracer simulations	Field (sandy humic soil with shallow water table): soil moisture profile and tracer concentration profile.
S	(Tiktak 2000)	(VARLEACH 2.0, LEACHM 3.1, PELMO 2.01, GLEAMS 2.1, PESTLA 2.31) << PESTRA < PRZM-2 < MACRO (in bentazone simulations) (PRZM-2 2.0, LEACHM 3.1, VARLEACH 2.0, PELMO 2.01, PESTRAS 3.1) < GLEAMS 2.1 < PESTLA 2.31 < MACRO 4.0 (in ethoprophos simulations)	Pesticide (bentazone, low sorption ethoprophos, high sorption and volatile) concentration profiles (Ranking orders based on the averages of the best and worst modeling efficiency produced by different users).
S	(Gottesbüren <i>et al.</i> 2000)	SIMULAT 2.3 < LEACHNP < (MACRO 3.1/4.0, WAVE and GLEAMS 2.10) => Choice of parameters overrides the model differences.	Field (silty, German soil): moisture, tracer and pesticide concentration profile.
L	(Bergström and Jarvis 1994)	(CALF, CMLS, GLEAMS, PELMO, PESTLA, PRZM) < (PLM and MACRO) => preferential flow important	Lysimeters in five sites: water flow and pesticide concentration in leachate.
L + S	(Styczen and Villholth 1995)	PESTLA < (LEACHM in sandy and MACRO in loamy soil)	Catchments: drainage flow, water table, pesticide concentration in suction cups
L + S	(Gottesbüren <i>et al.</i> 1995)	VARLEACH 2.0, LEACHP 3.1, PESTLA 2.3 < PELMO 1.5 < MACRO 3.1 => none of the models good enough	Lysimeters: pesticide concentration profile and water outflow.
L	(Vink <i>et al.</i> 1997)	(VARLEACH 2.0, LEACHP 3.1) < (PESTLA 2.3 and MACRO 3.1) < SIMULAT 2.4 => none of the models good enough	Clay soil column in laboratory: concentrations of leachate water.
L	(Francaviglia <i>et al.</i> 2000)	(PELMO 2.0, GLEAMS 2.10, PRZM-2) < SIMULAT 2.3 => none of the models good enough	Lysimeter data set: water flow, and tracer and pesticide concentrations in leachate..
L+S	(Malone <i>et al.</i> 1999)	PRZM-3 beta ~ GLEAMS 2.10 => neither is good enough	3 plots (160 m <sup>2</sup> ), slope 10%: water and erosion outflows, pesticide losses and concentrations in soil.
L	(Thorsen <i>et al.</i> 1998)	(PELMO 2.01 and PESTLA 2.3) < (MACRO 3.2 and MIKE SHE 5.23) => models containing macropores required less calibration	A soil column in laboratory and a field lysimeter: tracer and pesticide concentrations of leachate water.

Continues

**Table 6.** Continued.

L/S	Study	Order (from the worst to the best)	Data
L	(Armstrong <i>et al.</i> 2000a)	(PLM 3 and modified SIMULAT 2.3) < (CRACK-NP and MACRO 4.0) => Calibration needed	Field (cracking clay soil): pesticide losses into subsurface drainage water (tile depth: 55 cm).
L	(Beulke <i>et al.</i> 2001)	Uncalibrated: (MACRO-DB) < (CRACK-NP 2.0 and MACRO 4.0) < (PLM and SWAT) => none of the models were good enough; => uncalibrated modelling cannot be recommended for such artificially drained heavy clay soils.	Four plots in a heavy clay soil in England: drainage flow and pesticide (isoproturon) concentration in drainage water.

capacity type models (Zacharias *et al.* 1999, Tiktak 2000). Ten studied models (GLEAMS, LEACHP, MACRO, PELMO, PESTLA, PESTRAS, PRZM-2, SIMULAT, VARLEACH and WAVE) performed well in soil temperature simulation (at 2.5 cm depth from surface) even without calibration but failed in tracer simulations, and calibration improved only slightly the performance of the models (Vanclouster and Boesten 2000). CRACK-NP, EPIC or PLM were not included in any of these studies focusing on state variables.

Nine model comparison studies, which focused on mass balances and losses, are presented in Table 6. None of the models produced acceptable predictions without calibration. Moreover, the conclusion in four of the nine studies was that none of the included models could produce adequate estimations of pesticide losses (Gottesbüren *et al.* 1995, Vink *et al.* 1997, Malone *et al.* 1999, Francaviglia *et al.* 2000). A description of preferential pathways seemed to improve model performance. MACRO was included in seven studies and was classified to the best group of models in five of them. No comparison studies were found of the simulated losses of EPIC or RZWQM.

## Conclusions

### Fulfilment of predefined criteria

We compared pesticide fate models in order to select the appropriate model for herbicide fate simulations in Finnish sugar beet cultivation.

None of the models fulfilled all of the criteria which were composed for this specific purpose. An assessment of how each model fulfilled each criterion is presented in Table 7. Most of the models lack process descriptions for soil freezing and soil mixing by tillage. Only a few of the models take into account both surface losses and subsurface drainage losses. Many of the models are under a development process and improved model versions are expected in the near future. The documentation of a model, if it exists at all, refers seldom to the current version. The documentation of most of the models should be improved and the users should always indicate which version has been used.

### Selected models

The models were simply ranked according to the sum of the pluses and minuses given in Table 7. The five best models in this ranking list were MACRO (16), RZWQM (13), PEARL (11.5), GLEAMS (9.5) and PELMO (9). The order was the same even if the most subjective pluses of technical points and performance in model comparison test were excluded.

The best model in the ranking list, the Swedish MACRO version 4.1 (Jarvis and Larsson 1998) or later, was chosen for estimation of leaching and drainage losses of herbicides. Though MACRO fulfils most of the criteria, it has several limitations. The most important ones are the following: (1) It cannot be used for surface loss estimations, (2) tillage does not affect pesticide distribution in soil, (3) frozen

soil dynamic is not included in the model, (4) Source code of the model is not available, and (5) model requires a number of parameters, which are hardly available, and execution time is very long.

MACRO was not regarded sufficient to be used alone for herbicide fate simulations in Finnish sugar beet fields. Another model was needed for surface loss estimations. The American GLEAMS version 3.0 (Knisel and Davis 2000) was the best surface loss model in the ranking list. In this GLEAMS version, the erosion calculation has been modified to be suitable for northern Europe by reducing the rainfall energy. In addition, GLEAMS has a simple process

description for soil frost. GLEAMS uses a limited number of parameters and it is very quick to run. The source code is freely available but the Fortran code is poorly commented, and the program structure is unclear. The main limitations of the current version are that sorption coefficients can not be given separately for different layers and tillage does not affect pesticide distribution in soil. The model estimates the losses below the root zone, but the soil hydrology description is simple and preferential flow pathways or subsurface drainage are not included.

The other high regarded models in this review were RZWQM, PEARL and PELMO. If the selected MACRO or GLEAMS were

**Table 7.** Summary.

Model	Hydrology	Pesticide chemistry	Cultivation practices	Winter processes	Preferential flow	Technical points	Performance tests
CRACK-NP	(+)(+)+	++	–	–	+	+++	+
EPIC	+(+)		++(+)	+(?)		+++	?
GLEAMS	+(+)	++	++(+)	+(+)		(+)(+)+	X
LEACHP	+	++	+	–		?	X
MACRO	(+)++	+++	++(+)	+	++	+++	++
OPUS	+++	+	++?	+		?	+
PELMO	+(+)(+)	++	++?	+		++?+	–
PEARL	(+)++	+++	+++	–		++++	?
PESTLA	(+)++	+++	++	–		++	–
PLM	(+)(+)	++	–	–	+	?	X
PRZM	+(+)	(+)+	++(+)	+		+(+)??+	–
RZWQM	(+)++	++	+++(+)	+	+	++	+
SIMULAT	+	++	–	–	(+)	?	–

+ = positive features included (more detailed list below) or good performance in model comparison studies.

(+) = less than a full plus.

– = a required feature is lacking or weak performance in comparison studies.

? = no data found.

X = inconsistent result in performance studies.

Criteria for pluses:

Hydrology: a plus per (1) surface losses (includes erosion), (2) mechanistic water and solute transport in soil, (3) subsurface drainage flow.

Pesticide chemistry: a plus per (1) temperature and moisture dependent degradation, (2) ability to give sorption parameters separately for each layer, (3) metabolites.

Cultivation practices: a plus per (1) at least 10-year period and multiple application per summer, (2) foliar application, (3) tillage effect on pesticide distribution, (4) tillage effect on hydrology.

Winter hydrology: a plus per (1) snow accumulation and melting, (2) soil freezing and thawing and its effects on hydrology.

Preferential flow: a plus (1) if preferential flow is included, (2) a plus of the assumed quality of the description, (3) colloidal transport.

Technical points: a plus per (1) tight version control, (2) documentation for current version, (3) source code availability and quality, (4) model freely downloadable from internet.

abandoned, PELMO could replace GLEAMS, and either RZWQM or PEARL could replace MACRO. However, PEARL (SWAP) misses snow accumulation and melting routines, which must be added to model before simulating Finnish conditions. Technical points complicated the test use of RZWQM98 and the model can not be used in Finland before these are solved. Model requires detailed breakpoint rainfall data, which is available only for summer seasons. Moreover, the interface of RZWQM beta version is designed solely for U.S. users which caused problems in climate data importing. On the one hand the holistic viewpoint of RZWQM (especially the detailed crop growth model) is one of the strengths of the model, but on the other hand it calls for parameters not clearly related to pesticide fate.

### Need for further information

Particle facilitated colloidal transport phenomena may be an important process in pesticide transport (Jarvis *et al.* 1999, Worrall *et al.* 1999, Sprague *et al.* 2000). Due to lack of knowledge, no pesticide fate model currently considers this. Moreover, as Jarvis (2001) remarked, there are serious gaps in understanding surface processes, and how cultivation practices affect them. Therefore, these processes are not properly described in the models. Though thermal desorption is used as a cleaning method for pesticide contaminated soils (Sahle-Demessie and Richardson 2000), the effect of soil freezing and thawing on pesticide fate is not fully understood. This should be studied and, based on the outcome of the studies, the process could be incorporated into pesticide leaching models. In addition, the effect of soil freezing on hydrology, and pesticide redistribution after tillage practises, should be added into models.

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