RIVM report 711401 008, Alterra report 28

Manual of FOCUS PEARL version 1.1.1

A. Tiktak, F. van den Berg[a], J.J.T.I. Boesten[a],
D. van Kraalingen[a], M. Leistra[a] and A.M.A. van
der Linden

November 2000

a) *Co-authors from Alterra Green World Research*

Abstract

The PEARL model is used to evaluate the leaching of pesticide to the groundwater in support to the Dutch and European pesticide registration procedures. PEARL is an acrononym for Pesticide Emmission Assessment at Regional and Local scales. The model is a joint product of Alterra Green World research and the National Institute of Public Health and the Environment, and it has replaced the models PESTLA and PESTRAS since June 1st, 2000. Model and data can be accessed through a user-friendly Graphical User Interface for Windows 95/98/NT. All data are stored in a relational database. Both the Dutch standard scenario and the European standard scenario's as suggested by the FOCUS modeling working group can be accessed through the User Interface. This report gives a description of the processes and parameters included in PEARL version 1.1. It also contains a description of the Pearl User Interface and the input and output files. The Dutch standard scenario is described briefly.

Keywords:
Pesticides; leaching; groundwater; soil; risk-assessment; PEARL; FOCUS; graphical user interface

Preface

Pesticide leaching models have been developed and used in The Netherlands since the early seventies, but their use in pesticide registration was limited until 1989. In that year the PESTLA (PESTicide Leaching and Accumulation) model was launched and officially incorporated in the evaluation process. Initially, its use was limited to estimate leaching under standard soil and weather conditions in the first tier of the evaluation process, but within a few years its use was extended to higher tier assessments and evaluations outside the registration process.

The broader use stimulated the release of new versions of PESTLA, but also the development of the PESTRAS (PESTicide TRansport ASsessment) model; the latter especially developed for regional-scale applications. Although the description of pesticide behavior in both models was based on PESTLA, the two models produced different results. Although the differences were small, they were significant at the leaching level of 0.1 g ha^{-1}, which is relevant in the registration process. As this was considered unacceptable, the Ministry of Agriculture, Fisheries and Nature Preservation (LNV) and the Ministry of Housing, Spatial Planning and the Environment (VROM) charged Alterra Green World Research and the National Institute of Public Health and the Environment (RIVM) with the development of a consensus leaching model.

In 1997, a project team was formed to develop the new model. The team consisted of the authors of this report. The project team decided that PEARL (Pesticide Emission Assessment at the Regional and Local scale) should be more than a simple merger of the two precursors. The opportunity was taken to:
− include recent scientific developments
− upgrade the computer language to FORTRAN 95 and make use of object oriented techniques
− develop an object oriented database to assist in generating input and archiving
− develop a graphical user interface, called PUI (Pearl User Interface), consistent with the database, for easy use of the software.

Francisco Leus and Klaas Groen (RIZA) commented in the early stages on the concepts to be included in PEARL. Bernd Gottesbüren (BASF) and Helmut Schäfer (Bayer) reviewed the draft manuscripts and tested the software package. Their contributions are gratefully acknowledged.

The software package contains an e-mail address for communication with the developers. Users of PEARL are encouraged to report difficulties and errors they experience as well as suggestions for improvement.

Contents

List of Symbols and Units

Symbol	Description	Unit	Acronym
a	interception coefficient	m	*CofIntCrp*
$a_{C,g}$	coefficient in Currie diffusion equation for the gas phase	-	*CofDifGasCur*
$a_{C,L}$	coefficient in Currie diffusion equation for the liquid phase	-	*CofDifLiqCur*
a_g	parameter in bottom flux-phreatic head relationship	m d^{-1}	*CofFncGrwLev*
$a_{M,g}$	exponent in numerator of Millington equation for gas phase	-	*ExpDifGasMilNom*
$a_{M,L}$	exponent in numerator of Millington equation for liquid phase	-	*ExpDifLiqMilNom*
$a_{T,L}$	coefficient in Troeh diffusion equation for the liquid phase	m^3 m^{-3}	*CofDifLiqTro*
$a_{T,g}$	coefficient in Troeh diffusion equation for the gas phase	m^3 m^{-3}	*CofDifGasTro*
A_p	Areic mass of pesticide at the crop canopy	m d^{-1}	*AmaCrp*
$A_{d,p}$	Areic mass deposited on the plants	kg m^{-2}	*AmaAppCrp*
$A_{d,f}$	Areic mass deposited on the field	kg m^{-2}	*AmaApp*
$A_{d,s}$	Areic mass deposited on the soil surface	kg m^{-2}	*AmaAppSol*
b_g	parameter in bottom flux-phreatic head relationship	m^{-1}	*ExpFncGrwLev*
B	exponent for the effect of soil moisture on transformation	-	*ExpLiqTra*
$b_{C,g}$	exponent in Currie diffusion equation for the gas phase	-	*ExpDifGasCur*
$b_{C,L}$	exponent in Currie diffusion equation for the liquid phase	-	*ExpDifLiqCur*
$b_{M,g}$	exponent in denumerator of Millington equation for gas phase	-	*ExpDifGasMilNom*
$b_{M,L}$	exponent in denumerator of Millington equation for liquid phase	-	*ExpDifLiqMilNom*
$b_{T,g}$	exponent in Troeh diffusion equation for the gas phase	-	*ExpDifGasTro*
$b_{T,L}$	exponent in Troeh diffusion equation for the liquid phase	-	*ExpDifLiqTro*
c_a	concentration in air	kg m^{-3}	*ConAir*
C_a	volumic heat capacity of water	J m^{-3} K^{-1}	*NR*
C_{clay}	volumic heat capacity of clay	J m^{-3} K^{-1}	*NR*
$c*_{eq}$	pesticide concentration in the equilibrium domain of the soil	kg m^{-3}	*ConSysEql*
$c*_{ne}$	pesticide concentration in the non-equilibrium domain of the soil	kg m^{-3}	*ConSysNeq*
$C(h)$	differential water capacity	m^{-1}	*NR*
C_h	volumic heat capacity	J m^{-3} K^{-1}	*NR*
c_g	concentration in the gas phase	kg m^{-3}	*ConGas*
$c_{g,0}$	concentration in the gas phase at the soil surface	kg m^{-3}	*ConGasUbo*
$c_{g,1}$	concentration in the gas phase in center of top layer	kg m^{-3}	*ConGas(1)*
c_L	concentration in the liquid phase	kg m^{-3}	*ConLiq*
$c_{L,r}$	reference concentration in the liquid phase	kg m^{-3}	*ConLiqRef*
C_{om}	volumic heat capacity of organic matter	J m^{-3} K^{-1}	*NR*
C_{sand}	volumic heat capacity of sand	J m^{-3} K^{-1}	*NR*
C_w	volumic heat capacity of water		
d_a	thickness of air boundary layer	m	*ThiAirBouLay*
d_s	thickness of soil boundary layer	m	*ThiLay(1)/2*
D_a	pesticide diffusion coefficient in air	m^2 d^{-1}	*CofDifAir*
$D_{a,r}$	pesticide diffusion coefficient in air at reference temperature	m^2 d^{-1}	*CofDifAirRef*
$D_{dif,g}$	coefficient of pesticide diffusion in the gas phase	m^2 d^{-1}	*CofDifGas*
$D_{dif,L}$	coefficient of pesticide diffusion in the liquid phase	m^2 d^{-1}	*CofDifLiq*
$D_{dis,L}$	coefficient of pesticide dispersion in the liquid phase	m^2 d^{-1}	*CofDisLiq*
$DT_{50,r}$	half-life in equilibrium domain at reference temperature	d	*DT50Ref*
D_w	pesticide diffusion coefficient in pure water	m^2 d^{-1}	*CofDifWat*
$D_{w,r}$	pesticide diffusion coefficient in water at reference temperature	m^2 d^{-1}	*CofDifWatRef*
E_a	molar enthalpy of transformation	J mol^{-1}	*MolEntTra*
E_{max}	maximum soil evaporation flux based on Darcy equation	m^3 m^{-2} d^{-1}	*NR*

Symbol	Description	Unit	Acronym
ET_r	reference evapotranspiration according to Makkink	$m^3\ m^{-2}\ d^{-1}$	*NR*
E_s	actual flux of evaporation from the soil	$m^3\ m^{-2}\ d^{-1}$	*FlvLiqEvpSol*
E_p	potential flux of evaporation from the soil	$m^3\ m^{-2}\ d^{-1}$	*FlvLiqEvpSolPot*
ET_p	potential evapotranspiration flux	$m^3\ m^{-2}\ d^{-1}$	*NR*
ET_{p0}	idem, of a dry canopy, completely covering the soil	$m^3\ m^{-2}\ d^{-1}$	*NR*
ET_{w0}	idem, of a wet canopy, completely covering the soil	$m^3\ m^{-2}\ d^{-1}$	*NR*
f_c	empirical crop factor for transpiration	-	*FacCrpEvp*
f_d	factor for the effect of depth on transformation	-	*FacZTra*
$f_{d,p}$	fraction of dosage deposited on the plants	-	*FraAppCrp*
$f_{d,s}$	factor for the effect of depth on sorption	-	*FacZSor*
f_m	factor for the effect of soil moisture on transformation	-	*FacLiqTra*
$f_{K,ne}$	factor describing the ratio $K_{F,ne}/K_{F,eq}$	-	*FacSorNeqEql*
f_t	factor for the effect of temperature on transformation	-	*FacTemTra*
f_u	transpiration concentration stream factor	-	*FacUpt*
f_w	fraction of the day with wet canopy	-	*NR*
h	soil water pressure head	m	*PreHea*
H	hydraulic head	m	*NR*
$h_1..h_4$	critical soil water pressure heads in water uptake relationship	m	*HLim1..HLim4*
$J_{p,g}$	mass flux of pesticide in the gas phase	$kg\ m^{-2}\ d^{-1}$	*FlmGas*
$J_{p,L}$	mass flux of pesticide in the liquid phase	$kg\ m^{-2}\ d^{-1}$	*FlmLiq*
$J_{p,v}$	mass flux of pesticide volatilization	$kg\ m^{-2}\ d^{-1}$	*FlmGasVol*
$J_{v,a}$	volatilization flux through the air boundary layer	$kg\ m^{-2}\ d^{-1}$	*NR*
$J_{v,s}$	volatilization flux through the soil boundary layer	$kg\ m^{-2}\ d^{-1}$	*NR*
$J_{w,p}$	water flux from the crop canopy (canopy drip)	$m^3\ m^{-2}\ d^{-1}$	*NR*
K_a	dissociation constant for weak acids	$mol\ m^{-3}$	*Ka*
k_d	desorption rate coefficient	d^{-1}	*CofRatDes*
k_{dsp}	lumped rate coefficient for dissipation at the crop canopy	d^{-1}	*CofRatDisCrp*
$K_{F,eq}$	Freundlich sorption coefficient for the equilibrium domain	$m^3\ kg^{-1}$	*CofFreEql*
$K_{F,eq,r}$	Freundlich sorption coefficient at reference conditions	$m^3\ kg^{-1}$	*CofFreEql*
$K_{F,ne}$	Freundlich sorption coefficient for the non-equilibrium domain	$m^3\ kg^{-1}$	*CofFreNeq*
K_H	Henry coefficient for gas/liquid partitioning	$m^3\ m^{-3}$	*CofHenry*
$K(h)$	unsaturated hydraulic conductivity	$m\ d^{-1}$	*NR*
$K_{om,eq}$	coefficient of equilibrium sorption on organic matter	$m^3\ kg^{-1}$	*KomEql*
K_s	saturated hydraulic conductivity	$m\ d^{-1}$	*KSat*
k_t	rate coefficient for transformation in soil	d^{-1}	*CofRatTra*
$k_{t,par}$	rate coefficient for transformation of parent in soil	d^{-1}	*CofRatTraPrt*
$k_{t,p}$	rate coefficient for transformation at the crop canopy	d^{-1}	*CofRatTraCrp*
k_{vol}	rate coefficient for volatilization from the canopy	d^{-1}	*CofRatVolCrp*
LAI	Leaf Area Index	$m^2\ m^{-2}$	*LAI*
$L_{dis,L}$	dispersion length in the liquid phase	m	*LenDisLiq*
L_k	distance between drainage conduits of system k	m	*DstDra*
L_{root}	root length density	$m\ m^{-3}$	*NR*
M	molar mass	$kg\ mol^{-1}$	*MolMas*
N	Freundlich exponent	-	*ExpFre*
n	empirical parameter in Van Genuchten equation	-	*ParVgn*
m	empirical parameter in Van Genuchten equation	-	*ParVgm*
m_{om}	mass content of organic matter in soil	$kg\ kg^{-1}$	*CntOm*
P	volume flux of gross precipitation	$m^3\ m^{-2}\ d^{-1}$	*FlvLiqPrc*
P_i	precipitation intercepted by plant roots	m	*FlvLiqEvpInt*
P_{min}	Minimum precipitation to reset a soil surface drying cycle	m	*NR*

Symbol	Description	Unit	Acronym
P_n	volume flux of net-precipitation (throughfall)	$m^3\ m^{-2}\ d^{-1}$	*NR*
$p_{v,s}$	saturated vapor pressure	Pa	*PreVap*
$p_{v,s,r}$	saturated vapor pressure at reference temperature	Pa	*PreVapRef*
q	soil water flux	$m^3\ m^{-2}\ d^{-1}$	*FlvLiq*
q_b	soil water flux at the lower boundary	$m^3\ m^{-2}\ d^{-1}$	*FlvLiq(NumLay)*
$q_{d,k}$	flux of water to drainage system k	$m^3\ m^{-3}\ d^{-1}$	*NR*
R	molar gas constant	$J\ mol^{-1}\ K^{-1}$	*RGas*
$r_{a,v}$	resistance for volatilization through the air boundary layer	$d\ m^{-1}$	*RstAirLay*
R_{dsp}	areic mass rate of pesticide dissipation at the crop canopy	$kg\ m^{-2}\ d^{-1}$	*AmrDspCrp*
R_d	volumic mass rate of lateral pesticide discharge by drainage	$kg\ m^{-3}\ d^{-1}$	*VmrDra*
$R_{d,L}$	volumic volume rate of lateral water discharge	$m^3\ m^{-3}\ d^{-1}$	*VvrDraLiq*
$R_{d,L,k}$	rate of lateral water discharge to drainage system k	$m^3\ m^{-3}\ d^{-1}$	*NR*
R_f	volumic mass rate of formation	$kg\ m^{-3}\ d^{-1}$	*VmrFor*
$R_{f,par,dau}$	volumic mass rate of transformation from parent to daughter	$kg\ m^{-3}\ d^{-1}$	*VmrTraParDau*
$R_{v,p}$	areic mass rate of penetration into the plants	$kg\ m^{-2}\ d^{-1}$	*AmrPenCrp*
R_s	volumic mass rate of sorption in non-equilibrium domain	$kg\ m^{-3}\ d^{-1}$	*VmrSorNeq*
$r_{s,v}$	resistance for volatilization through the soil boundary layer	$d\ m^{-1}$	*RstSolLay*
R_t	volumic mass rate of transformation	$kg\ m^{-3}\ d^{-1}$	*VmrTra*
$R_{t,p}$	areic mass rate of transformation on the plants	$kg\ m^{-2}\ d^{-1}$	*AmrVolCrp*
$R_{t,par}$	areic mass rate of transformation of parent	$kg\ m^{-2}\ d^{-1}$	*AmrTraPrt*
$R_{v,p}$	areic mass rate of volatilisation from the plants	$kg\ m^{-2}\ d^{-1}$	*AmrVolCrp*
R_u	volumic mass rate of pesticide uptake	$kg\ m^{-3}\ d^{-1}$	*VmrUpt*
$R_{u,L}(z)$	actual rate of water uptake by plant roots	$m^3\ m^{-3}\ d^{-1}$	*VvrUptLiq*
$R_{u,L,p}(z)$	potential rate of water uptake by plant roots	$m^3\ m^{-3}\ d^{-1}$	*VVrUptLiqPot*
$R_{w,p}$	areic mass rate of wash-off from the crop canopy	$kg\ m^{-2}\ d^{-1}$	*AmrWasCrp*
SC	fraction of the soil covered by crop	$m^2\ m^{-2}$	*FraCovCrp*
S_e	relative water saturation	-	*NR*
S_w	solubility in water	$kg\ m^{-3}$	*SlbWat*
$S_{w,r}$	solubility in water at reference temperature	$kg\ m^{-3}$	*SlbWatRef*
t	time	d	*Tim*
T	temperature	K	*Tem*
T_{air}	daily average air temperature	K	*TemAir*
T_a	actual plant transpiration flux	$m^3\ m^{-2}\ d^{-1}$	*FlvLiqTrp*
T_r	reference temperature	K	*TemRef*
T_0	freezing point	K	*TemFrozen*
TL	thickness of soil layer	m	*ThiLay*
T_p	potential plant transpiration flux	$m^3\ m^{-2}\ d^{-1}$	*FlvLiqTrpPot*
w_p	washability factor	m^{-1}	*FacWasCrp*
X_{eq}	mass content sorbed in the equilibrium domain	$kg\ kg^{-1}$	*CntSorEql*
X_{ne}	mass content sorbed in the non-equilibrium domain	$kg\ kg^{-1}$	*CntSorNeq*
z	position or depth in soil	m	*Z*
z_{root}	rooting depth	m	*ZRoot*
z_{til}	depth of tillage layer	m	*ZTil*
α	reciprocal of air entry value (Van Genuchten parameter)	m^{-1}	*ParVgAlpha*
$\alpha_w(h)$	factor for root water uptake as a function of pressure head	-	*NR*
β	parameter for reduction of soil evaporation due to drying	$m^{1/2}$	*CofRedEvp*
β_{gwl}	shape factor for groundwater surface	-	*FacShapeGrwLev*
γ_{aqt}	vertical resistance of semi-confining aquifer	d	*RstAqt*
$\gamma_{dr,k}$	resistance of drainage system k	d	*RstDra*
ΔH_d	molar enthalpy of dissolution	$J\ mol^{-1}$	*MolEntVap*

Symbol	Description	Unit	Acronym
ΔH_v	molar enthalpy of vaporisation	J mol^{-1}	*MolEntVap*
Δz_i	distance between nodal point i and $i+1$	m	*DelZ*
ε	volume fraction of air in the soil system	m^3 m^{-3}	*Eps*
θ	volume fraction of water in the soil system	m^3 m^{-3}	*Theta*
θ_{fc}	volume fraction of water at field-capacity	m^3 m^{-3}	*ThetaRef*
θ_{clay}	volume fraction of clay in the soil system	m^3 m^{-3}	*NR*
θ_{om}	volume fraction of organic matter in the soil system	m^3 m^{-3}	*NR*
θ_r	residual volume fraction of water in the soil system	m^3 m^{-3}	*ThetaRes*
θ_s	saturated volume fraction of water in the soil system	m^3 m^{-3}	*ThetaSat*
θ_{sand}	volume fraction of sand in the soil system	m^3 m^{-3}	*NR*
κ	extinction coefficient for global solar radiation	-	*CofExtRad*
ξ_g	relative diffusion coefficient for the gas phase	m^2 m^{-2}	*CofDifGasRel*
ξ_L	relative diffusion coefficient for the liquid phase	m^2 m^{-2}	*CofDifLiqRel*
λ	empirical parameter in hydraulic conductivity function	-	*ParVgl*
λ_h	effective heat conductivity of soil	J m^{-1} d^{-1} K^{-1}	*NR*
ρ_b	dry bulk density of the soil	kg m^{-3}	*Rho*
Φ_{avg}	average hydraulic head of phreatic groundwater	m	*NR*
Φ_{aqf}	average hydraulic head in semi-confining aquifer	m	*HeaAqfAvg*
Φ_d	hydraulic head of drainage base	m	*HeaDraBase*
Φ_{gwl}	hydraulic head of phreatic groundwater	m	*GrwLev*
$\chi_{p,d}$	molar fraction of parent transformed to daughter	-	*FraPrtDau*

Samenvatting

In 1989 werd het PESTLA (PESTicide Leaching and Accumulation) model door de Nederlandse overheid geïntroduceerd als standaardinstrument voor de beoordeling van de uitspoeling van bestrijdingsmiddelen naar het ondiepe grondwater. Dit model werd aanvankelijk uitsluitend gebruikt om de uitspoeling onder standaard weer- en bodemcondities te berekenen. Al snel ontstond er ook interesse in evaluaties buiten de officiële beoordeling. Dit heeft niet alleen geleid tot de ontwikkeling van nieuwe versies van PESTLA, maar ook tot de ontwikkeling van het (regionale) PESTRAS (PESticide TRansport ASsessment) model. Hoewel beide modellen nagenoeg dezelfde modelconcepten hanteerden, waren er kleine verschillen in de resultaten van beide modellen. Alhoewel de verschillen gering waren, werd de afwijking op het voor de toelating van belang zijnde niveau van 0.1 g ha^{-1} niet acceptabel gevonden. Om deze reden werd door de Ministeries van LNV en VROM een opdracht verleend aan het toenmalige SC-DLO (tegenwoordig Alterra) en RIVM om een op consensus gebaseerd nieuw uitspoeling-model te ontwikkelen.

Het nieuwe model kreeg de naam PEARL (Pesticide Emission Assessment at Regional and Local scales). Eigenschappen van het model zijn o.a. (i) het model is object georiënteerd geprogrammeerd, waardoor onderhoud van de broncode vereenvoudigd wordt, (ii) model en data zijn toegankelijk via een Graphical User Interface voor Windows 95/98/NT, (iii) data en scenario's zijn opgeslagen in een relationele database, (iv) het is eenvoudig het model te koppelen aan andere programma's, zoals Geografische Informatie Systemen en programmatuur voor inverse modellering en (v) door bundeling van krachten is een 'state-of-the-art' model ontstaan, zowel wat betreft de ontwikkeling van procesformuleringen als wat betreft de validatiestatus van het model.

Het model zal gebruikt worden als nieuw standaardinstrument voor de beoordeling de uitspoeling van bestrijdingsmiddelen. Het model is geschikt voor de Nederlandse en de Europese beoordeling. Het model ondersteunt n.l. de scenario's die opgezet zijn door het Forum voor Internationale Coördinatie van modellen van het gedrag van bestrijdingsmiddelen (FOCUS). Een metamodel van PEARL is opgenomen in USES 3.0. Het model is tevens geschikt voor evaluatie van gevoerd beleid. Op korte termijn is toepassing voorzien in het kader van het Meerjaren Plan Gewasbescherming (MJP-G), MB/MV en het Gewasbeschermingsplan 2000^{+}.

Dit rapport geeft een beschrijving van de processen en parameters in PEARL 1.1-sr3. Tevens wordt een beschrijving gegeven van de PEARL user interface en de in- en uitvoerbestanden. Het Nederlands standaardscenario wordt kort beschreven.

Summary

In 1989, the PESTLA (PESTicide Leaching and Accumulation) model was launched and officially incorporated in the pesticide registration process. Initially, its use was limited to estimate leaching under standard soil and weather conditions, but within a few years its use was extended to evaluations outside the registration process. The broader use stimulated the release of new versions of PESTLA, but also the development of the PESTRAS (PESTicide TRansport ASsessment) model; the latter especially developed for regional-scale applications. Although the description of pesticide behavior in both models was based on PESTLA, the two models produced different results. Although the differences were small, they were significant at the leaching level of 0.1 g ha^{-1}, which is relevant in the registration process. As this was considered unacceptable, the Ministry of Agriculture, Fisheries and Nature Preservation (LNV) and the Ministry of Housing, Spatial Planning and the Environment (VROM) charged Alterra Green World Research and the National Institute of Public Health and the Environment (RIVM) with the development of a consensus leaching model.

This new model, PEARL, is presented in this report. PEARL is an acronym of *Pesticide Emission Assessment at Regional and Local scales*. Important features of the model are: (i) object oriented design guaranteeing easy maintenance of the source code, (ii) model and data can be accessed through a user-friendly Graphical User Interface for Windows 95/98/NT, (iii) data and scenarios are stored in a relational database, (iv) easy link with external programs, such as Geographical Information Systems and inverse modeling tools, and (v) maximum benefit is taken from the experience of both modeling groups, both with respect to the development of new process descriptions, and with respect to the validation status of the model. The model is the new official tool in Dutch pesticide registration procedures. It is also suitable for European applications, as the model supports the target quantities and scenarios set by the Forum for International Co-ordination of pesticide fate models and their Use (FOCUS). A meta-model of PEARL has been incorporated into USES 3.0 (Uniform System for the Evaluation of Substances). The model is also suitable for policy evaluation. Model use is foreseen in the context of the Multi Year Crop Protection Plan (MJP-G), the project 'State of the Environment' and the Crop Protection Plan 2000^{+}.

This report gives a description of the processes and parameters included in PEARL version 1.1. It also contains a description of the Pearl User Interface and the input and output files. The Dutch standard scenario is described briefly.

1   Introduction

1.1   General introduction

The potential threat of pesticides to the environment has been recognized for decades. Approximately 50 pesticides have been detected in the groundwater in western Europe and the USA (Leistra and Boesten, 1989; Hallberg, 1989). Today, the usage of hazardous products is prevented by legislation that is based on quantitative and objective criteria. The modeling of the fate of pesticides in soil has contributed to the development of these legislation procedures (Van der Linden and Boesten, 1989; Boesten and van der Linden, 1991; Brouwer *et al.*, 1994). Using pesticide properties measured in the laboratory as input data, the fate of pesticides in the soil can be simulated under various environmental scenarios (Tiktak *et al.*, 1996ab).

In the Netherlands, PESTLA 1.1 (*Pesticide Leaching and Accumulation*; Van der Linden and Boesten, 1989) has been used on a regular basis for assessing the accumulation and leaching of pesticides in soil. As early as 1976, precursors of the PESTLA model were operational as tools for Dutch legislation purposes (Leistra and Dekkers, 1976). Versions 1.x of the PESTLA model were written in CSMP. The most important limitation of this model version was its inflexibility: Pesticide properties, hydrological conditions and weather data were introduced into the source code. This inflexibility stimulated the development of new models and model versions. The PESTLA model was further developed by Van den Berg and Boesten (1998). This model was loosely coupled with the hydrological model SWAP (*Soil Water Atmosphere Plant model*), which also provided the heat flow algorithm (Van Dam *et al.*, 1999). Processes like adsorption-desorption kinetics, the formation and behavior of reaction products, and vapor diffusion in the gas phase were included. In the mid-nineties, the PESTRAS (*Pesticide Transport Assessment*) model was developed by Tiktak *et al.* (1994) and Freijer *et al.* (1996). PESTRAS was developed primarily for regional-scale applications (Tiktak *et al.*, 1996ab). The description of pesticide behavior in soil was similar to that in PESTLA. However, PESTRAS was coupled to a different model for soil water flow (i.e. the SWIF model developed by Tiktak *et al.*, 1992) and heat transport. The description of vapor transport (both convective and diffusive) was taken from Freijer (1994). Concepts were developed on the volatilization of pesticide from a film residing at the soil surface. The model further included a comprehensive description of the formation of reaction products.

Although the description of pesticide behavior in both models was based on PESTLA 1.1, the two models predicted slightly different leaching rates into the groundwater (see e.g. Boesten, 2000). This has lead to confusion in the pesticide registration procedure, particularly if both models were used for one pesticide. For this reason, the authorities asked for a consensus model simulating the behavior of pesticides in soil and their emissions from soil systems. This new model was given the name PEARL, which is an acronym for *Pesticide Emission Assessment at Regional and Local scales*). Important features of the model are: (i) object

oriented design guaranteeing easy maintenance of the source code, (ii) model and data can be accessed through a user-friendly Graphical User Interface for Windows 95/98/NT, (iii) data and scenarios are stored in a relational database, (iv) easy link with external programs, such as Geographical Information Systems and inverse modeling tools, and (v) maximum benefit is taken from the experience of both modeling groups, both with respect to the development of new process descriptions, and with respect to the validation status of the model.

PEARL is a joint product of Alterra Green World Research and the National Institute of Public Health and the Environment, and it has replaced PESTLA and PESTRAS since January 1, 2000. The model is the new official tool in Dutch pesticide registration procedures. It is also suitable for European applications, as the model supports the target quantities and scenarios set by the Forum for International Co-ordination of pesticide fate models and their Use (FOCUS). A metamodel of PEARL was incorporated into USES 3.0 (Uniform System for the Evaluation of Substances). The model is also suitable for policy evaluation. Model use is foreseen in the context of the Multi Year Crop Protection Plan (MJP-G), the project 'State of the Environment' and the Crop Protection Plan 2000^{+}.

1.2   Accompanying reports

The primary aim of this document is to provide a guidance to the use of PEARL 1.1. Both the command-line version, the Graphical User Interface, and the database structure are described. This document contains a chapter on process descriptions. However, the reader is referred to the accompanying report by Leistra *et al.* (2000) for a comprehensive overview of the theory, including references and background information. They also describe the code verification and the comparison of PEARL with previous models. The hydrological model SWAP, which is partly embedded in PEARL, is briefly described. A full description of this model can be found in Van Dam *et al.* (1997) and Kroes *et al.* (1999). A full description of the PEARL implemetation of the nine FOCUS scenarios for European pesticide registration can be found in FOCUS (2000).

It should be noted that the model has not yet been applied to field studies. The model has, however, been compared with the previous models. These models have been applied to a number of field studies. Results from these model applications were published in a series of reports and in the scientific literature (Boekhold *et al.*, 1993; Van den Bosch and Boesten, 1994; Tiktak *et al.*, 1998; Boesten, 2000; Boesten and Gottesbüren, 2000; Tiktak, 2000; Vanclooster and Boesten, 2000; Vanclooster *et al.*, 2000). In short term, the model will be further tested. This work will be carried out within the framework of the EU project APE-COP, which is an acronym for 'effective approaches for Assessing the Predicted Environmental COncentrations of Pesticides'.

1.3   Reporting of errors

The software package contains an e-mail address for communication with the developers. Users of PEARL are encouraged to report difficulties and errors they experience as well as suggestions for improvement. The e-mail address for PEARL is:

lbg-pearl@rivm.nl

This central PEARL e-mail adress is configured for archiving and automatic forwarding to the PEARL developers, so do not use one of the e-mail addresses of the authors.

1.4   Structure of report

Chapter 2 gives an overview of the theory and the mathematical formulations included in the model. This chapter is subdivided into sections on hydrology, heat flow and pesticide behavior in soil and on the canopy. Chapter 3 gives details on model parameterization. Chapter 4 describes the so-called command-line version of PEARL. The core of this chapter consists of a comprehensive description of the model-inputs. Chapter 5 describes the Graphical User Interface. After a description of the database structure and the data model, the individual screens are described. It will be shown that there is a close relationship between the screens in the GUI and the database structure. Chapter 6 gives some examples, including the Dutch standard scenario.

2   Model description

This chapter gives a brief overview of PEARL 1.1. PEARL 1.1 is linked with the SWAP model (version 2.0.7c). A comprehensive description of SWAP is given by Van Dam *et al.* (1997), a comprehensive description of the processes in PEARL is given by Leistra *et al.* (2000).

2.1   Overview

PEARL (Pesticide Emission Assessment at Regional and Local scales) is a one-dimensional, dynamic, multi-layer model that describes the fate of a pesticide and relevant transformation products in the soil-plant system. The model is linked with the Soil Water Atmosphere Plant (SWAP) model (figure 1). Pesticides can enter the system by direct application or by atmospheric deposition. The application methods described in PEARL are spraying of pesticide on the soil surface, spraying on the crop canopy, incorporation of pesticide into the topsoil (e.g. by rototillage), and injection of pesticide into the topsoil. PEARL and SWAP describe the following processes: Transient state soil water flow, potential evapotranspiration, interception of water, water uptake by plant roots, evaporation of water from the soil surface, lateral dis-
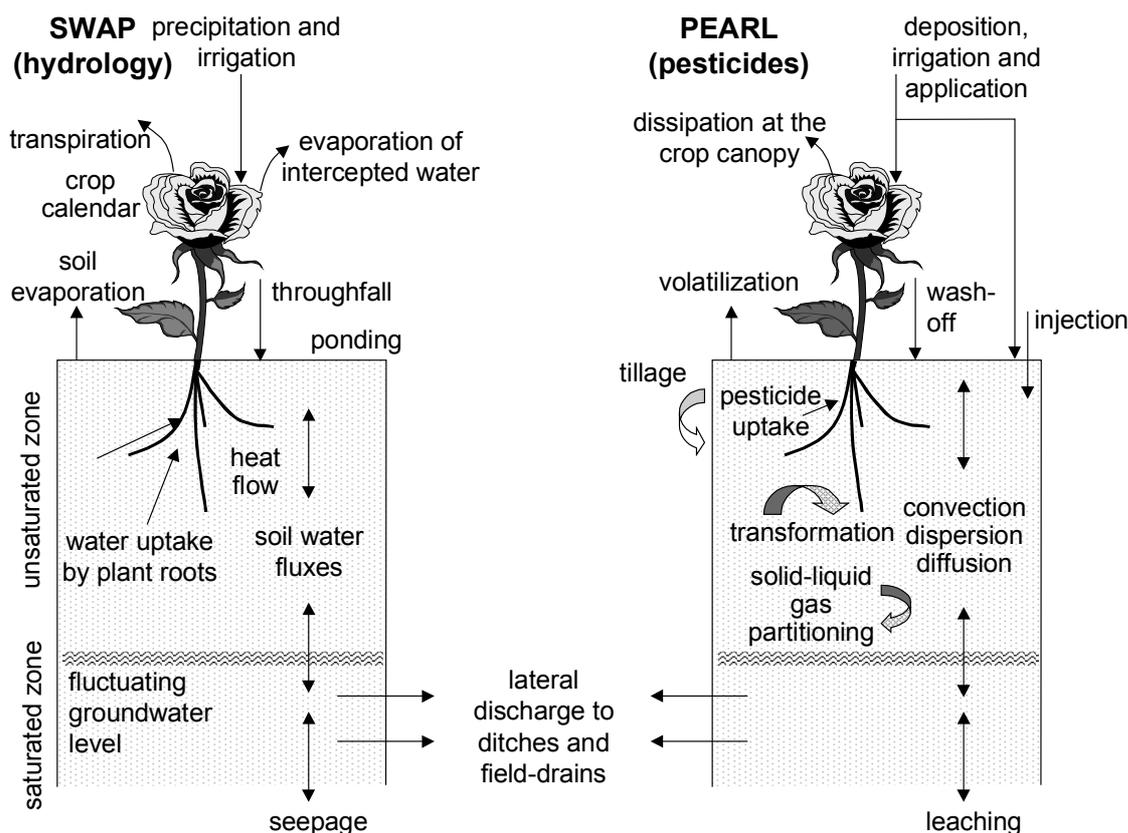
Figure 1 Overview of processes included in the PEARL model.

charge, heat flow, pesticide application, dissipation of pesticide from the crop canopy, convective and dispersive transport of pesticide in the liquid phase, diffusion of pesticide through

the gas and liquid phases, equilibrium sorption and non-equilibrium sorption, first-order transformation kinetics, uptake of pesticide by plant roots, and volatilization of pesticide at the soil surface.

The core of the model is driven by a Graphical User Interface (the PEARL user interface), which is available for Windows 95/98/NT. Figure 2 shows the linkage between the individual components of PEARL. The actual linkage between the individual components is established through text and binary files (i.e. the components are loosely coupled). The basic data are stored in a relational database. The Graphical User Interface generates the input files for PEARL. SWAP input files are created by PEARL, so it is always guaranteed that both models use the same data. This is particularly important if the model is used independently from the GUI, which is the case when performing Monte Carlo simulations or inverse modeling exercises. Relevant outputs of SWAP are transferred to PEARL through a binary datafile. Summary model-outputs of PEARL are transferred to the database, where they can be retrieved and viewed by the user. Comprehensive model-outputs (e.g. vertical profiles and daily values) can be viewed with the graphical program *XY*, which is also driven by the PEARL user interface.
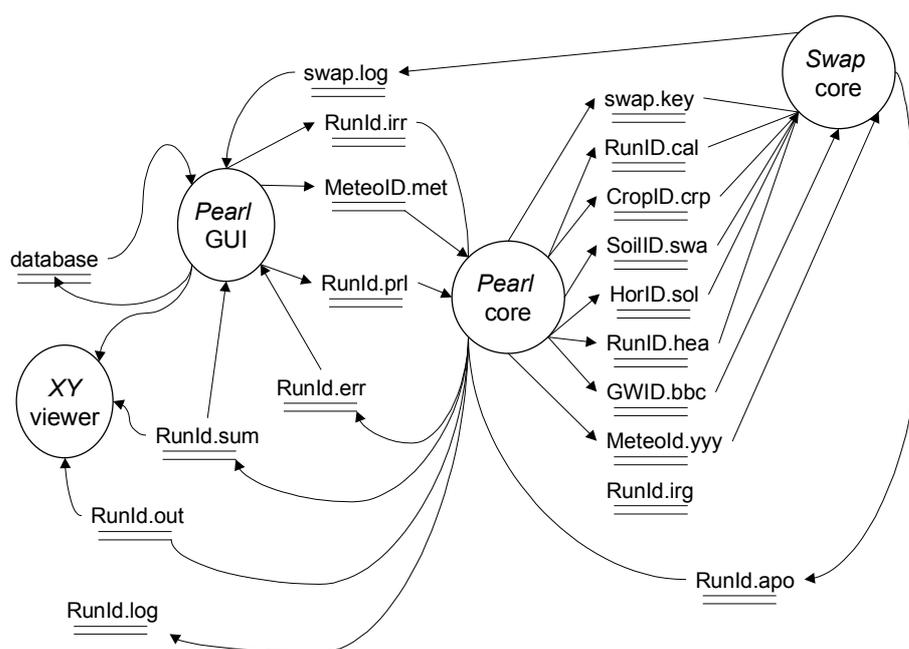
Figure 2 Dataflow diagram (DFD) for the PEARL model. Text files are double underlined.

2.2   Vertical discretization

In PEARL, soil properties are specified as a function of soil horizons. A soil horizon is assumed to have uniform chemical and physical properties. The current system allows for the definition of up to 10 soil horizons. Soil horizons are divided into numerical soil layers. Soil

layers are represented by nodal points, which are situated in the center of these layers (See Figure 3, which gives an example for 9 soil layers and 3 soil horizons). The maximum number of nodal points is currently set at 500. Nodal points are characterized by a nodal height, z (m), which is negative downwards. The distance between two nodal points, Δz (m) is calculated from:

$$\Delta z_i = z_{i+1} - z_i \tag{1}$$

The maximum distance between two nodal points is given by:

$$\Delta z < 2 L_{dis,L} \tag{2}$$

where $L_{dis,L}$ (m) is the dispersion length (see section 2.5).
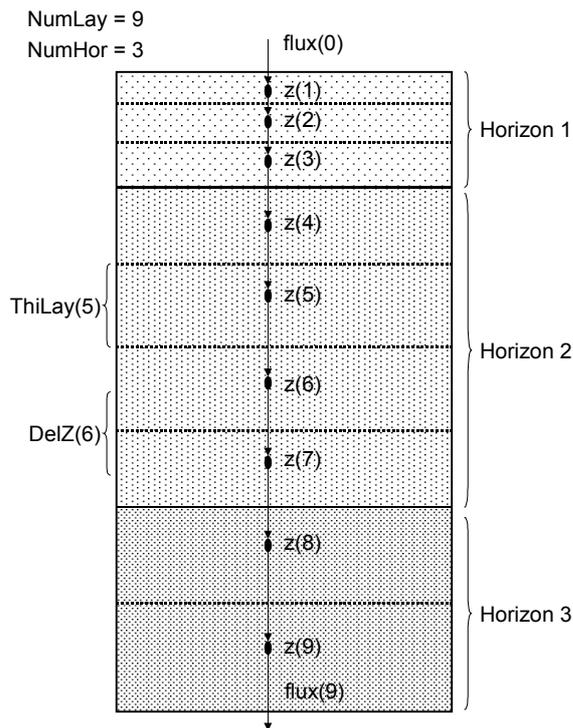
Figure 3 Vertical discretization of the soil in the PEARL model.

2.3   Hydrology

2.3.1   Soil water flow

The SWAP model (Van Dam *et al.*, 1997) uses a finite-difference method to solve the Richards equation:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] - R_{u,L} - R_{d,L} \tag{3}$$

where $C(h)$ (m^{-1}) is differential water capacity, t (d) is time, z (m) is vertical position, h (m) is soil water pressure head, $K(h)$ ($m\ d^{-1}$) is unsaturated hydraulic conductivity, $R_{u,L}$ ($m^3\ m^{-3}\ d^{-1}$) is volumic volume rate of root water uptake, and $R_{d,L}$ ($m^3\ m^{-3}\ d^{-1}$) is volumic volume rate of lateral discharge by drainage. SWAP can handle tabular data and analytical functions to de-

scribe the soil hydraulic properties. In the PEARL context, only the analytical equations proposed by Van Genuchten (1980) are supported:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha \mid h \mid)^n]^m} \qquad (4)$$

and

$$K(h) = K_s S_e^{\lambda} \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \qquad (5)$$

where θ_s (m^3 m^{-3}) is the saturated volume fraction of water, θ_r (m^3 m^{-3}) is the residual volume fraction of water, α (m^{-1}) reciprocal of the air entry value, K_s (m d^{-1}) saturated hydraulic conductivity, n (-) and λ (-) are parameters, $m = 1-1/n$, and S_e (-) is the relative saturation, which is given by:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad (6)$$

2.3.2 Potential evapotranspiration

The potential evapotranspiration, ET_p (m d^{-1}) is the key variable affecting the uptake of water by plant roots and soil evaporation. SWAP uses a slightly modified version of the Penman-Monteith equation (Monteith, 1965; Van Dam *et al.*, 1997) to calculate the potential evapotranspiration. Recent comparative studies have shown a good performance of the Penman-Monteith approach under varying climatic conditions (Jensen *et al.*, 1990). Potential and even actual evapotranspiration calculations are possible with the Penman-Monteith equation, through the introduction of canopy and air resistance's to water vapor diffusion. However, canopy and air resistance's may not be available. For this reason, SWAP follows a classical two step approach, i.e. (i) the calculation of the potential evapotranspiration, using the minimum value of the canopy resistance and the actual air resistance, and (ii) the calculation of the actual evapotranspiration using a reduction function (section 2.3.4). Application of the Penman-Monteith equation requires values of the air temperature, solar radiation, wind speed and air humidity. Feddes and Lenselink (1994) proposed a methodology to use *daily* values of these parameters. This approach is used in SWAP. See Van Dam *et al.* (1997) for details. SWAP calculates three quantities with the Penman-Monteith equation:

− ET_{w0} (m d^{-1})   potential evapotranspiration of a *wet* canopy, completely covering the soil
− ET_{p0} (m d^{-1})   potential evapotranspiration of a *dry* canopy, completely covering the soil
− E_{p0} (m d^{-1})   potential evaporation of a *wet,* bare soil.

As wind speed and air humidity are not always available, PEARL can alternatively calculate the reference evapotranspiration according to Makkink (1957), which requires daily values of temperature and solar radiation only. This equation, however, has some limitations: (i) it is developed for Dutch climatological conditions, and (ii) due to the lack of a ventilation term its performance in winter conditions is relatively poor. In this case, the potential evapotranspiration rate of a *dry* canopy, ET_{p0} (m d^{-1}) is calculated by:

$$ET_{p0} = f_c ET_r \qquad (7)$$

where f_c (-) is an empirical crop factor, which depends on the crop type, and ET_r (m d^{-1}) is the reference evapotranspiration. Notice that this approach does not allow differentiation between a dry crop, a wet crop and wet soil. SWAP therefore assumes that these quantities are equal.

2.3.3 Potential transpiration and potential evaporation

The potential evapotranspiration is partitioned into the potential transpiration and the potential soil evaporation (Belmans, 1983). The potential evaporation rate from a partly covered soil, E_p (m d^{-1}) is given by

$$E_p = e^{-\kappa LAI} E_{p0} \tag{8}$$

where LAI (m^2 m^{-2}) is the Leaf Area Index, κ (-) is the extinction coefficient for global solar radiation, and E_{p0} (m d^{-1}) is the potential evaporation rate of a *wet* bare soil. As mentioned above, E_{p0} is equal to ET_{p0} if the Makkink equation has been used.

SWAP assumes that the evaporation rate of the water intercepted by the canopy is equal to ET_{w0}, independent of the soil cover fraction. The ratio of the daily amount of intercepted precipitation (see eqn. 14), P_i and ET_{w0} indicates the fraction of the day that the canopy is wet, f_w (-):

$$f_w = \frac{P_i}{ET_{w0}} \tag{9}$$

SWAP calculates a daily average of the potential transpiration rate, taking into account the fraction of the day that the canopy is wet (cf. Bouten, 1992):

$$T_p = (1 - f_w)ET_{p0} - E_p \qquad \text{with} \quad T_p \geq 0 \tag{10}$$

where T_p (m d^{-1}) is the potential transpiration rate in the case of a partly soil cover.

2.3.4 Uptake of water by plant roots

The maximum possible root water extraction rate, integrated over the rooting depth, is equal to the potential transpiration rate, T_p (m d^{-1}). The potential root water extraction rate at a given depth, $R_{u,L,p}(z)$ (m^3 m^{-3} d^{-1}), is calculated from the volumic root length, $L_{root}(z)$ (m m^{-3}) at that depth as a fraction of the integrated volumic root length (Tiktak and Bouten, 1992):

$$R_{u,L,p}(z) = \frac{L_{root}(z)}{\int_{z_{root}}^{0} L_{root}(z)\mathrm{d}z} T_p \tag{11}$$

Notice that SWAP does not account for preferential uptake from layers with high relative water saturation (Herkelrath *et al.*, 1977; Tiktak and Bouten, 1992). The actual root water extraction rate, $R_{u,L}$, is calculated using a reduction function (Figure 4, Feddes *et al.*, 1978):

$$R_{u,L}(z) = \alpha_w R_{u,L,p}(z) \tag{12}$$
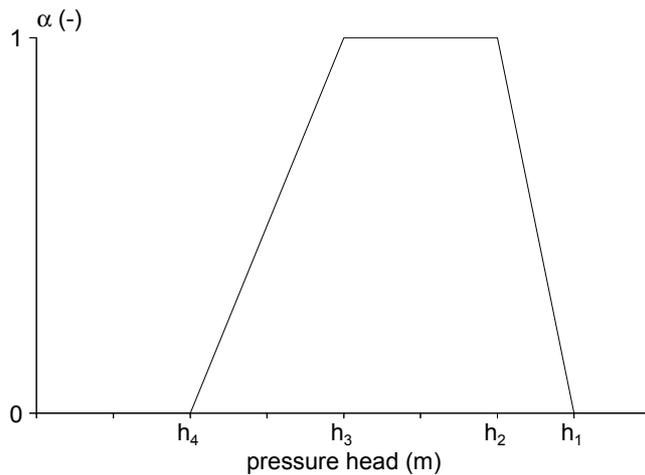
Figure 4 Reduction coefficient for root water uptake, α, as a function of soil water pressure head.

2.3.5   Evaporation of water from the soil surface

To calculate the actual soil evaporation rate, the potential soil evaporation rate is first limited to the maximum flux calculated from the Darcy equation for the top nodal point, E_{max}. The soil evaporation flux is additionally reduced according to the method proposed by Boesten and Stroosnijder (1986), who calculated the maximum actual soil evaporation, E_a (m) during a drying cycle:

$$\sum E_a = \sum E_p \qquad \text{if} \quad \sum E_p \leq \beta^2$$
$$\sum E_a = \beta \sqrt{\sum E_p} \qquad \text{if} \quad \sum E_p > \beta^2 \tag{13}$$

where β ($m^{1/2}$) is an empirical parameter.

2.3.6   Interception of rainfall

Interception of rainfall by the crop canopy is calculated from the empirical equation (Braden, 1985):

$$P_i = a\,LAI\left[1 - \frac{1}{1 + (SC\,P)/(aLAI)}\right] \tag{14}$$

where P_i ($m^3\ m^{-2}\ d^{-1}$) is intercepted precipitation, P ($m^3\ m^{-2}\ d^{-1}$) is precipitation, SC (-) is the fraction of the soil covered by the crop, and a is an empirical parameter. In SWAP, the fraction of the soil covered by the crop is approximated by $LAI/3$ (Van Dam *et al.*, 1997).

2.3.7   Bottom boundary conditions

SWAP makes a distinction between the local drainage flux to ditches and drains and the seepage flux due to regional groundwater flow. The seepage flux due to regional groundwater flow is the lower boundary flux (q_b), the local drainage flux is treated as a sink term ($R_{d,L}$). The following lower boundary conditions of SWAP can be used via the PEARL model:

1. Groundwater level, Φ_{gwl} (m), specified as a function of time.
2. Regional bottom flux q_b ($m^3\ m^{-2}\ d^{-1}$) specified as a function of time (Neumann condition).
3. Regional bottom flux is calculated using the hydraulic head difference between the phreatic groundwater and the groundwater in the semi-confined aquifer (pseudo two-dimensional Cauchy condition; Figure 5):

$$q_b = \frac{\Phi_{aqf} - \Phi_{avg}}{\gamma_{aqt}} \tag{15}$$

where Φ_{aqf} (m) is hydraulic head of the semi-confined aquifer, Φ_{avg} (m) is average phreatic head, and γ_{aqt} (d) is vertical resistance of the aquitard. The average phreatic head is determined by the shape of the groundwater level in a field. The average phreatic head is calculated using the drainage base, Φ_d (m) and a shape-factor, β_{gwl}:

$$\Phi_{avg} = \Phi_d + \beta_{gwl}(\Phi_{gwl} - \Phi_d) \tag{16}$$

Possible values for the shape factor are 0.64 (sinusoidal), 066 (parabolic), 0.79 (elliptic) and 1.00 (no drains present). Seasonal variation of the bottom flux can be induced through a sine-wave of the hydraulic head in the semi-confined aquifer.

4. q_b is calculated from an exponential flux-groundwater level relationship (Cauchy condition):

$$q_b = a_g e^{b_g |\Phi_{avg}|} \tag{17}$$

with a_g (m d^{-1}) and b_g (m^{-1}) as empirical coefficients.

5. Pressure head of the bottom soil layer specified as a function of time (Dirichlet condition).

6. Zero flux at bottom of soil profile: $q_b = 0$ (special case of Neumann condition).

7. Free drainage of soil profile, in which case unit gradient is assumed at the lower boundary: $q_b = -K_{NumLay}$ (special case of Neumann condition).

8. Lysimeter boundary condition: Outflow only occurs if the pressure head of the bottom soil layer is above zero (special case of Neumann condition).

2.3.8 Lateral discharge of soil water

Lateral discharge rates can be calculated for a maximum number of five local drainage systems (e.g. drainage tiles and field-ditches). PEARL uses the following equation to calculate the flux to drainage system k:

$$q_{d,k} = \frac{\Phi_{avg} - \Phi_{d,k}}{\gamma_{d,k}} \tag{18}$$

where $q_{d,k}$ (m^3 m^{-2} d^{-1}) is the flux of water to local drainage system k, $\Phi_{d,k}$ (m) is hydraulic head of drainage system k, and $\gamma_{d,k}$ (d) is drainage resistance. In order to distribute the discharge rates over the soil layers, first a discharge layer is determined by considering a travel-time distribution. The most important assumption in this computational procedure is that lateral discharge occurs to parallel, equidistant water courses (distance L_k (m)). See chapter 10.1 in Van Dam *et al.* (1997) for details. Within this discharge layer, the lateral drainage from soil layer i to local drainage system k, $R_{d,L,k,i}$, is calculated with the equation:

$$R_{d,L,k,i} = \frac{q_{d,k}}{\Delta z_i} \frac{K_{s,i} \Delta z_i}{\sum (K_{s,i} \Delta z_i)} \tag{19}$$

The total lateral drainage is calculated by summing the lateral drainage for all local drainage systems.
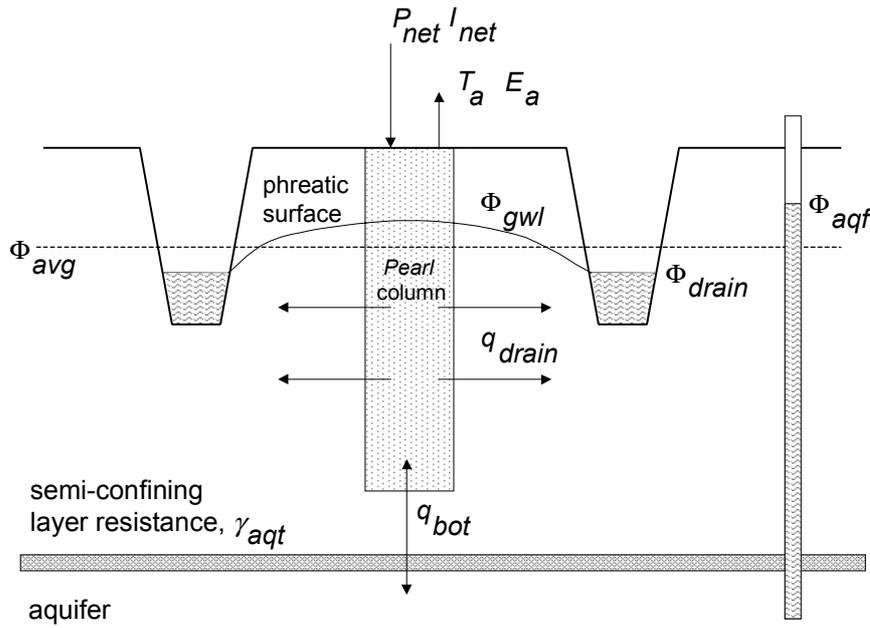
Figure 5 Pseudo two-dimensional Cauchy lower boundary condition, in case of drainage to ditches (Van Dam et al., 1997).

2.4   Heat flow

The model SWAP (Van Dam *et al.*, 1997) calculates conductive transport of heat in soil:

$$\frac{\partial C_h T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda \frac{\partial T}{\partial z}\right] \tag{20}$$

where C_h (J m^{-3} K^{-1}) is the volumic heat capacity, T (K) is temperature, and λ (J m^{-1} d^{-1} K^{-1}) is the effective heat conductivity. The volumic heat capacity is calculated as the weighted mean of the heat capacities of the individual soil components (De Vries, 1963):

$$C_h = \theta_{sand} C_{sand} + \theta_{clay} C_{clay} + \theta_{om} C_{om} + \theta C_w + \varepsilon C_a \tag{21}$$

where θ_{sand}, θ_{clay}, θ_{om} and θ (m^3 m^{-3}) are the volume fractions of sand, clay, organic matter and water, ε (m^3 m^{-3}) is the air-filled porosity, and C_{sand}, C_{clay}, C_{om}, C_w and C_a (J m^{-3} K^{-1}) are the volumic heat capacities of the individual components. Table 1 gives an overview of the volumic heat capacity for the individual soil components. The volume fractions of sand, clay and organic matter are calculated from the mass percentages of sand, clay and organic matter, which are input to the model. The thermal conductivity is calculated according to the procedure described by Ashby *et al.* (1996), which accounts for both soil composition and soil geometry.

Table 1 Volumic heat capacity and thermal conductivity of the individual soil components (after Van Dam et al., 1997).

Component	Volumic heat capacity (J cm^{-3} K^{-1})	Thermal conductivity (J cm^{-1} K^{-1} d^{-1})
Sand	2.128	7603
Clay	2.385	2523
Organic matter	2.496	216
Water	4.180	492
Air (293 K)	1.212	22

The upper boundary condition for the soil heat-flow model is the daily average air temperature, T_{air} (K); the lower boundary condition is a zero-flux boundary condition. The heat flow equation is solved using a numerical method.

2.5   Pesticide fate

2.5.1   Pesticide application

Various factors affect the fraction of the dosage that is introduced into the soil system. During spraying, a fraction of the nominal dosage may be intercepted by the crop canopy. A part of the nominal dosage may drift from the field to adjacent ditches and fields. Another part may dissipate at the soil surface by processes like film volatilization and photochemical transformation. In PEARL, the user can choose from two general methods to describe the dosage introduced into the system:

1. Pesticide losses above the soil system are estimated beforehand, and the net load is introduced directly into the soil system.
2. The processes at the soil surface and plant surface are simulated in a simplified way.

2.5.2   Canopy processes

When a pesticide is sprayed on a field grown with plants, the nominal dosage has to be distributed over the plant canopy and the soil surface:

$$A_{d,p} = SC \, A_{d,f} \tag{22}$$

and

$$A_{d,s} = (1 - SC) A_{d,f} \tag{23}$$

where $A_{d,f}$ (kg m^{-2}) is the areic mass of pesticide applied to the field, $A_{d,p}$ (kg m^{-2}) is the areic mass of pesticide applied to the crop canopy, $A_{d,s}$ (kg m^{-2}) is the areic mass of pesticide deposited on the soil, and SC (-) is the fraction of the soil surface covered by the crop. All areic masses are expressed per m^2 field surface. Methods are being developed for more targeted spraying on plants or on the soil surface, so the soil cover fraction may not be appropriate. In this particular case, the fraction of the dosage that is deposited onto the crop canopy can be introduced by the user.

The following processes are described at the plant surface: (i) volatilization into the air, (ii) penetration into the plant, (iii) transformation at the plant surface, and (iv) wash-off via rainfall. The first three processes are described by first-order kinetics:

$$R_{dsp} = k_{v,p} A_p + k_{p,p} A_p + k_{t,p} A_p \qquad (24)$$

where R_{dsp} (kg m^{-2} d^{-1}) is the areic mass rate of dissipation of pesticide at the plant surface, $k_{v,p}$ (d^{-1}) is rate coefficient for volatilization, $k_{p,p}$ (d^{-1}) is rate coefficient for penetration, $k_{t,p}$ (d^{-1}) is rate coefficient for transformation at the plant surface, and A_p (kg m^{-2}) is areic mass of pesticide at the crop canopy. Alternatively, the user can introduce an overall dissipation rate coefficient, k_{dsp} (d^{-1}) for the three processes. The areic mass rate of pesticide wash-off is taken proportional to the canopy drip flux:

$$R_{w,p} = w_p (SC\, P - P_i) A_p \qquad (25)$$

where $R_{w,p}$ (kg m^{-2} d^{-1}) is the areic mass rate of pesticide wash-off from the crop canopy, w_p (m^{-1}) is an empirical wash-off factor, P (m d^{-1}) is precipitation, and P_i (m d^{-1}) is intercepted water. The following mass balance applies for the crop canopy:

$$\frac{\partial A_p}{\partial t} = -R_{w,p} - R_{dsp} \qquad (26)$$

2.5.3 Mass balance equations

Pesticide can be found in the equilibrium domain and in the non-equilibrium domain of the soil system (Figure 6), so two mass balances apply:

$$\frac{\partial c^*_{eq}}{\partial t} = -R_s - \frac{\partial J_{p,L}}{\partial z} - \frac{\partial J_{p,g}}{\partial z} - R_t + R_f - R_u - R_d \qquad (27)$$

and

$$\frac{\partial c^*_{ne}}{\partial t} = R_s \qquad (28)$$

Here, c^*_{eq} (kg m^{-3}) is the pesticide concentration in the equilibrium domain of the soil system, c^*_{ne} (kg m^{-3}) is the pesticide concentration in the non-equilibrium domain of the soil system, R_s (kg m^{-3} d^{-1}) is the volumic mass rate of pesticide sorption, $J_{p,L}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the liquid phase, $J_{p,g}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the gas phase, R_t (kg m^{-3} d^{-1}) is the transformation rate, R_f (kg m^{-3} d^{-1}) is the formation rate, R_u (kg m^{-3} d^{-1}) is the rate of pesticide uptake by plant roots, and R_d (kg m^{-3} d^{-1}) is the lateral discharge rate of pesticides.

2.5.4 Transport in the liquid phase

Transport of the pesticide in the liquid phase of the soil is described by an equation including convection, dispersion and diffusion:

$$J_{p,L} = q c_L - D_{dis,L} \frac{\partial c_L}{\partial z} - D_{dif,L} \frac{\partial c_L}{\partial z} \qquad (29)$$

where $J_{p,L}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the liquid phase, q (m^3 m^{-2} d^{-1}) is the soil water flux, $D_{dis,L}$ (m^2 d^{-1}) is coefficient of pesticide dispersion in the liquid phase, z (m) is vertical position, and $D_{dif,L}$ (m^2 d^{-1}) is the coefficient of pesticide diffusion in the liquid phase. The dispersion coefficient is taken to be proportional to the soil water flux:

$$D_{dis,L} = L_{dis,L} |q| \qquad (30)$$

with $L_{dis,L}$ (m) as the dispersion length. The diffusion of pesticide in the liquid phase is described by Fick's law. The coefficient for diffusion of pesticide in the liquid phase is calculated by:

$$D_{dif,L} = \zeta_L D_w \qquad (31)$$

where ζ_L (-) is the relative diffusion coefficient in the liquid phase, and D_w (m^2 d^{-1}) is the coefficient of pesticide diffusion in pure water.

Figure 6 Diagram of equilibrium and non-equilibrium domains of the soil system.

The relative diffusion coefficient is a function of the volume fraction of liquid. PEARL offers three methods do describe this function. By default, the function proposed by Millington and Quirk (1960) is used:

$$\zeta_L = \theta^{a_{M,L}} / \theta_s^{b_{M,L}} \qquad (32)$$

where θ (m^3 m^{-3}) is the volume fraction of liquid, θ_s (m^3 m^{-3}) is the volume fraction of liquid at saturation, and $a_{M,L}$ (-) and $b_{M,L}$ (-) are empirical parameters. The second type of equation is the one used by Currie (1960):

$$\zeta_L = a_{C,L} \theta^{b_{C,L}} \qquad (33)$$

where $a_{C,L}$ (-) and $b_{C,L}$ (-) are empirical coefficients. The third equation is suggested by Troeh *et al.* (1982). In this approach, diffusion in the liquid phase is taken to be zero in a range of (low) volume fractions of water. In this range, the water-filled pores are assumed to be discontinuous:

$$\zeta_L = \begin{cases} \left(\dfrac{\theta - a_{T,L}}{1 - a_{T,L}} \right)^{b_{T,L}} & \text{if} \quad \theta > a_{T,L} \\ 0 & \text{if} \quad \theta \leq a_{T,L} \end{cases} \qquad (34)$$

where $a_{T,L}$ (m^3 m^{-3}) is the volume fraction of water at the air-entry point, and $b_{T,L}$ (-) is an empirical parameter.

The value of the diffusion coefficient in water is temperature dependent, mainly because the viscosity of water depends on the temperature. In PEARL, the theoretically derived Stokes-Einstein equation (Tucker and Nelken, 1982) is approximated by:

$$D_w = 1 + 0.02571(T - T_r)D_{w,r}$$ (35)

where T (K) is temperature, T_r (K) is reference temperature, and $D_{w,r}$ (m^2 d^{-1}) is the diffusion coefficient in water at reference temperature. See Leistra *et al.* (2000) for details.

2.5.5   Transport in the gas phase

Transport of pesticide in the gas phase is described by Fick's law:

$$J_{p,g} = -D_{dif,g} \frac{\partial c_g}{\partial z}$$ (36)

where $J_{p,g}$ (kg m^{-2} d^{-1}) is mass flux of pesticide in the gas phase, and $D_{dif,g}$ (m^2 d^{-1}) is coefficient of pesticide diffusion in the gas phase. The coefficient for diffusion of pesticide in the gas phase is calculated by:

$$D_{dif,g} = \zeta_g D_a$$ (37)

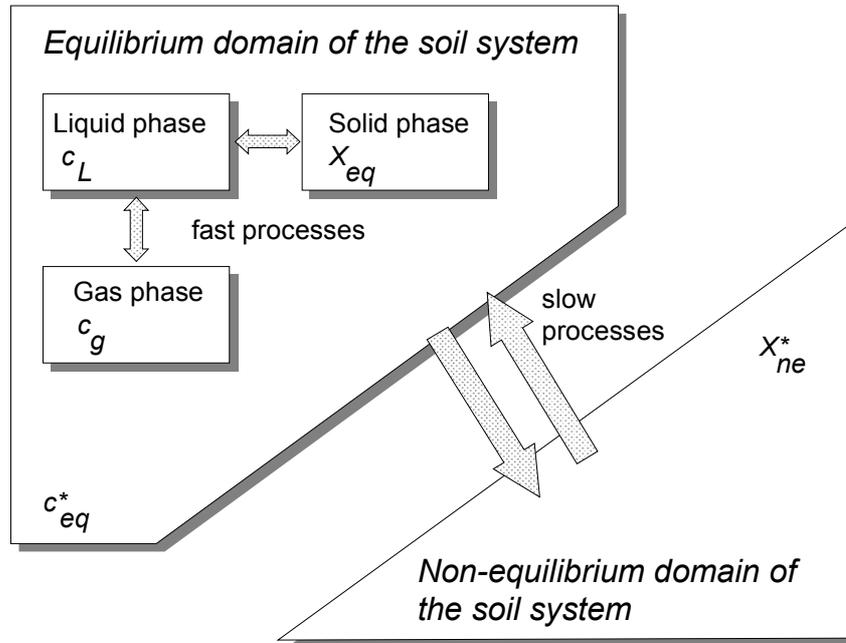where ζ_g (-) is the relative diffusion coefficient in the gas phase, and D_a (m^2 d^{-1}) is the coefficient of pesticide diffusion in air. The relation between D_a and temperature is described by:

$$D_a = \left(\frac{T}{T_r}\right)^{1.75} D_{a,r}$$ (38)

where $D_{a,r}$ (m^2 d^{-1}) is the diffusion coefficient in air at reference temperature. The relative diffusion coefficient is a function of the volume fraction of the gas phase. It is calculated analogous to the relative diffusion coefficient in the liquid phase (eqn. 32-34).

2.5.6   Initial and boundary conditions

The initial condition for the model is defined by profiles of the concentration of pesticide in the equilibrium domain of the soil system, $c*_{eq}$ (kg m^{-3}), and in the non-equilibrium domain of the soil system, $c*_{ne}$ (kg m^{-3}). It is further assumed that at the start of the simulation the areic mass of pesticide at the plant surface, A_p, is zero.

The boundary condition at the soil surface is a flux boundary condition. The user can enter deposition fluxes of pesticide as a function of time. Pesticides entering the system by deposition are subject to canopy processes. The user can also specify the concentration of pesticide in irrigation water, in which case the user has to choose between surface irrigation (i.e. application of irrigation water directly to the soil system) and sprinkler irrigation (application to the crop canopy).

At the lower boundary of the soil system, dispersive and diffusive fluxes of pesticide are assumed to be zero. In the case of infiltration of water from a deep aquifer, the pesticide concentration is set to zero.

Diffusion of pesticide vapor in the gas phase of the soil is included in the model, which implies that a description of pesticide volatilization at the soil surface is required. In the current model version, the diffusion of vapor through the soil and a laminar air-boundary layer are the limiting factors for volatilization (cf. Jury *et al.*, 1990):

$$J_{p,v} = \frac{c_g}{r_{s,v} + r_{a,v}}$$

(39)

where $J_{p,v}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide volatilization, c_g (kg m^{-3}) is concentration of pesticide in the gas phase of the top layer, $r_{s,v}$ (d m^{-1}) is resistance of the soil boundary layer, and $r_{a,v}$ (d m^{-1}) is resistance of the air boundary layer. The resistance's of the boundary layers are calculated by:

$$r_{s,v} = \frac{d_s}{D_{dif,g}} \qquad \text{and} \qquad r_{a,v} = \frac{d_a}{D_a}$$

(40)

where d_s (m) is thickness of soil boundary layer, $D_{dif,g}$ (m^2 d^{-1}) is the coefficient for diffusion of pesticide in the gas phase of the soil system, d_a (m) is the thickness of the laminar air-boundary layer, and D_a (m^2 d^{-1}) is coefficient for diffusion of pesticide in air. It should be noted that the current description of pesticide volatilization is subject to considerable uncertainty, particularly for surface-applied pesticides where initial volatilization is hardly limited by the soil boundary layer. For this reason, at present research aimed at improving the sub-model for pesticide volatilization is being carried out. See Leistra *et al.* (2000) for further considerations.

2.5.7 Partitioning over the three soil phases

The sorption of pesticide on the soil solid phase is described with a Freundlich equation. Both equilibrium and non-equilibrium (kinetic) sorption are considered. Equilibrium sorption is described by the equation:

$$X_{eq} = K_{F,eq} c_{L,r} \left(\frac{c_L}{c_{L,r}} \right)^N$$

(41)

in which X_{eq} (kg kg^{-1}) is pesticide content in the equilibrium sorption phase, $K_{F,eq}$ (m^3 kg^{-1}) is Freundlich coefficient for the equilibrium-sorption phase, c_L (kg m^{-3}) is concentration in the liquid phase, $c_{L,r}$ (kg m^{-3}) is reference concentration in the liquid phase and N is the Freundlich exponent. Notice that a particular type of Freundlich equation is used in the model, by introducing the reference concentration. The advantage of this type of equation is that the unit of the Freundlich coefficient becomes independent of the exponent.

The Freundlich coefficient may depend on various soil properties, such as organic matter content, oxide content and pH. For most pesticides, the following equation is appropriate:

$$K_{F,eq} = m_{om} K_{om,eq}$$

(42)

where m_{om} (kg kg^{-1}) is mass content of organic matter in soil and $K_{om,eq}$ (m^3 kg^{-1}) is the coefficient of equilibrium sorption on organic matter.

PEARL contains a description of the sorption of weak acids, which is *p*H dependent:

$$K_{F,eq} = m_{om} \frac{K_{om.eq,ac} + K_{om,eq,ba} \frac{M_{ba}}{M_{ac}} 10^{pH-pKa-\Delta pH}}{1 + \frac{M_{ba}}{M_{ac}} 10^{pH-pKa-\Delta pH}}$$ (43)

where $K_{om,eq,ac}$ (m^3 kg^{-1}) is the coefficient for sorption on organic matter under acidic conditions, $K_{om,eq,ba}$ (m^3 kg^{-1}) is the coefficient for sorption on organic matter under basic conditions, M (kg mol^{-1}) is molar mass, *p*Ka is the negative logarithm of the dissociation constant, and ΔpH is a *p*H correction factor. See Leistra et al. (2000) for the derivation of this equation.

The sorption of some specific pesticides cannot be described with the organic matter equilibrium constant. This is particularly true for those pesticides that sorb preferentially on clay and oxides. In this case, the user should specify the Freundlich coefficient of the topsoil and a depth-effect factor:

$$K_{F,eq} = f_{d,s} K_{F,eq,r}$$ (44)

where $K_{F,eq,r}$ (m^3 kg^{-1}) is the Freundlich coefficient in the topsoil, and $f_{d,s}$ (-) is an empirical depth-effect factor.

Pesticide sorption to the non-equilibrium phase is described by a first-order rate equation:

$$R_s = \rho_b k_d \left[f_{K,ne} K_{F,eq} c_{L,r} \left(\frac{c_L}{c_{L,r}} \right)^N - X_{ne} \right]$$ (45)

where R_s (kg m^{-3} d^{-1}) is rate of sorption in the non-equilibrium domain of the soil system, ρ_b (kg m^{-3}) is the dry bulk density of the soil, X_{ne} (kg kg^{-1}) is pesticide content at non-equilibrium sorption sites, k_d (d^{-1}) is desorption rate coefficient, and $f_{K,ne}$ (-) is factor describing the ratio $K_{F,ne}/K_{F,eq}$, with $K_{F,ne}$ (m^3 kg^{-1}) as the Freundlich coefficient for the non-equilibrium sorption phase. See Leistra *et al.* (2000) for a discussion of the theoretical background of this equation.

The partitioning of the pesticide between the gas phase and the liquid phase is described by Henry's law:

$$c_g = K_H c_L$$ (46)

in which c_g (kg m^{-3}) is the concentration of pesticide in the gas phase and K_H (m^3 m^{-3}) is the Henry coefficient, which is calculated by:

$$K_H = \frac{p_{v,s} M}{S_w RT}$$ (47)

where $p_{v,s}$ (Pa) is the saturated vapor pressure, M (kg mol^{-1}) is molar mass, S_w (kg m^{-3}) is solubility in water, R (J mol^{-1} K^{-1}) is the molar gas constant, and T (K) is the temperature. PEARL describes the temperature dependence of both $p_{v,s}$, which requires the molar enthalpy of vaporization, ΔH_v (J mol^{-1}), and S$_w$, which requires the molar enthalpy of dissolution, ΔH_d (J mol^{-1}):

$$p_{v,s} = p_{v,s,r} \exp\left[\frac{-\Delta H_v}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \tag{48}$$

and

$$S_w = S_{w,r} \exp\left[\frac{-\Delta H_d}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \tag{49}$$

Here, $p_{v,s,r}$ (Pa) is the saturated vapor pressure at reference temperature T_r (K) and $S_{w,r}$ (kg m^{-3}) is the pesticide solubility in water at reference temperature.

The total concentration of pesticide in the equilibrium domain of the soil system (kg m^{-3}) is given by:

$$c_{eq}^* = \varepsilon c_g + \theta c_L + \rho_b X_{eq} \tag{50}$$

where ε (m^3 m^{-3}) is volume fraction of the gas phase, c_g (kg m^{-3}) is concentration of pesticide in the gas phase, θ (m^3 m^{-3}) is volume fraction of the liquid phase, c_L (kg m^{-3}) is concentration of pesticide in the liquid phase, ρ_b (kg m^{-3}) dry bulk density of the soil, and X_{eq} (kg kg^{-1}) is pesticide mass content in the equilibrium phase. The total concentration of pesticide in the non-equilibrium phase (kg m^{-3}) is given by:

$$c_{ne}^* = \rho_b X_{ne} \tag{51}$$

with X_{ne} (kg kg^{-1}) as the pesticide mass content in the non-equilibrium phase.

2.5.8 Transformation of pesticide in soil

Transformation of pesticides may lead to reaction products (*daughters*) that may show a certain degree of persistence and mobility in soils. For this reason, the formation and behavior of the most important daughters is included in PEARL. The first step in the definition of the reaction scheme is to set up the list of compounds that will be considered. The second step is the definition of the pathways of pesticide transformation. Consider the example shown in Figure 7. The reaction scheme presented in Figure 7 can be represented in matrix notation as shown in Table 2. This example shows that a compound may transform into various products and that they may be formed from more than one precursor compound.
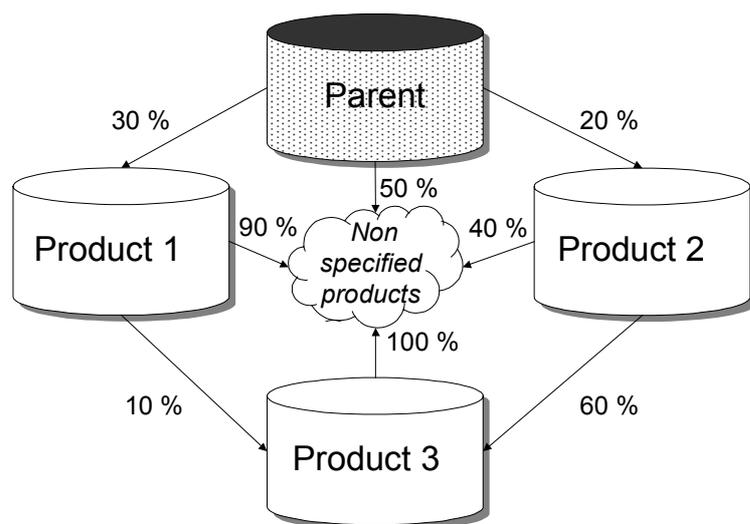
Figure 7 Example of a reaction scheme of a pesticide.

Table 2 Example of a matrix, which represents the reactions between one parent and three reaction products. A value of zero indicates no interaction.

	Parent	Product 1	Product 2	Product 3
Parent	0.0	0.3	0.2	0.0
Product 1	0.0	0.0	0.0	0.1
Product 2	0.0	0.0	0.0	0.6
Product 3	0.0	0.0	0.0	0.0

In PEARL 1.1, the rate of transformation of a precursor (*parent*) is described by a first-order rate equation:

$$R_{t,par} = k_{t,par} c^*_{eq,par}$$
(52)

in which $R_{t,par}$ (kg m^{-3} d^{-1}) is the rate of transformation of the parent pesticide, $k_{t,par}$ (d^{-1}) is the transformation rate coefficient, and $c^*_{eq,par}$ (kg m^{-3}) is the concentration of the parent pesticide in the equilibrium domain of the soil. *Notice that pesticide residing in the non-equilibrium domain is not transformed.* The rate of formation of a daughter from a parent, $R_{f,par,dau}$ (kg m^{-3} d^{-1}), is subsequently calculated by:

$$R_{f,par,dau} = \chi_{par,dau} \frac{M_{dau}}{M_{par}} R_{t,par}$$
(53)

where $\chi_{par,daugher}$ (-) is the molar fraction of parent transformed to daughter, and M (kg mol^{-1}) is the molar mass.

The rate of pesticide transformation in soil depends on the temperature, soil moisture content and the depth in soil:

$$k_t = f_t f_m f_d k_{t,r}$$
(54)

where f_t (-) is the factor for the effect of temperature, f_m (-) is the factor for the effect of soil moisture, f_d (-) is the factor for the effect of depth in soil, and $k_{t,r}$ (d^{-1}) is the rate coefficient at reference conditions, which is calculated from:

$$k_{t,r} = \frac{\ln(2)}{DT_{50,r}} \tag{55}$$

where $DT_{50,r}$ (d) is the half-life of the pesticide in the well-moistened plough layer at reference temperature. The effect of temperature on the pesticide transformation rate is described by the Arrhenius equation:

$$f_t = \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \tag{56}$$

where E_a (J mol^{-1}) is molar activation energy, R (J mol^{-1} K^{-1}) is the molar gas constant, and T (K) is temperature. The Arrhenius equation is assumed to be valid from 5 to 35 ^{o}C. Above 35 ^{o}C, the factor for the effect of temperature is kept constant. At temperatures below zero, the factor for the effect of temperature is set to zero (Jarvis, 1994). This implies that no pesticide transformation is simulated in frozen soil. The equation for the effect of soil water on transformation reads (Walker, 1974):

$$f_m = \min\left[1, \left(\frac{\theta}{\theta_{fc}}\right)^B\right] \tag{57}$$

where θ (m^3 m^{-3}) is volume fraction of soil water, B (-) is empirical factor for the effect of soil moisture, and the suffix fc refers to field capacity. The effect of depth on the rate of transformation in soil is described by a tabular relationship.

2.5.9 Pesticide uptake

The uptake of pesticide by plant roots is described by the equation:

$$R_u = R_{u,L} f_u c_L \tag{58}$$

where R_u (kg m^{-3} d^{-1}) is volumic mass rate of pesticide uptake, $R_{u,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of water uptake, and f_u (-) is an empirical transpiration stream concentration factor.

2.5.10 Lateral discharge of pesticides

The rate of water discharged by the tile-drainage system is calculated by the hydrological submodel (eqn. (19)). The lateral discharge of pesticides is taken proportional to the water fluxes discharged by the tile-drainage system:

$$R_d = R_{d,L} c_L \tag{59}$$

where R_d (kg m^{-3} d^{-1}) is volumic mass rate of pesticide discharge, and $R_{d,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of water discharge. Equation 59 implies that it is assumed that concentration gradients in the lateral direction are negligible (i.e. no diffusion/dispersion).

3   Model parameterization

In a ring-test of 9 European pesticide leaching models (Vanclooster *et al.*, 2000), subjectivity in the derivation of model inputs was the major source of differences between model results (Tiktak, 2000; Boesten, 2000). An important recommendation was to provide to model-users with strict guidelines and additional tools for deriving model inputs. We therefore included this chapter, which gives an overview of methods to derive the most important model inputs.

In the pesticide registration procedure (e.g. Linders *et al.*, 1994), several stages can be distinguished. In first-tier assessments, the model is used to get a first indication of the leaching potential of a pesticide. To minimize user subjectivity during this stage, the model is used in combination with *standardized* scenario's (FOCUS, 2000). These scenario's are supported by PEARL (chapter 5). The following steps should be followed:

1. Specification of pesticide properties, including the half-life at reference temperature ($DT_{50,r}$, see section 3.2.9), the coefficient for sorption on organic matter ($K_{om,eq}$, see section 3.2.6), the saturated vapor pressure at reference temperature ($p_{v,s,r}$, see section 3.2.8), and the solubility in water ($S_{w,r}$, see section 3.2.8).
2. Selection of crop type.
3. Selection of one or more locations.
4. Selection of application schedule (annual, biennial, triennial) and the actual application dates.

By selecting a combination of location, crop type and application schedule most model-inputs are fixed.

During the second and higher tiers of the registration procedure, field studies and lysimeter experiments may become important. During this stage, the model should preferably be used in combination with *on-site measured data*. Guidelines for model parameterization follow below.

3.1   Hydrology

3.1.1   Soil water flow

Soil water transport is described with the Richards equation (eqn. 3). The soil hydraulic properties are described with analytical functions (eqn. 4 and 5). Parameter values can be obtained by fitting experimentally derived retention data to eqn. 4 and 5, using the RETC program (Van Genuchten *et al.*, 1991). See Van Dam *et al.* (1997) for an overview of experimental procedures to obtain the soil hydraulic characteristics. Parameter values for the Van Genuchten (1980) analytical functions can be found in a number of international and

Table 3 Dataset of soil hydraulic functions (Wösten et al., 1994), based on Dutch texture classes (Table 4). The function are described with the analytical model of Mualem-Van Genuchten (1980).

TOP Soils	θ_r (m3 m^{-3})	θ_s (m3 m^{-3})	K_s (cm d^{-1})	α (cm^{-1})	λ (-)	n (-)
Sand						
B1	0.01	0.43	17.46	0.0249	-0.140	1.507
B2	0.02	0.43	9.65	0.0227	-0.983	1.548
B3	0.01	0.45	17.81	0.0152	-0.213	1.412
B4	0.01	0.42	54.80	0.0163	0.177	1.559
Loam						
B7	0.00	0.40	14.07	0.0194	-0.802	1.250
B8	0.00	0.43	2.25	0.0096	-2.733	1.284
B9	0.00	0.43	1.54	0.0065	-2.161	1.325
Clay						
B10	0.01	0.42	1.17	0.0118	-4.795	1.224
B11	0.00	0.60	5.26	0.0243	-5.395	1.111
B12	0.00	0.55	15.46	0.0532	-8.823	1.081
Silt						
B14	0.01	0.42	0.80	0.0051	0.000	1.305
Peat						
B16	0.00	0.73	13.44	0.0134	0.534	1.320
B17	0.00	0.72	4.46	0.0180	-0.350	1.140
B18	0.00	0.77	6.67	0.0197	-1.845	1.154

SUB Soils	θ_r (m3 m^{-3})	θ_s (m3 m^{-3})	K_s (cm d^{-1})	α (cm^{-1})	λ (-)	n (-)
Sand						
O1	0.01	0.36	13.21	0.0224	0.000	2.167
O2	0.02	0.38	15.56	0.0214	0.039	2.075
O3	0.01	0.34	18.30	0.0211	-0.522	1.564
O4	0.00	0.36	53.10	0.0216	-0.520	1.540
O5	0.01	0.32	43.55	0.0597	0.343	2.059
O6	0.00	0.41	5.48	0.0291	-6.864	1.152
Loam						
O8	0.00	0.47	9.08	0.0136	-0.803	1.342
O9	0.00	0.46	2.23	0.0094	-1.382	1.400
O10	0.00	0.49	2.22	0.0107	-2.123	1.280
Clay						
O11	0.00	0.42	13.79	0.0191	-1.384	1.152
O12	0.00	0.56	1.14	0.0095	-4.171	1.159
O13	0.00	0.57	3.32	0.0171	-4.645	1.110
Silt						
O14	0.00	0.38	0.36	0.0025	0.057	1.686
O15	0.01	0.41	3.70	0.0071	0.912	1.298
Peat						
O16	0.00	0.89	1.07	0.0103	-1.411	1.376
O17	0.00	0.86	2.75	0.0127	-1.832	1.274

Table 4 Silt fraction, clay fraction, median particle size and organic matter content for the units of the Staring Series (Table 3)

SUB Soils	Nomenclature	f_{silt} (%)	f_{clay} (%)	m_{om} (%)	M50 (µm)
Sand					
B1	Loam-poor fine sand	0-10		0-15	105-210
B2	Slightly loamy fine sand	10-18		0-15	105-210
B3	Loamy fine sand	18-33		0-15	105-210
B4	Very loamy fine sand	35-50		0-15	105-210
Loam					
B7	Light sandy clay		8-12	0-15	
B8	Sandy clay		12-18	0-15	
B9	Heavy sandy clay		18-25	0-15	
Clay					
B10	Light clay		25-35	0-15	
B11	Clay		35-50	0-15	
B12	Heavy clay		50-100	0-15	
Silt					
B14	Silty loam	85-100		0-15	
Peat					
B16	Sandy peat		0-8	23-100	
B17	Peaty clay		8-100	16-45	
B18	Clayey peat		8-100	25-70	

SUB soils	Nomenclature	f_{silt} (%)	f_{clay} (%)	m_{om} (%)	M50 (µm)
Sand					
O1	Loam-poor fine sand	0-10		0-3	105-210
O2	Slightly loamy fine sand	10-18		0-3	105-210
O3	Loamy fine sand	18-33		0-3	105-210
O4	Very loamy fine sand	35-50		0-3	105-210
O5	Coarse sand			0-3	210-2000
O6	Glacial till	0-50		0-3	50-2000
Loam					
O8	Light sandy clay		8-12	0-3	
O9	Sandy clay		12-18	0-3	
O10	Heavy sandy clay		18-25	0-3	
Clay					
O11	Light clay		25-35	0-3	
O12	Clay		35-50	0-3	
O13	Heavy clay		50-100	0-3	
Silt					
O14	Sandy loam	50-85		0-3	
O15	Silty loam	85-100		0-3	
Peat					
O16	Sandy peat		0-8	35-100	
O17	Clayey peat		8-100	35-100	

national databases (e.g. Carsel and Parrish, 1988; Yates *et al.*, 1992; Wösten *et al,* 1994; Leij *et al.*, 1996). Table 3 summarizes parameter values derived from a database of over 600 soil

samples in the Netherlands, known as the Staring Series (Wösten *et al.,* 1994). The Staring Series correspond to the legend of the 1 : 50 000 soil map of the Netherlands. The definition of the classes is primarily based on soil texture and organic matter content (Table 4), with a distinction between top- and sublayers. The Staring Series can be used in first-tier assessments and regional-scale applications. In the case of more detailed studies (e.g. field-studies), on-site measured data should preferably be used (Tiktak *et al.*, 1998).

3.1.2   Potential evapotranspiration

Depending on the data availability, three methods can be chosen for the calculation of the potential evapotranspiration (section 2.3.2). Because of good performance of the Penman-Monteith equation, we recommend the use of this equation if daily value of air-temperature, solar radiation, wind-speed and air-humidity are available. In other cases the simpler (and empirical) Makkink equation can be used.

If the Penman-Monteith equation is used, SWAP additionally requires the crop height as a function of crop development stage and the minimum canopy resistance. The minimum canopy resistance ranges from 30 s m^{-1} for arable crops to 150 s m^{-1} for trees in forests. See Allen *et al.* (1989) for parameter values.

If the Makkink equation is used, crop-factors should be entered as a function of crop development stage. Crop factors in relation to the Makkink approach were presented by Feddes (1987) for some common Dutch arable crops. The FOCUS modeling Working group (FO-CUS, 2000) compiled crop factors for common European crops. For the partitioning of the potential evapotranspiration, SWAP requires the Leaf Area Index as a function of development stage (see FOCUS (2000) for examples) and the extinction coefficient, κ (eqn. 8). Feddes *et al.* (1978) used $\kappa = 0.39$ for common arable crops. More recent studies showed that κ is crop dependent.

3.1.3   Uptake of water by plant roots

The depth distribution of water uptake is based on the root length distribution (eqn.11). The FOCUS modeling Working Group (FOCUS, 2000) compiled an overview of the maximum rooting depth as a function of development stage for some European crops. See also Van den Berg *et al.* (2000).

SWAP uses a trapezoidal function to describe the ratio between actual and potential transpiration rate (Figure 4). Table 5 gives a summary of critical pressure heads for some arable crops.

Table 5 Critical pressure heads (cm) of the sink term reduction function (Figure 4) for some main arable crops (Wesseling, 1991).

Crop	h_1	h_2	h_{3h}	h_{3l}	h_4
Potato	-10	-25	-320	-600	-16000
Sugar beet	-10	-25	-320	-600	-16000
Wheat	0	-1	-500	-900	-16000
Pasture	-10	-25	-200	-800	-8000
Corn	-15	-30	-325	-600	-8000

3.1.4   Evaporation of water from the soil surface

PEARL calculates the actual soil evaporation rate using eqn. 13 (Boesten and Stroosnijder, 1986). Wesseling *et al.* (1990) gave values for β in the range of 0.54 to 0.96 cm^{½}. Boesten (1986) analyzed literature data and concluded that there was no significant correlation between soil texture and β. This implies, that the full range (0.54 to 0.96 cm^{½}) applies to any soil type.

3.1.5   Interception of rainfall

Interception of rainfall is calculated with eqn. 14. This equation shows that at increasing rainfall amounts, the amount of intercepted water asymptotically reaches *a*LAI. Braden (1985) analyzed interception data for a number of agricultural crops and found that parameter *a* is approximately 0.25 for common agricultural crops. This value is also the default value in PEARL.

3.1.6   Bottom boundary conditions

The bottom boundary condition in PEARL is considered separately from lateral drainage fluxes. The lateral drainage fluxes apply to local groundwater flow, which is directly affected by local surface water management, whereas the bottom boundary conditions describe the influence of regional groundwater flow, which is not affected by local surface water management.

As mentioned in section 2.3.7, the user can choose between 8 types of lower boundary conditions. One of these relationships (option 4) is a lumped empirical relationship, describing both the influence of local and regional groundwater flow. The type of option to be chosen is dependent upon data-availability and the hydrological conditions.

3.2   Pesticide fate

3.2.1   Compounds and transformation scheme

PEARL can simulate the fate of a parent pesticide and its formation products (metabolites) in soils. PEARL uses a code with a maximum length of 5 alphanumerical characters to distinguish between compounds. The default code for the parent pesticide (i.e. the compound that has been applied) is 'pest'. For each compound, the molar mass must be specified. Data on molecular masses of compounds are reported in Tomlin (1994).

Usually a pesticide registration dossier states the transformation scheme of a compound, including the amounts of transformation products formed relative to the initial amount of the pesticide. The formation fractions – sometimes stated as percentages – may be based on masses (kg) or on molar fractions. PEARL needs data on molar fractions. For relatively simple transformation schemes (parent and first generation daughters only) the molar fraction data can be used directly in the transformation matrix (Table 2). For second (or higher) generation transformation products the molar fractions usually have to be recalculated from the original data; PEARL needs the molar fraction of each single reaction. If the data is not available from the dossier, data might be obtained by fitting the reaction model (scheme) to the experimental data. Several software packages, e.g. TOPFIT and SIMUSOLV are commercially available for this purpose.

Figure 9 shows the transformation curves of a pesticide with two metabolites. The transformation route is an ordinary chain reaction (Figure 8). The registration dossier of this pesticide states half-lives of 2.4, 22 and 48 days for the parent, the first metabolite and the second metabolite, respectively. Formation fractions are 0.76 for the first metabolite and 0.5
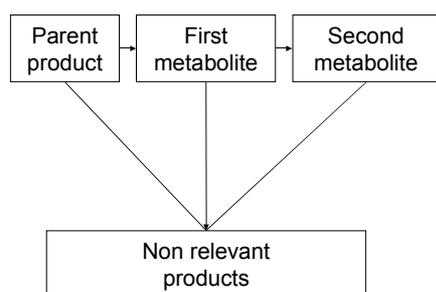
Figure 8 Simple chain reaction scheme for the example described

for the second metabolite, *both relative to the parent*. The half-lives and formation fractions can be introduced into PEARL as given in the dossier. However, the formation fraction of the second reaction must be recalculated, because the fraction should be introduced into PEARL relative to the first metabolite. Therefore, 0.658 (=0.5/0.76) should be used for the second reaction in the transformation table of PEARL. If data are calculated from experimental results one must be careful; if the results are expressed as mass versus time, data should be corrected for the relative molar mass.

From Figure 9 it becomes clear that the graphical method for estimating transformation fractions may lead to erroneous results. In this methodology, the peak values of the curves are often used as an approximation of the formation fractions. In this case, transformation fractions of 0.61 and 0.44 (=0.27/0.61) could be derived from Figure 9. As these values are far below the real values, we strongly recommend to use the parameter estimation method.
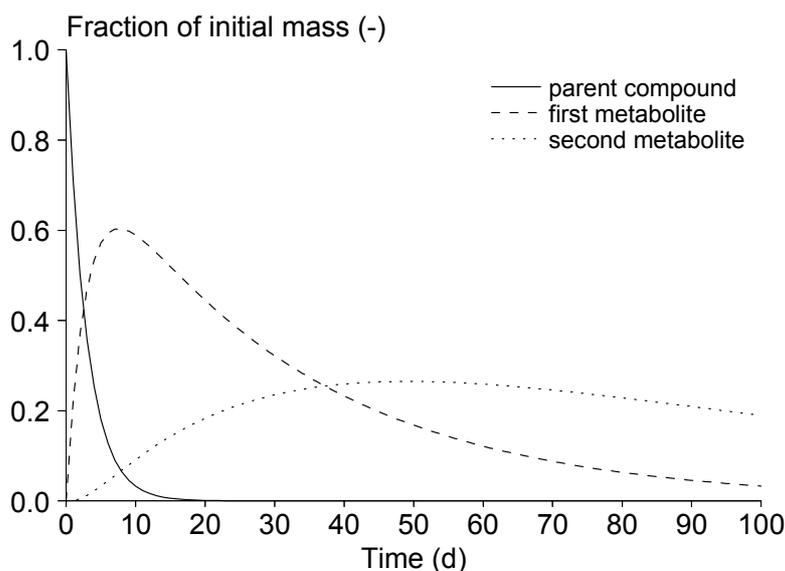
Figure 9 Example of a simple incubation experiment

3.2.2 Pesticide application

PEARL supports four types of pesticide application, i.e. spraying of pesticide onto the crop canopy, spraying of pesticide onto the soil surface, incorporation of pesticide into the topsoil and injection of pesticide at some depth in the soil.

3.2.3 Initial and boundary conditions

For each compound, the initial concentration in the soil system must be provided as a function of depth. PEARL needs the concentration in the equilibrium domain, c^*_{eq}, and the concentration in the non-equilibrium domain, c^*_{ne}. The default value is zero, which means that the simulations start with pesticide free soil.

The calculation of the volatilization flux requires the thickness of the laminar air boundary layer (eqn. 40). There is considerable uncertainty about the thickness of the air boundary layer. Also it is not yet known whether this layer exists permanently in space and time (Freijer *et al.*, 1996). Values that have been published for the thickness of the laminar layer range from a few mm to a few cm (e.g. Jury *et al.*, 1983).

3.2.4 Transport in the liquid phase

Transport of a compound in the liquid phase is described with the convection-dispersion equation (eqn. 29), which requires the coefficient of dispersion and the coefficient of diffusion.

The coefficient of dispersion is calculated with eqn. 30. The dispersion length, $L_{dis,L}$, of the soil generally varies between 0.03 and 0.10 m (Van Ommen *et al.* (1989). The default value in PEARL is set to 0.05 m, which is the average of values reported by Van Ommen *et al.* (1989).

The coefficient of diffusion in the liquid phase is calculated from the diffusion coefficient in pure water and a relative diffusion coefficient (eqn. 31). The diffusion coefficient in pure water is temperature dependent (eqn. 35). Therefore, the temperature reflecting the experimental conditions, T_r, must be provided together with the diffusion coefficient at the temperature reflecting the experimental conditions. The diffusion coefficient can be estimated from the molecular structure of a compound using the method described by Reid and Sherwood (1966). The value of the diffusion coefficient in water at 20 ^{o}C will be approximately 4.3 10^{-5} m^2 d^{-1} for compounds with a molar mass of 200 g mol^{-1} (Jury $et\ al.$, 1983). This is also the default value in PEARL. Notice that this value is slightly different from the value in the old Dutch standard scenario, which was 4 10^{-5} m^2 d^{-1}.

The relative diffusion coefficient can be calculated according to Millington and Quirk (1960), Currie (1960) and Troeh $et\ al.$ (1982). The Millington and Quirk relationship (eqn. 32) requires two parameters, $a_{M,L}$ (-) and $b_{M,L}$ (-). Based on Jin and Jury (1996), these parameters are set to 2 and 2/3, respectively. Also the Currie relationship (eqn. 33) requires two parameters, i.e. $a_{C,L}$ (-) and $b_{C,L}$ (-). Parameter values for this relationship have been reported for a wide range of Dutch soils in Bakker $et\ al.$(1987). The default values in PEARL are 2.5 and 3.0, respectively. These values are valid for weakly and moderately aggregated plough layers of loamy and humic sandy soils. The default values for $a_{T,L}$ and $b_{T,L}$ in the Troeh relationship (eqn. 34) are 0.05 m^3 m^{-3} and 1.4, respectively. More detailed information on these parameters is given in Jin and Jury (1996).

3.2.5   Transport in the gas phase

Transport of a compound in the gas phase is described with Fick's law (eqn. 36), which requires the coefficient of the coefficient of diffusion in the gas phase. This coefficient is calculated from the diffusion coefficient in air and a relative diffusion coefficient (eqn. 37). The diffusion coefficient in air is temperature dependent (eqn. 38). Therefore, the temperature reflecting the experimental conditions, T_r, must be provided together with the diffusion coefficient at the temperature reflecting the experimental conditions. The diffusion coefficient can be estimated from the molecular structure of a compound using the method described by Reid and Sherwood (1966). The value of the diffusion coefficient in air at 20 ^{o}C will be approximately 0.43 m^2 d^{-1} for compounds with a molar mass of 200 g mol^{-1} (Jury $et\ al.$, 1983). This is also the default value in PEARL. For some compounds, particularly soil fumigants, the coefficients for diffusion in air are substantially higher than the default value. Van Den Berg (1992) estimated the coefficient for the diffusion of 1,3-dichloropropene in air at 20 ^{o}C to be 0.69 m^2 d^{-1}.

The relative diffusion coefficient in the gas phase is calculated analogous to the relative diffusion coefficient in the liquid phase.

3.2.6   Freundlich equilibrium sorption

The sorption of pesticides is described with a Freundlich equation (eqn. 41). We recommend to derive the Freundlich equilibrium parameters from the conventional slurry experiments in which soil-water suspensions are equilibrated for about one day. The value of the reference

concentration, $c_{L,r}$, must be within the concentration range of the simulation study. Its default value is 1 mg L^{-1}.

In the most common approach, the Freundlich coefficient is calculated on the basis of the coefficient of equilibrium sorption on organic matter, $K_{om,eq}$ (eqn. 42). This equation requires two parameters, i.e. $K_{om,eq}$ and N. Average values of $K_{om,eq}$ have been compiled by Linders *et al.* (1994). The exponent, N, is usually in the range between 0.7 and 1.1 (Calvet, 1980). The average value of N is 0.9, which is also the default value in PEARL (Boesten and Van der Linden, 1991). These average values can be used for first-tier assessments. However, in more detailed field studies, the sorption coefficient and exponent should be obtained from soil material collected on-site (Boesten, 1991; Tiktak, 2000). The obtained sorption points should be fitted to the Freundlich model (eqn. 41). Tiktak *et al.* (1998) give an example for bentazone and ethoprophos.

If the Freundlich coefficient is dependent on the *p*H, the dissociation constant, *p*Ka, must be specified (eqn. 43). The *p*Ka can be taken from a handbook on chemical properties of pesticides (e.g. Tomlin, 1994). Eqn. 43 further requires two coefficients for sorption on organic matter, i.e. $K_{om,eq,ac}$ and $K_{om,eq,ba}$. These two parameters can be obtained by fitting eqn. 43 to experimental sorption data. Figure 10 gives the results of a sorption experiment with flumetsulam (Fontaine *et al.*, 1991). In this experiment, the *p*H was varied from well below to well above the *p*Ka of flumetsulam. The lines show the results of two fittings: (i) with the *p*H correction fixed to zero, and (ii) with the *p*H correction fitted. In this particular case, both equation fitted the data well. In such a case, the equation without *p*H correction is preferred.
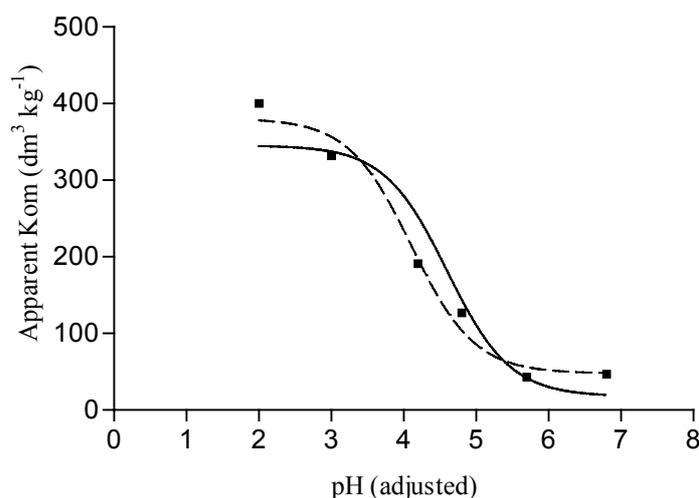

Figure 10 pH dependent sorption of flumetsulam

If a fitting program is unavailable, the user can alternatively decide to take the apparent K_{om} at *p*H values well below (more than 2 *p*H units), respectively well above the pKa value of the compound. Another use of the *p*H correction in equation 43 is to account for differences in

experimental methods to measure the soil pH. The sorption of pesticides is often measured in a 0.01 M CaCl$_2$ solution. If the soil pH has been measured in a different way (e.g. pH-KCl), a correction may be required. The pH correction, ΔpH, may vary between -1 and 2. See Leistra et al. (2000) for further considerations.

3.2.7   Freundlich non-equilibrium sorption

Non-equilibrium sorption is described in equation (45). This equation requires two additional parameters, i.e. the desorption rate coefficient, k_d, and the factor describing the ratio $K_{F,ne}/K_{F,eq}$, where $K_{F,ne}$ is the Freundlich coefficient at the non-equilibrium site and $K_{Fe,eq}$ is the Freundlich coefficient at the equilibrium site. Equation (45) shows that non-equilibrium sorption will not be simulated if k_d is set to zero.

Boesten et al. (1987) found values of $K_{F,ne}/K_{F,eq}$ ranging from 0.3 to 0.4 and k_d values ranging from 0.01-0.02 d^{-1} for cyanazine and metribuzin in a sandy soil. Boesten and Gottesbüren (2000) found a value of $K_{F,ne}/K_{F,eq}$ of 0.55 and a k_d value of 0.015 d^{-1} for bentazone in a sandy soil. If no further information is available, we recommend to use 0.5 for $K_{F,ne}/K_{F,eq}$ and 0.01 d^{-1} for k_d as default values.

A compound residing in the non-equilibrium domain is not subject to transformation (Figure 6), which implies that the half-life of transformation refers to the equilibrium domain only. An important consequence is that the transformation half-life, which usually refers to the total mass content, should be obtained in a slightly different way (page 51). This alternative experimental procedure also returns the two parameters mentioned here.

3.2.8   Gas-liquid phase partitioning

The gas-liquid phase partitioning coefficient is affected by basic compound properties (eqn. 47), that can be taken from a handbook on chemical properties of pesticides (e.g. Tomlin, 1994; Hornsby et al., 1996).

The saturated vapor pressure is temperature dependent (eqn. 48). For this reason, both the temperature reflecting the experimental conditions, T_r, and the saturated vapor pressure at that temperature, $p_{v,s,r}$, must be provided. The saturated vapor pressure shows a wide range of values. Smit et al. (1997) have compiled data on the saturated vapor pressure. The default value of $p_{v,s,r}$ in PEARL is set to zero, which means that there will be no compound in the gas phase. The default value of the enthalpy of vaporization, ΔH_v, is 95 kJ mol^{-1}, which is the average of available measurements as collected by Smit et al. (1997). Their data show a range from 58 to 146 kJ mol^{-1}.

The solubility of a compound in water should be provided together with the temperature reflecting the experimental conditions, T_r. The effect of soil temperature on the water solubility is described in equation 49. The default value for the molar enthalpy of dissolution, ΔH_d, is 27 kJ mol^{-1}, which is the average of measurements by Smit et al. (1997). Their data, which are all based on Bowmans and Sans (1985), show a range from -17 to $+156$ kJ mol^{-1}.

3.2.9   Transformation of the compound

In PEARL, transformation is described with first-order kinetics (eqn. 52 and 55). Average values for the half-life of 243 pesticides have been reported by Linders *et al.* (1994). These average values can be used for first-tier assessments. However, in more detailed field studies, the half-life time should be obtained by incubating soil material collected on-site (Boesten, 1991; Tiktak, 2000). The normal procedure is that top-soil material is incubated for periods with different length. Then, first-order rate constant, k_t (d^{-1}), is calculated using linear regression of ln-transformed data or non-linear curve fitting. The experiment is optionally repeated to obtain the half-life in subsoil material and the temperature dependence of transformation. See Tiktak *et al.* (1998) for an example.

The transformation half-life time is temperature (eqn. 56), soil-moisture (eqn. 57) and depth (eqn. 54) dependent. The half-life time that is input in PEARL should be representative for transformation in the topsoil. This half-life time must further be accompanied with the conditions reflecting the experimental conditions, i.e. the temperature (^{o} C) and the water content (kg kg^{-1}). The half-life time is often measured at 20 ^{o}C and at a liquid content reflecting field-capacity (*p*F 2). These values are taken as the default experimental conditions in PEARL.

The dependency of the transformation rate coefficient on the temperature is described with eqn. 56. Using the results of some 50 experiments, Boesten (1991) found an average value of the molar Activation energy in this equation of 55 kJ mol^{-1}, which was the value in the old Dutch standard scenario (Van der Linden and Boesten, 1989). The standard deviation for the activation energy was calculated to be 15 kJ mol^{-1}, with values ranging between 20 and 100 kJ mol^{-1}. In a more recent review, the FOCUS Soil Modeling Working Group (1997), found an average activation energy of 54 kJ mol^{-1}. This value is the default value in PEARL.

The effect of soil water on the rate coefficient is described with eqn. 57. Boesten (1986) reviewed the results of some 40 experiments with a range of compounds and soils, and found an average value of the exponent of 0.7. Its range was between zero and 2.8. This value is taken to be the default value in PEARL. In a more recent review (based on more data) the FOCUS Soil Modelling Working Group (1997) found the same average value of 0.7.

The factor f_d (eqn. 54), which accounts for the decrease of the rate of transformation with increasing depth must be introduced for each soil layer. This is soil and compound dependent. The default values have been taken from a literature review by Boesten and Van der Linden (1991). Additional information can be found in Walker *et al.* (1989, 1992).

In the case of pesticides that show sorption/desorption kinetics, a different procedure should be used to obtain the transformation half-life (see section 3.2.10).

3.2.10 Transformation of the compound in case of sorption/desorption kinetics

Commonly reported half-lives refer to the total mass content of pesticide. As PEARL assumes that transformation of pesticide occurs in the equilibrium domain only, a slightly different

experimental set-up should be used to obtain the half-life of pesticides that show desorp-tion/sorption kinetics. In this new experimental set-up, both the total mass of pesticide, M_p, and the concentration in the liquid phase, c_L, should be available as a function of time. We developed a simple model, PEARLNEQ, describing the processes occurring during this experi-ment. Using this model and the PEST parameter optimization tool (Doherty *et al.*, 1994), the first-order rate transformation constant, k_t (d^{-1}), the desorption rate coefficient, k_d (d^{-1}), and the ratio $K_{F,ne}/K_{F,eq}$ can be obtained. The molar activation energy, E_a (J mol^{-1}) can be fitted simultaneously, provided the incubation experiments were carried out at different tempera-tures. In addition to the transformation experiment, an equilibrium sorption experiment should be carried out. PEARLNEQ is provided with the PEARL model. PEST is *not* distributed with the PEARL package but should be ordered directly from a commercial supplier. Please check the internet for addresses by typing pest+optimaztion in the search engine box. See appendix 3 for a manual of the PEARLNEQ-PEST combination.

PEARLNEQ contains a subset of processes described by PEARL. Analogous to eqn. 50, the total mass of pesticide in the system is described by the equation:

$$M_p = V_L c_L + m_s K_{F,eq} c_{L,r} \left(c_L / c_{L,r} \right)^N + m_s X_{ne} \tag{60}$$

where M_p (µg), is the total mass of pesticide in the system, V_L (mL) is the volume of liquid, c_L (µg mL^{-1}) is the concentration of pesticide in the liquid phase, and m_s (g) is the dry mass of soil. As we assume that the transformation rate in the system is proportional to the equilib-rium domain, the following rate equation applies:

$$\frac{dM_p}{dt} = k_t \left(V_L c_L + m_s K_{F,eq} c_{L,r} \left(c_L / c_{L,r} \right)^N \right) \tag{61}$$

where k_t (d^{-1}) is the transformation rate coefficient, which is described as a function of tem-perature (eqn. 56). The system is further characterized by the sorption isotherm for the equi-librium sites (eqn. 41) and the sorption rate equation for the non-equilibrium sites (eqn. (45).

As an example, we used the bentazone incubation study described by Boesten and van der Pas (1999). They simultaneously measured the decline of the total amount of bentazone in moist soil and the soil pore water concentration for about 400 d (Figure 11). The experiments were carried out at 5 °C and 15 °C. In a separate experiment, they measured the sorption of bentazone via shaking a soil suspension for 24 h. We assumed that the shaking period for the soil suspension experiment was long enough to obtain equilibrium for the equilibrium iso-therm and that it was short enough to be able to ignore sorption to the non-equilibrium site. Boesten and Gottesbüren (2000) fitted the equilibrium sorption isotherm and found $K_{F,eq} = 0.10$ L kg^{-1} and $N = 0.82$. With these parameter values, k_t at 20 °C, E_a, $K_{F,ne}/K_{F,eq}$ and k_d were optimized with the PEARLNEQ-PEST combination. Figure 11 shows the lines that result from the fitting procedure.
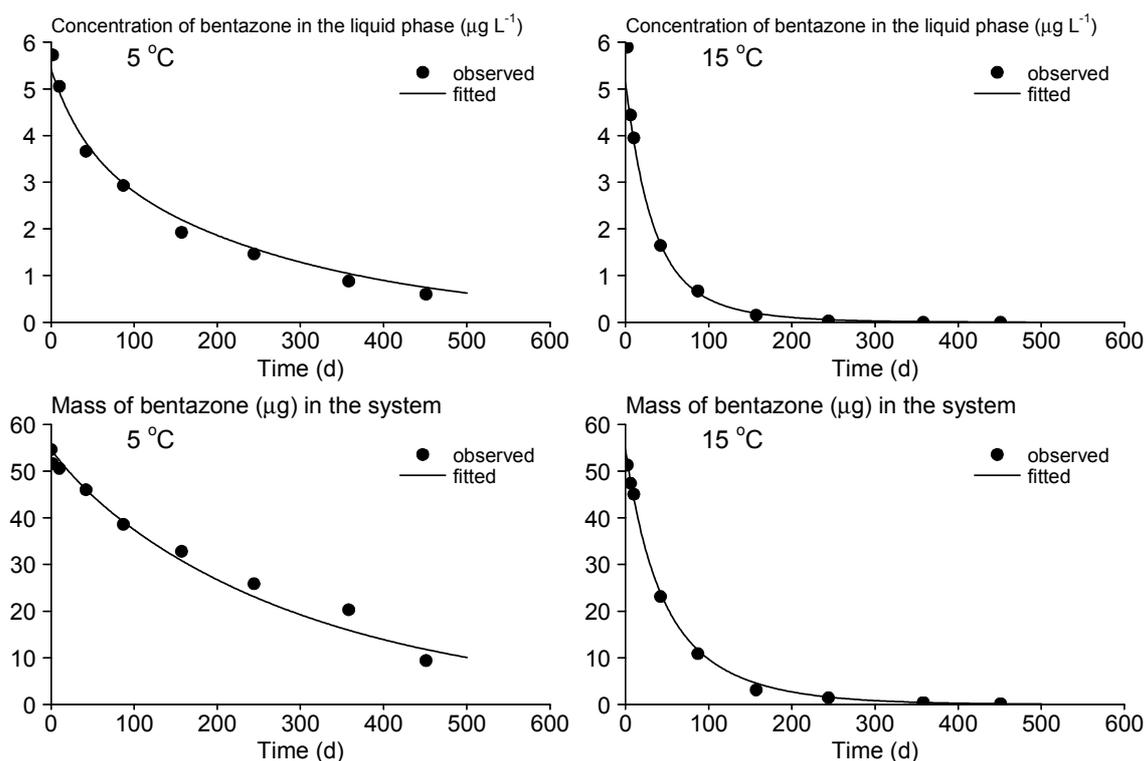
Figure 11 Concentration in the liquid phase and total mass of bentazone as a function of incubation time as measured in laboratory incubation experiments at 5 °C and 15 °C (markers). The lines refer to the results of the PEARLNEQ-PEST optimization (see further text).

Table 6 Fitted parameter values for the desorption rate constant, pesticide transformation half-life, molar-activation energy and the ration $K_{F,ne}/K_{F,eq}$ obtained from the laboratory incubation experiments shown in Figure 11.

Parameter	Unit	Estimated value	95 % confidence limits[a]	
			Lower limit	Upper limit
$K_{F,ne}/K_{F,eq}$	(-)	0.728	0.305	1.152
k_d	(d^{-1})	0.0193	0.0083	0.0304
DT$_{50}$	(d)	13.73	9.45	18.01
E_a	(kJ mol^{-1})	110	98	122

a) Confidence intervals provide only an indication of parameter uncertainty. They rely on a linearity assumption which may not extend as far in parameter space as the confidence intervals themselves.

Correlation matrix

	$K_{F,ne}/K_{F,eq}$	k_d	DT$_{50}$	E_a
$K_{F,ne}/K_{F,eq}$	1.000	-0.5712	-0.1420	0.04388
k_d	-0.5712	1.000	0.1077	-0.1211
DT$_{50}$	-0.1420	0.1077	1.000	-0.9052
E_a	0.04388	-0.1211	-0.9052	1.000

The figure shows that the decline of both the mass and the concentration in the liquid phase could be well described with the PEARLNEQ-PEST combination. Table 6 shows the fitted parameter values and their 95 % confidence limits. The fitted parameter values compare well to results from the studies by Boesten and Gottesbüren (2000) and Tiktak *et al.* (1998). PEST also gives the correlation coefficient matrix. Inspection of this table reveals that with the exception of E_a and DT$_{50}$, the model parameters are only slightly correlated, which means that the experimental set-up is suitable for deriving the four model parameters.

3.2.11 Compound uptake

The only parameter in the equation for uptake of compounds (eqn. 58) is the coefficient for the uptake by plant roots, f_u. This coefficient is sometimes known as the transpiration stream concentration factor, F. For non-ionic compounds, this factor can be estimated from the octanol-water partitioning coefficient as described by Briggs *et al.* (1982). For these compounds, this factor will be between 0 and 1. For ionic compounds no reliable estimation methods exist and the factor may be greater than 1. For example, Shone and Wood (1974) found a value of 3 for the 2,4-D anion. The default value in PEARL is 0.5, which is the average of values reported in Briggs *et al.* (1982).

4   User's guide for the command line version of PEARL

This chapter contains a description of the command-line version of PEARL. The command-line version is interesting for those who want to use PEARL in a batch environment. It also interesting for performing uncertainty- and sensitivity analyses or inverse modeling exercises. In all other cases we recommend the use of the PEARL User Interface (chapter 5). This interface has some distinct advantages, such as automatic generation of input files, data-storage in a relational data-base, easy access to scenarios, and an integrated viewer. Please realize that the command-line version is only suitable for experienced users.

4.1   Running the model

After you have installed the model (section 5.16), a copy of the PEARL kernel will be available in the bin directory of the PEARL package. Copies of the input file are availble in the defscen directory of the PEARL package. These input files can be used as a basis for further processing. It is a good practice to copy all input files to a working directory. *Do not edit the original files, so they can serve as a back-up.* The defscen directory contains the following three files:

- a general input file, defscen.prl
- the file containing weather data, defscen.met
- an optional file containing irrigation data, defscen.irr

You can change the name of the input files, but the extensions are fixed.

Assuming that you have installed PEARL in the directory c:\Program Files\Pearl, you can start the model by typing:

```
"C:\program files\pearl\bin\pearlmodel" RunID
```

where RunID is the first part of the name of the general input file. If, for example, the name of the input file is 'atra.prl', you can start the PEARL kernel by typing:

```
"C:\program files\pearl\bin\pearlmodel" atra
```

The Run ID has a maximum length of eight alphanumerical characters. Please notice that the quotes are obligatory, because the path contains a space. If you wish to run the model several times, it may be handy to create a batch file "pearl.bat", which contains the following two lines:

```
@echo off
"C:\program files\pearl\bin\pearlmodel" %1
```

If put in the working directory, the model can be run by typing pearl, followed by the RunID.

4.2   Description of the PEARL file

4.2.1   Structure of records in the PEARL input file

The PEARL input file consists of obligatory and optional records. Each record contains the following fields:

- An obligatory field containing the identifier
- One or more fields containing the actual data
- An optional field containing the dimension of the data
- Comment fields

Figure 12 shows the sequence of actions that are undertaken when an input parameter is read. First, the model looks for the record containing the requested identifier. The entire input file
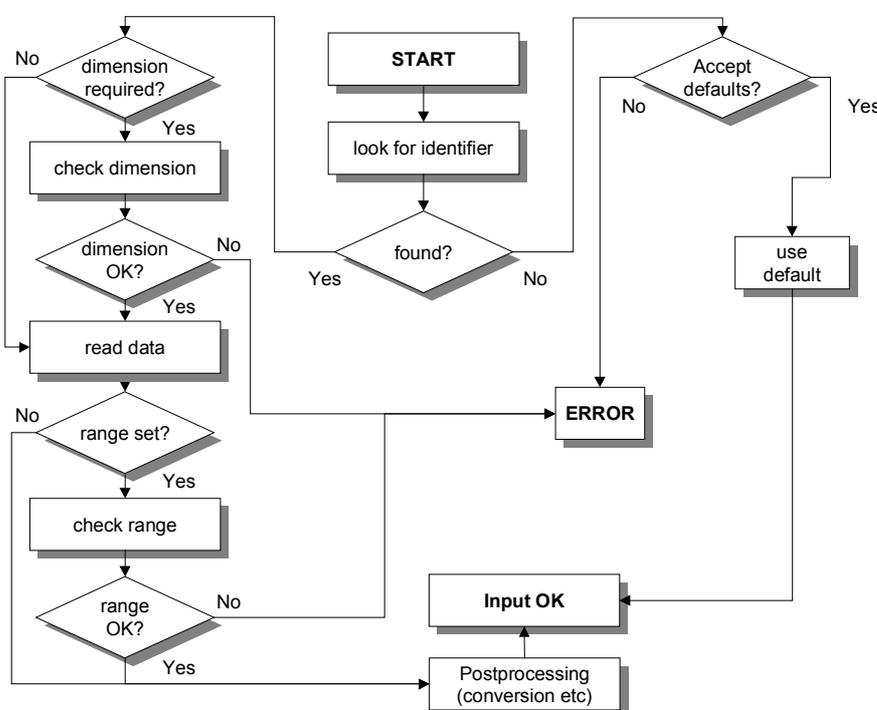
Figure 12 Flow chart showing the sequence of actions when reading an input parameter

is scanned, so the sequence of records is free. If the requested record is missing (right-hand side of diagram), the model either uses default values, or prints an error message. If the requested record is found, the model proceeds with verifying the dimension field. This step is followed by the actual data input. Finally, the lower- and upper bounds of the model inputs are checked. In some cases, additional actions are undertaken: Model inputs that are specified as a function of soil horizon are allocated to numerical soil layers, and model inputs that are specified in user-friendly units are converted to units used within the model (i.e. kg, m, mol and d). The data are echoed to the log file *after conversion,* so the user can check whether the model has interpreted the inputs correctly.

PEARL distinguishes the following type of records:

- Numerical records
- Option records
- Date records
- Soil properties
- Compound properties
- Crop properties

Numerical records

These records are meant for single numerical values, such as the initial groundwater level. Numerical records consist of an input field (field 1), an identifier (field 2), an optional dimension field (field 3), and a comment field (rest of record). See the following example:

```
1.00           ZGrwLevSta   (m)   Initial groundwater level [0|50]
```

Option records

Option records consist of the input field (field 1), an identifier (field 2) and a comment field (rest of record):

```
Penman         OptEvp             Evapotranspiration: Input, Penman or Makkink
```

Date records

Date records consist of the input field (field 1), an identifier (field 2) and a comment field (rest of record). Dates are input in the format dd-mmm-yyyy. The following month names are valid: Jan, Feb, Mar, Apr, May, Jun, Jul, Aug, Sep, Oct, Nov and Dec.

```
01-Jan-1980    TimStart           Begin time of simulation [01-Jan-1900|-]
```

Soil properties

The input of soil properties starts with the definition of the soil profile in the SoilProfile table (see page 61). Soil properties can then be input as a function of depth (interpolate option) or as a function of soil horizon (horizon option). In the first case, the values specified by the user are linearly interpolated onto the numerical grid given in the SoilProfile table. In the second case, the horizon definitions given in the table are used as a key. Soil property tables consist of the following lines: (i) the identifier line, containing the key-word 'table', followed by the input option (horizon or interpolate), the identifier field and the dimension, (ii) the actual input records (one for each soil horizon), and (iii) the obligatory line containing the word 'end_table'. Comment between the identifier line and the end_table line is illegal:

```
table horizon Rho            (kg.m-3)   Bulk-density of the soil [100|2000]
1    1310.0
2    1540.0
3    1640.0
4    1650.0
5    1650.0
end_table
```

Multiple soil properties can be input in one table. In this case, two extra lines are added to the header of the table. These lines contain the identifiers of the individual columns and the dimension for the individual columns. Consider the following example.

```
table   horizon SoilProperties
Nr      FraSand   FraSilt   FraClay   CntOm     pH
        (kg.kg-1) (kg.kg-1) (kg.kg-1) (kg.kg-1) (-)
1       0.92      0.05      0.03      0.0470    4.7
2       0.96      0.02      0.02      0.0080    4.4
3       0.95      0.03      0.02      0.0019    4.6
4       0.94      0.04      0.02      0.0014    4.6
5       0.93      0.05      0.02      0.0000    4.6
end_table
```

Compound properties

Values have to be supplied for all compounds considered in a simulation run. First, the user has to specify compound names in the compounds table (page 65). Compound properties that are independent from the soil profile are input through a series of numerical records. Consider the following example:

```
70.00          KomEql_atra  (L.kg-1)   Coefficient for equilibrium sorption
40.00          KomEql_DEA   (L.kg-1)   Coefficient for equilibrium sorption
45.00          KomEql_DIA   (L.kg-1)   Coefficient for equilibrium sorption
```

Depth dependent compound properties are input through tables (SoilCompound properties) as described in the soil properties section:

```
table interpolate ConSysEql        (kg.m-3)
z         pest    DEA     DIA
0.0       0.0     0.0     0.0
5.0       0.0     0.0     0.0
end_table
```

Notice that the compound names are specified at the second line of the table.

Crop properties

Crop properties are input in an equivalent way as compound properties. Consider the following example:

```
-10.0          HLim1_Maize  (cm)      Anaerobiosis point  [-100|0]
```

4.2.2 General rules for variable names

To improve the readability of the PEARL input file, a systematic approach has been followed for nomenclature of variables in the input file. Names were constructed using the three-letter codes listed in Table 7. These codes are usually used from left to right, and only if they are

considered necessary. Sometimes several codes from one column were used, in which case they appear in alphabetical order.

Table 7 Notation of variable names in the PEARL input file.

Nature of quantity		Quantity		Process		Compartment		Specification	
Code	Description	Code	Description	Code	Description	Code	Description	Code	Description
Cof	coefficient	Alt	Altitude	Ant	Anthesis	Air	air	Act	actual
Del	difference	Ama	areic mass	App	Application	Aqf	aquifer	Amp	amplitude
Exp	exponent	Amr	areic mass rate	Cnv	Convection	Aqt	aquitard	Avg	average
Fac	factor	Avo	areic volume	Dep	Deposition	Clay	clay	Bou	boundary
Fra	fraction	Cnt	Content	Dif	Diffusion	Crp	crop	Cum	cumulative
Mol	molar	Con	Concentration	Dis	Dispersion	Gas	gas	Cur	currie
Num	number	Day	Day	Dra	Drainage	Grw	groundwater	Dau	daughter
Opt	option	DT50	half-life	Dsp	Dissipation	Lay	layer	Den	denominator
		Ent	Enthalpy	Emg	Emergence	Lbo	lower bound	End	final
		Eps	Volume fraction of gas	Evp	Evaporation	Liq	liquid	Eql	equilibrium
		Flm	mass flux	Ext	Extinction	Om	organic matter	Err	error
		Flv	volume flux	For	Formation	Pro	profile	Fre	Freundlich
		Hea	Head	Har	Harvest	Sand	sand	Foc	FOCUS
		Itr	Iteration	Hyd	Hydrology	Silt	silt	Max	maximum
		K	Conductivity	Inf	Infiltration	Sol	soil	Mil	millington
		Kom	K_{om}	Int	Interception	Sys	system	Min	minimum
		LAI	leaf area index	Irr	Irrigation	Ubo	upper bound	Neq	non-equilibrium
		Lat	Latitude	Mat	Maturity	Wat	water	Nom	nominator
		Len	Length	Pen	Penetration			Pot	potential
		Lev	Level	Pnd	Ponding			Prn	print
		Mas	mass flux	Prc	Precipitation			Prt	parent
		pKa	PKa	Sor	Sorption			Red	reduction
		Pre	Pressure	Til	Tillage			Ref	reference
		Rat	Rate	Tra	Transformation			Rel	relative
		Rho	bulk density	Trp	Transpiration			Res	residual
		Rst	Resistance	Upt	Uptake			Sat	saturated
		Slb	Solubility	Vap	Vaporisation			Scr	screen
		Tem	Temperature	Vol	Volatilisation			Sta(rt)	start
		Theta	volume fraction of liquid	Was	wash-off			Sum	sum
		Thi	Thickness					Tro	troeh
		Vvr	Volumic volume rate						
		Z	Depth						

4.2.3 Getting started with the command-line version

As mentioned in chapter 3, PEARL can be used for first- and higher tier pesticide leaching assessments. In the first case, many model-inputs can be set at default values. The second case requires more specific input. We recommend to use the file 'default.prl' for first-tier assessments with the Dutch standard scenario. In this file, most model-input are fixed, and the user only specifies the most important compound parameters, such as $DT_{50,r}$ and $K_{om,eq}$. The file 'expert.prl' (appendix 2) can be used for simulating field-studies and lysimeter experiments.
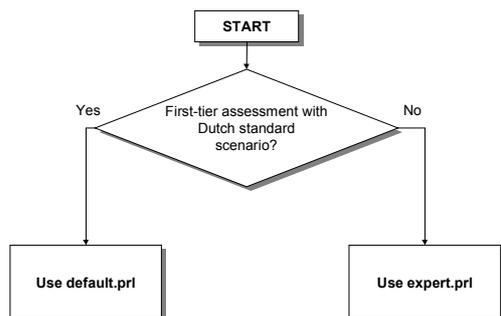
Figure 13 Decision between expert and default mode.

4.2.4 Overview of sections in the PEARL files

Table 8 gives an overview of sections in the PEARL files.

Table 8 Overview of sections in the PEARL files

Nr	Section name	Kind of model parameters
1.	Simulation control	Simulation options
2.	Soil profile and soil properties	Soil profile, soil properties
3.	Weather and irrigation data	File names for weather and irrigation data
4.	Boundary conditions of hydrological model	Lower boundary flux and drainage/infiltration parameters
5.	Compound properties	Compound properties
6.	Management	Application and tillage
7.	Initial and boundary conditions	Initial pesticide concentration and deposition
8.	Crop section	Crop calendar and crop properties
9.	Output control	Input/output options

4.2.5 Section 1: Simulation control

The control section contains general options for the simulation run, such as the time-domain, print time and minimum and maximum time-step for the hydrological model.

Using default values

PEARL can use default values from the new Dutch standard scenario. This scenario is based on Van der Linden and Boesten (1989), but uses a variable groundwater table instead of a fixed groundwater table. If AcceptDefaults is set to Yes, the standard scenario will be used and input of parameters that have been given a default value will not be necessary (see *Figure 12*).

Time-domain

The time-domain for the simulation is specified with the variables TimStart and TimEnd. PEARL internally uses the day number since 01-Jan-1900, but the date-format specified at page 57 can be used in the input file. Please notice that the time-domain is fixed in the case of running FOCUS scenarios and the Dutch standard scenario. According to guidelines of the FOCUS soil modeling Working group (1997), FOCUS simulations must start at 1-Jan-1901. The length of the run should be 26 years in the case of annual applications, 46 years in the

case of biennial applications and 66 years in the case of triennial applications. The time-domain for the Dutch standard scenario is 1-Jan-1980 until 31-Dec-2000.

Additional stop criterion.
The variable <u>AmaSysEnd</u> can be used as an additional stop criterion. The simulations will stop if the areic mass of pesticide in the soil system has become less than AmaSysEnd. This variable will be ignored if set to zero.

Control of the hydrological model SWAP.
The other variables in the control section control the hydrological model SWAP. The <u>Re-peatHydrology</u> option can be used to repeat weather and irrigation data. If set to Yes, weather and irrigation data of one year are constantly repeated. This option is intended to be used in combination with Dutch standard scenario, which repeats weather data from the year 1980. The hydrology option (<u>OptHyd</u>) determines how PEARL calls the hydrological model SWAP. The following options are availabe:
–   <u>OffLine</u>: PEARL assumes that SWAP has already been run. A hydrological datafile (RunId.pfo) must be prepared in advance.
–   <u>OnLine</u>: PEARL generates the input files for swap and runs SWAP.
–   <u>Automatic</u>: PEARL checks if the hydrological datafile (RunId.pfo) is already available. In this case, the hydrological calculations will be skipped.
–   <u>Only</u>: The hydrological model is run, but the rest of the simulations is skipped. This switch is interesting for users who want to test or calibrate the hydrological model, without (already) running the pesticide part. Output is written in PEARL format.
–   <u>GenerateInput</u>: PEARL creates input for the hydrological model only.

Accuracy of the hydrological model.
The variables <u>DelTimSwaMin</u> and <u>DelTimSwaMax</u> determine the minimum and maximum time-steps in the SWAP model. The model will look for the optimal time step between the preset limits. Making the time-step too large could lead to instability, while making it too small will increase the computation time substantially. The stop criterion for the iteration procedure (<u>ThetaTol</u>) defines the accuracy of the simulations. Choosing it too large could introduce a numerical water balance error.

4.2.6   Section 2: Soil properties and soil profile
In this section, the soil profile, vertical discretization and soil properties have to be specified.

The soil profile
The vertical discretization is input through the <u>SoilProfile</u> table. For each soil horizon, the thickness of the horizon, and the number of soil layers used in the finite-difference scheme (see Figure 3) must be provided. The maximum number of soil horizons is currently set to 10, the maximum number of numerical soil layers is set to 500. The number of soil layers is a compromise between accuracy and computation time. Computation time increases approximately with the square of the number of soil layers. On the other hand, predictions may

become inaccurate if the layer thickness is taken too large. This is particularly true if the expected concentration in the groundwater is lower than 0.001 µg L^{-1} (Leistra et al., 2000). For most simulations, however, a layer-thickness of 2.5 cm in the top 30 cm, 5 cm in the 0.3-1 m soil layer and 10 cm in the layer below 1 m is fair compromise.

Basic soil properties
Basic soil properties are input in the SoilProperties table. For each soil horizon, the textural distribution (FraSand, FraSilt and FraClay), the mass content of organic matter (CntOm) and the pH have to be specified. Notice that the textural distribution refers to the mineral soil only, so the sum of the sand, silt and clay fractions should be one. The mass content of organic matter refers to dry soil. The *p*H is used for the sorption model of weak acids. As most sorption experiments are being carried out in 0.01 *M* CaCl$_2$, the *p*H-CaCl$_2$ is preferred. If the *p*H-CaCl$_2$ is not available, the user should set the pHCorrection variable unequal to zero (page 66).

Soil physical properties
Parameters of the Van Genuchten functions (eqn. 4 and 5) are input in the VanGenuchtenPar table. The columns should contain θ_s (ThetaSat), θ_r (ThetaRes), α (Alpha), n (n), K_s (KSat) and λ (l). If the bulk-density is unknown, it can be calculated by the model (OptRho). If set to Calculate, the model uses the pedo-transfer function (Bollen *et al.*, 1995):

$$\rho_b = 1800 + 1236 m_{om} - 2910\sqrt{m_{om}} \qquad (r^2 = 0.91) \qquad (62)$$

where ρ_b (kg m^{-3}) is the dry bulk density and m_{om} (kg kg^{-1}) is mass content of organic matter. If OptRho is set to Input, the bulk density should be provided in table Rho.

Ponding and air boundary layer.
The maximum ponding layer thickness (ZPndMax) determines the maximum thickness of the water layer that can be present on the soil profile before surface runoff starts. The thickness of the air boundary layer must be specified in the ThiAirBouLay record.

Soil evaporation parameters
The potential evaporation calculated by eqn. 8 can be corrected by a factor FacEvpSol. This is particularly important in the case of a small soil cover fraction, because eqn. 8 has been derived for situations where the canopy shades the ground. FacEvpSol can be given a value between 0.5 and 1.5. The actual soil evaporation rate is calculated using hydraulic properties and an empirical reduction function (eqn. 13). Parameter β in this relationship must be provided in the CofRedEvp record.

Parameter values of the functions describing the relative diffusion coefficients
The diffusion of compounds is affected by the diffusion coefficient in water and air and by the relative diffusion coefficient. The diffusion coefficients are compound properties, the relative diffusion coefficients are soil properties. Three functions can be used for the relative diffusion coefficient, i.e. the functions published by Millington and Quirk (eqn. 32), Currie

(eqn. 33), and Troeh *et al.* (eqn. 34). The value of the option <u>OptCofDifRel</u> determines which of the three functions is used by the model. The following parameters should further be specified:

- If OptCofDifRel is set to MillingtonQuirk: a_M (<u>ExpDifLiqMilNom</u>) and b_M (<u>ExpDifLiq-MilDen</u>) for diffusion in the liquid phase; ExpDifGasMilNom and ExpDifGasMilDen for diffusion in the gas phase.
- If OptCofDifRel is set to Currie: a_C (<u>CofDifLiqCur</u>) and b_C (<u>ExpDifLiqCur</u>) for diffusion in the liquid phase; CofDifGasCur and ExpDifGasCur for diffusion in the gas phase.
- If OptCofDifRel is set to Troeh: a_T (<u>CofDifLiqTro</u>) and b_T (<u>ExpDifLiqTro</u>) for diffusion in the liquid phase; CofDifGasTro and ExpDifGasTro for diffusion in the gas phase.

See page 48 for a discussion on parameterization.

Dispersion length
The dispersion length, $L_{dis,L}$ (eqn. 30) should be given for each soil horizon (table <u>LenDisLiq</u>). Please notice that the distance between the nodal points, Δz, should be small enough to meet the Peclet condition (eqn. 2). Some information about the dispersion length is given at page 47).

4.2.7   Section 3: Weather and irrigation data
In this section, the names of the files with weather and irrigation data should be specified. This section further contains some options.

Weather data
The name of the file with weather data should be specified in the <u>MeteoStation</u> record. The altitude (<u>Alt</u>) and latitude (<u>Lat</u>) are also required. The name should be given without the extension, and has a maximum length of eight alphanumerical characters. PEARL automatically adds the extension .met to the file name, so in the above listed example the full name is debilt.met. The format of the file with weather data is described in section 4.2.14. PEARL needs some additional information. First, the user should specify which method is chosen for the computation of the potential evapotranspiration (<u>OptEvp</u>). Three options are available: (i) the potential evapotranspiration is input by the model, (ii) the Penman-Monteith equation is used, and (iii) the Makkink equation is used. If Penman-Monteith is selected, solar radiation, minimum and maximum air temperature, air humidity, wind speed and precipitation are required. If Makkink is selected, only minimum and maximum air temperature, solar radiation and precipitation are necessary.

Soil temperatures
To calculate the initial soil temperature profile, PEARL requires the temperature at the lower boundary (<u>TemLboSta</u>). If measured data are unavailable, we recommend the use of the long-term average air-temperature.

Irrigation
The name of the file with weather data should be specified in the IrrigationData record. The name should be given without the extension, and has a maximum length of eight alphanumerical characters. PEARL automatically adds the extension .irr to the file name, so in the above listed example the full name is debilt.irr. The format of the file with irrigation data is described in section 4.3. Irrigation water can be added to the crop canopy (Sprinkler irrigation) or to the soil surface (Surface irrigation). The type of irrigation should be specified in the OptIrr record.

4.2.8 Section 4: Boundary and initial conditions of the hydrological model

In this section, the boundary conditions of the hydrological model are specified. SWAP makes a distinction between the seepage flux due to regional groundwater flow and the local drainage flux to ditches and drains (see Figure 5). The seepage flux due to regional groundwater flow is the lower boundary condition of the model (section 4a of input file), the local drainage flux is considered a sink term (section 4b of input file).

Initial conditions
It is assumed that initally the pressure head of each nodal point is in hydrostatic equilibrium with the groundwater table. This implies that the pressure head at the groundwater table equals zero, and that the pressure head of each nodal point decreases linearly with height towards the soil surface. The user only needs to specify the initial depth of the groundwater table (ZGrwLevSta). If, however, OptLbo (see next paragraph) is set to GrwLev, the model uses the appropriate record in the GrwLev table.

Lower boundary conditions
As described in section 2.3, SWAP offers eight options for the lower boundary condition. The value of OptLbo determines which type of boundary condition is used by the model. The following options are available (see page 28 for description of options): (1) GrwLev, (2) Flux, (3) Head, (4) FncGrwLev, (5) Dirichlet, (6) ZeroFlux, (7) FreeDrain and (8) Lysimeter. For option 1-5, the user should specify additional information.

If OptLbo is set to GrwLev, the groundwater level should be specified as a function of time (table GrwLev). Normal data-format can be used. If RepeatHydrology is Yes (see page 61), the year can be omitted.

If OptLbo is set to Flux, a sine function is applied to generate the daily regional bottom flux. The user should specify the mean (FlvLiqLboAvg) and amplitude (FlvLiqLboAmp) of the annual bottom flux. Also the date at which the maximum of the sine wave occurs should be given (DayFlvLiqLboMax). Notice that negative values denote downward fluxes and positive fluxes denote upward values.

If OptLbo is set to Head, the regional bottom flux is calculated using the head difference between the phreatic groundwater and the groundwater in the semi-confining aquifer (see

Figure 5 and eqn.15). The average groundwater level in the field, Φ_{avg}, is affected by the drainage base (HeaDraBase) and by the shape of the groundwater table (OptShapeGrwLev), which can be Elliptic, Parabolic, Sinusoidal or NoDrains. The daily value of the hydraulic head in the semi-confining aquifer, Φ_{aqf} is described by a sine-wave. The user must specify its annual average value (HeaAqfAvg), the amplitude (HeaAqfAmp) and the date at which the maximum hydraulic head occurs (TimHeaAqfMax). The bottom flux (eqn.15) is also affected by the vertical resistance of the aquitard (RstAqt, γ_{aqt}).

If OptLbo is set to FncGrwLev, the bottom flux is calculated as a function of the groundwater level (eqn. 17). If this option is chosen, the model needs the coefficient (CofFncGrwLev) and the exponent (ExpFncGrwLev). Please realize that this option is only valid for deep, sandy areas. The calculated bottom flux includes local drainage to surface waters and drains, so local drainage should be set to zero if this option is used.

If OptLbo is set to Dirichlet, the pressure head at the lower boundary should be specified as a function of time (table h). Normal data-format can be used. If RepeatHydrology is Yes (see page 61), the year can be omitted.

The FreeDrain, Lysimeter and ZeroFlux options do not require additional input.

Local drainage fluxes to ditches and drains
If OptLbo is set to GrwLev, Flux, Head, Dirichlet or ZeroFlux, a local drainage flux can be defined in addition to the regional seepage flux. The user must first specify if local drainage should be simulated (OptDra). Then the number of local drainage systems, such as drainage-tiles and field-ditches) must be provided (NumDraLev). SWAP can simulate up to 5 local drainage systems.

For each local drainage system, a drainage flux is calculated according to eqn. 18. The model needs information about the bottom of the drainage system (ZDra) and the drainage resistance (RstDra) . The procedure that distributes the drainage flux over the individual soil layers additionally requires information about the drainage type (DraTyp) and the distance between the drainage systems (DistDra). To distinguish between the local drainage systems, the sequence number of each local drainage system should be concatenated to the record identifiers specified above, so we get DraTyp_1, DraTyp_2, etc.

4.2.9   Section 5: Compound properties
In this section, the properties of all compound must be specified. In this section, the identifier names are concatenated with compound names (in this example 'pest').

Compound table
The compounds section starts with the list of compound codes (the compounds table). The maximum length of each code is five letters. For each compound, the molar mass (MolMas) must be specified (section 3.2.1).

Reaction scheme
The reaction scheme (see Figure 7 for an example and section 3.2.1 for guidance) is input in the <u>FraPrtDau</u> table. For each parent compound j, the molar fraction of compound transformed into daughter i (variable $\chi_{i,j}$ in eqn 53) must be specified. The input file contains examples for one and three compounds.

Transformation rate parameters
This section contains the variables that affect the transformation rate of the compound. The transformation half-life time (<u>DT50Ref</u>) must be specified together with the temperature reflecting the experimental conditions during the incubation study (<u>TemRefTra</u>). Then, the user must specify whether the experiments have been carried out under optimum moisture conditions (i.e. wetter than pF 2). Record <u>OptCntLiqTraRef</u> can be used for this purpose, its value is Optimum or NonOptimum. If set to NonOptimum, PEARL needs information about the moisture content during the incubation study (<u>CntLiqTraRef</u>). The temperature dependence of transformation is described with eqn. 56; the molar activation energy is input in record <u>MolEntTra</u>. The effect of soil water on the rate coefficient is described with eqn. 57. The exponent in this equation should be specified in record <u>ExpLiqTra</u>. The effect of depth on transformation rate must be introduced in the <u>FacZTra</u> table. See section 3.2.9 for further information on transformation parameters.

Freundlich equilibrium sorption
The sorption of compounds is described with a Freundlich equation (eqn. 41). The value of the reference concentration must be introduced in the <u>ConLiqRef</u> record. Its value must be within the concentration range of the simulation study. The default value is 1 mg L^{-1}.

Three methods are available to describe the Freundlich coefficient; the desired approach must be specified in the <u>OptCofFre</u> record. The most common approach (OptCofFre is pH-independent) is to calculate the Freundlich coefficient from the organic matter content and the coefficient for sorption on organic matter (eqn. 42). If OptCofFre is set to pH-dependent, the Freundlich coefficient is calculated with eqn. 43. This equation applies to the sorption of weak-acids. In cases that the sorption of pesticides is not dependent on the organic matter content, the Freundlich coefficient can be introduced directly (eqn. 44). In these cases, OptCofFre should be set to CofFre.

In the most common approach (OptCofFre is pH-independent), only two parameters have to be introduced, i.e. the coefficient for sorption on organic matter, $K_{om,eq}$ (<u>KomEql</u>) and n (<u>ExpFre</u>). See section 3.2.6 for further guidance and backgrounds.

If OptCofFre is set to pH-dependent, two coefficients for sorption on organic matter must be specified (section 3.2.6), i.e. <u>KomEqlAcid</u> ($K_{om,eq,ac}$) and <u>KomEqlBase</u> ($K_{om,eq,ba}$). In addition, the negative logarithm of the dissociation constant (<u>pKa</u>) and a <u>pHCorrection</u> are required.

If OptCofFre is set to CofFre, the user should specify the Freundlich coefficient measured in the top-soil (CofFre) and the factor to describe the depth dependence of sorption (FacZSor). The factor to describe the depth dependence of sorption should be 1 in the top-soil.

Non-equilibrium sorption
Non-equilibrium sorption is described in equation (45). This equation requires two additional parameters, i.e. the desorption rate coefficient, k_d, and the factor describing the ratio $K_{F,ne}/K_{F,eq}$, where $K_{F,ne}$ is the Freundlich coefficient at the non-equilibrium site and $K_{Fe,eq}$ is the Freundlich coefficient at the equilibrium site (FacSorNeqEql).

The desorption rate coefficient should be specified in the CofRatDes record. Please notice that non-equilibrium sorption will not be simulated if CofRatDes is set equal to zero. See further section 3.2.7.

Gas-liquid partitioning
The gas-liquid phase partitioning coefficient is affected by compound properties that can be taken from a handbook on chemical properties of pesticides (e.g. Tomlin, 1994, Hornsby *et al.*, 1996). PEARL needs the saturated vapor pressure (PreVapRef), the temperature at which this parameter is determined (TemRefVap), the enthalpy of vaporization MolEntVap, the solubility of pesticide (SlbWatRef), the temperature at which the water solubility is obtained (TemRefSlb) and the molar enthalpy of dissolution (MolEntSlb). See section 3.2.8 for further guidance.

Pesticide uptake
The only parameter in the equation for uptake of pesticides (eqn. 58) is the coefficient for the uptake by plant roots, FacUpt. See further section 3.2.11.

Diffusion coefficients
The diffusion coefficients of pesticides in pure water (CofDifWatRef) and air (CofDifAirRef) are compound properties and must be specified in this section. Parameters for the relative diffusion coefficient are specified in the soil section (see page 62). The diffusion coefficients are temperature dependent. The reference temperature should be introduced in record TemRefDif.

Pesticide fate at the crop canopy
In the last part of the compound section, parameter values must be given for the submodel on pesticide fate at the crop canopy. In this submodel only the parent compound is considered, as the reaction scheme (Figure 7) is derived for products formed in the soil. For this reason, the pesticide code should not be concatenated to the identifiers below.

Processes that occur at the plant canopy are volatilization, penetration into the plant and (photochemical) transformation (page 28). These processes are described with first-order rate reactions. The user can make a choice between a lumped description of the processes at the

crop canopy, or a full description of dissipation (record OptDspCrp). If set to 'Specified', the user should specify the half-life due to penetration (DT50PenCrp), volatilization (DT50VolCrp) and transformation (DT50TraCrp). If set to 'Lumped'. an overall half-life (DT50DspCrp) is sufficient.

The wash-off of pesticides is described with a zero-order equation with one parameter (FacWasCrp).

4.2.10 Section 6: Management

This section contains data on pesticide applications and tillage. First, a variable DelTimEvt should be specified. This variable determines the repeat interval in years of the event table. If cset to 2, for example, biennial applications are simulated. If set to NoRepeat, the application table will not be repeated.

The actual applications are specified in the Applications table. The first column in this table contains the application date. Normal date format can be used, but the year is only required if DelTimEvt has been set to NoRepeat. The second column contains the application type, which must have one of the following values:

−   Application to the soil surface (AppSolSur).
−   Incorporation (AppSolTil). If this option is chosen, the user must specify the tillage depth in the third column.
−   Injection (AppSolInj). If this option is chosen, the user must specify the injection depth in the third column.
−   Application to the crop canopy; fraction intercepted user specified (AppCrpUsr). The interception fraction must be specified in column 3.
−   Application to the crop canopy; fraction intercepted calculated on the basis of the soil cover fraction (eqn. 22; AppCrpLAI).

Tillage events must be introduced into the TillageDates table. Column 1 contains the tillage date, column 2 contains the tillage depth. Please notice that the DelTimEvt switch operates on both the Applications and the TillageDates tables.

4.2.11 Section 7: Initial and boundary conditions

In this section, the initial and boundary conditions of PEARL must be specified.

Initial conditions

Both the mass content of pesticide in the equilibrium domain (CntSysEql) and the non-equilibrium domain of the soil system (CntSysNeq) should be specified in this section. The initial concentration is usually set to zero, i.e. the simulation starts with pesticide-free soil. Only in the case of previous pesticide applications, the initial pesticide concentration should be set unequal to zero. The intial mass content of metabolites cannot be specified.

Upper boundary condition

The upper boundary of the system is the crop canopy. This implies that pesticide entering the soil by deposition is always subject to dissipation at the crop canopy. Deposition fluxes should be specified in the FlmDep table. Deposition fluxes are linearly interpolated between two dates, so in the case of a constant deposition rate only two dates need to be specified (see the example). The user can also specify the concentration in irrigation water (ConIrr). If OptIrr is set to Sprlinkler (page 64), dissipation at the crop canopy will be calculated. Please notice that only one concentration can be specified, which applies to all irrigation events.

4.2.12 Section 8: Crop properties

This section contains the crop properties. PEARL uses a simple crop growth model, i.e. the relevant crop parameters have to be provided by the user as a function of development stage (see below). Notice that most identifiers in this section have been concatenated with crop names. In the example below, only one crop named 'Maize' is described.

Crop calendar

The crop section starts with the crop calendar. The user should first specify whether the calendar must apply to all years (option RepeatCrops). Secondly, the actual crop calendar must be provided (table Crops). The crop calendar consists of three columns: (i) emergence (*not* seeding) date of crop, (ii) harvest date of crop, and (iii) crop name. A single crop can occur several times in the crop table, but the following restrictions apply: (i) the length of the growing season must constant, and (ii) a crop is linked to a single development stage table (see below). If the user wants the crop to have different development stages over the years, a unique crop name must be specified for each year, e.g. Maize80, Maize81, etc. During periods that no crop is present, the model will use parameter values for bare soil.

Course of development stage with time

Dynamic crop properties, such as the Leaf Area Index and the rooting depth are input as a function of the development stage. The development stage is 0 at emergence, 0.5 at flowering (anthesis) and 1 at maturity (notice that in the original publication by Van Heemst (1986), the development stage is between 0 and 2.

The course of development stage with time can either be controlled by the temperature sum, or can be linear in time. One of these two options should be chosen with the switch OptLenCrp. If set to 'Fixed' (development stage linear with time) no additional parameters are required. If set to 'Variable', the user should specify the temperature sum at emergence (TemSumSta), the temperature sum from emergence to anthesis (TemSumEmgAnt), and the temperature sum from anthesis to maturity (TemSumAntMat). The advantage of this option is that regional differentiation of crop growth can be made on the basis air temperature.

Dynamic crop properties
The Leaf Area Index (LAI), crop factor (FacCrp), rooting depth (ZRoot) and crop height (HeightCrp) are input in table CrpPar. A maximum number of 36 rows can be entered in the table. One table must be provided for each crop considered.

Root density table
The user may define up to 11 data pairs to define the relative root density distribution as a function of the relative rooting depth (table RootDensity). Any unit can be used, the model will normalize the root density distribution in such a way that the integral of root density times depth over the root zone equals one.

Crop water use
The user must enter the pressure heads defining the root water extraction function (Figure 4). HLim1 is the anaerobiosis point, HLim2 is the reduction point at near-saturation, HLim3 is the reduction point at dry conditions, and HLim4 is the wilting point. If these values are available for *p*F values instead of pressure heads, they should be converted (i.e. $h = -10^{pF}$).

Light extinction and interception
PEARL needs the extinction coefficient of global solar radiation, κ, (eqn. 8). The interception coefficient (CofIntCrp) controls the amount of interception by the crop canopy (parameter *a* in eqn. 14). In case of ordinary agricultural crops, *a* may be set to 0.25. If set to zero, no interception will be calculated (in fact PEARL will substitute a very small value in the SWAP files to prevent division by zero). Please notice that at high precipitation rates, the interception rate asymptotically reaches *a*LAI.

4.2.13 Section 9: Control of daily output
In this section, the daily output is controlled. The following steps must be followed:
1. First specify whether the daily output file should be saved (OptDelOutput). If set to Yes, the daily output file will be removed. This option saves time if summary information is required only.
2. Specify the desired (fixed) output interval (record DelTimPrn). If set to zero, PEARL will calculate the output interval based on the begin and end date of the simulation. It is important to realize that PEARL generates *averages* over the print interval and *not point values*. This implies that a larger print interval generates a smoother picture (Figure 14).
3. Specify whether fluxes should be cumulated over the entire simulation period (PrintCumulatives).
4. Specify the desired format of the date (DateFormat) and the actual values in the output file (OutputFormat). The DateFormat can be set to DaysFromSta (print the number of days since the start of the simulation), DaysFrom1900 (print the number of days since 1-Jan-1900) or Years (print the number of years since the start of the simulation). To specify the output format, normal FORTRAN notation should be used (see the example in appendix 3).
5. Specify the depths for which output is requested (OutputDepths)

6. Specify for each variable whether output is wanted or not (print_)
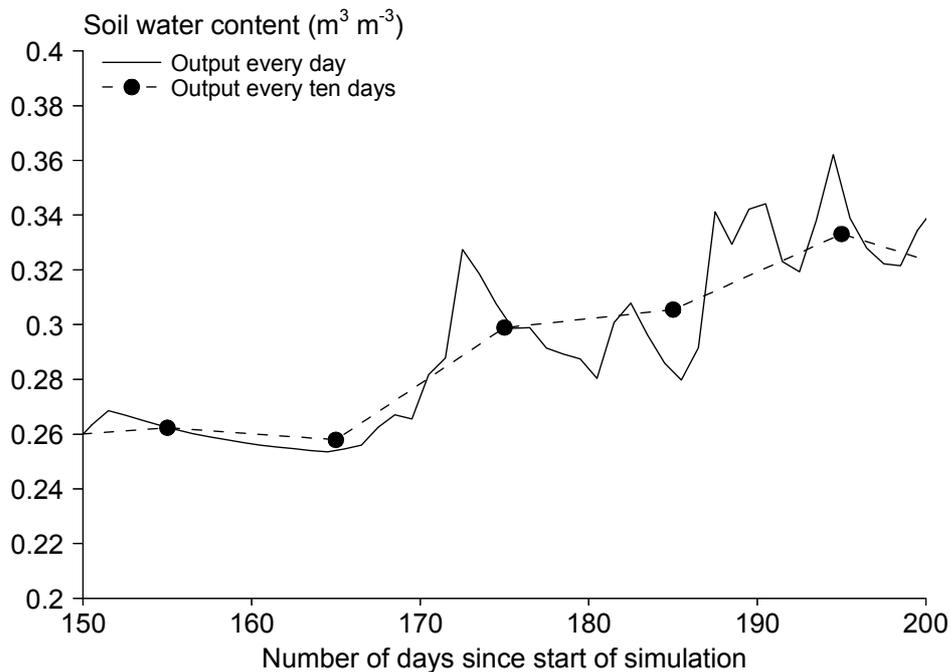
Figure 14 Example of the effect of the print interval on the generated model output.

Output of vertical profiles

The user can specify a number of dates at which vertical profiles of the most important state variables are produced (table (VerticalProfiles).

4.2.14 Description of the weather data file

PEARL uses daily weather data. These data must be specified in a file with extension .met (e.g. debilt.met). The datafile consists of 11 columns. Depending on the value of OptEvp (see page 63), one or more columns can be left blank. See Table 9.

Table 9 Contents of the weather data file

Column name	Required in the case of OptEvp =		
	Penman	Makkink	Input
Meteostation code. The Meteostation code must be the same as the code specified in the Meteostation record of the PEARL file (see page 63).	Yes	Yes	Yes
Day, between 1 and 31	Yes	Yes	Yes
Month, between 1 and 12	Yes	Yes	Yes
Year, between 1900 and 3000	Yes	Yes	Yes
Daily global radiation (kJ m^{-2} d^{-1}), between 0 and 5 10^6	Yes	Yes	No
Minimum daily temperature (^{o}C), between −50 and 35	Yes	Yes	Yes
Maximum daily temperature (^{o}C), between −30 and 60	Yes	Yes	Yes
Average vapor pressure (kPa), between 0 and 10	Yes	No	No
Average windspeed (m s^{-1}), between 0 and 50	Yes	No	No
Daily precipitation (mm d^{-1}), between 0 and 1000	Yes	Yes	Yes
Reference evapotranspiration (mm d^{-1}), between 0 and 100	No	No	Yes

If a column is left blank, -99.9 should be specified. The following example shows a part of the weather data file, with OptEvp is Input.

```
*************************************************************************
* File name: detbilt.met
* Meteo data for the Dutch standard scenario
*************************************************************************
* Station   DD MM YYYY      RAD    Tmin    Tmax     HUM     WIND    RAIN     ETref
*              nr nr   nr  kJ.m-2     C       C      kPa    m.s-1  mm.d-1  mm .d-1
 'debilt'    1  1 1980   -99.9      .9      .9   -99.9    -99.9     5.8      0.0
 'debilt'    2  1 1980   -99.9     -.4     -.4   -99.9    -99.9     0.6      0.0
 'debilt'    3  1 1980   -99.9    -2.3    -2.3   -99.9    -99.9     1.3      0.0
...
...
 'debilt'   30 12 1989   -99.9     7.7     7.7   -99.9    -99.9     0.0      0.2
 'debilt'   31 12 1989   -99.9     7.3     7.3   -99.9    -99.9     0.0      0.2
```

Figure 15 File debilt.met: Daily weather data

4.3   Description of the irrigation data file

Two types of irrigation can be specified in PEARL, i.e. sprinkler irrigation and surface irrigation. In the case of sprinkler irrigation, interception at the crop canopy will be calculated. The choice between both types of irrigation has to be specified in the OptIrr record of the PEARL input file (see page 64). The actual irrigation data must be specified in an irrigation event table, IrrTab. The concentration of pesticide in irrigation water can be specified in the ConIrr record of the PEARL file (see page 64).

```
* Example of an irrigation table
table   IrrTab   (mm)
12-Jul-1980   12.3
01-Aug-1980   17.1
03-Aug-1980   3.4
end_table
```

Figure 16 The irrigation datafile.

The first column of this table contains the date. Normal data-format can be used. The second column contains the irrigation depth (mm). Please notice that the irrigation table is repeated if the RepeatHydrology switch has been set to Yes. In this case, specification of the year is not required.

4.4   Description of the comprehensive output file

As described at page 70, the output is rather flexible. The print interval can be set (record DelTimPrn), a format for the date can be set (record DateFormat), output depths can be specified (table OutputDepths), and for each variable in the output list, a print flag can be set indicating whether a variable is to be printed (record print_).

Two types of output are written to the comprehensive output file:
1. Output as a function of time. This type of output is produced at regular intervals. This interval is controlled by the variable DelTimPrn (see page 70).
2. Output as a function of depth. This type of model output is produced only at the dates specified in the VerticalProfiles table (page 71).

All types of model outputs are written in records.

4.4.1   Output as a function of time

Time dependent model outputs are written in records with the following general format:

```
Time    Date    Identifier   Value(1)   …   Value(n)
```

where *n* is:
- one in the case of ordinary (depth independent) variables
- the number of depths specified in the OutputDepths table

The box below shows a part of the output file, which was produced with the following control settings:
1. DateFormat was set at DaysFromSta
2. RealFormat was set at g12.4
3. OutputDepths was set at 0.25 and 0.50 m. These depths are in the 0.225-0.250 m and 0.475-0.500 m layers with nodal points situated at 0.2375 m and 0.4875 m depth. These depths are listed in record Z, directly after the header.
4. Output was requested for the variables Tem, GrwLev, FlvLiqPrc, ConSys, ConSysEql, ConLiq and FlmLiq.

```
--------------------------------------------------------------------------------
######                                    ###
 ##  ##                                    ##
 ##  ##    #####    #####    ## ###        ##
 #####   ##    #        #    ### ##        ##
 ##      #######  ######    ##             ##
 ##         ##     #  ##    ##             ##
####       #####   #### ##  ####          ####  (c) RIVM/Alterra
Pesticide Emission Assessment for Regional and Local scales
--------------------------------------------------------------------------------
RIVM                    Alterra
PO BOX 1                PO BOX 47
3720 BA Bilthoven       6700 AA Wageningen
the Netherlands         the Netherlands
a.tiktak@rivm.nl        f.vandenberg@alterra.wag-ur.nl
--------------------------------------------------------------------------------
   0.000                          Z    0.2375      0.4875
… … …
 192.000 10-Jul-1980              Tem   14.3500     13.7900
 192.000 10-Jul-1980           GrwLev   0.2200E-01
 192.000 10-Jul-1980         FlvLiqPrc   0.1060E-01
 192.000 10-Jul-1980       ConSys_pest   0.8934E-07   0.1345E-19
 192.000 10-Jul-1980    ConSysEql_pest   0.8934E-07   0.1345E-19
 192.000 10-Jul-1980       ConLiq_pest   0.5202E-08   0.9874E-22
 192.000 10-Jul-1980       FlmLiq_pest  -0.1409E-09  -0.2740E-23
```

Figure 17 Example of comprehensive output file

4.4.2 Vertical profiles of some selected variables

Vertical profiles are produced only at times specified in the Events table. For each requested time and for each compound, a series of records is produced with the name Profile_pest (where pest must be substituted by the appropriate compound name). The following variables are output:

1. Volumetric soil water content, θ ($m^3\,m^{-3}$)
2. Soil water pressure head, h (m)
3. Soil temperature, T (^{o}C)
4. Concentration in the system, c^* ($kg\,m^{-3}$)
5. Concentration in the equilibrium domain of the soil system, c^*_{eq} ($kg\,m^{-3}$)
6. Concentration in the non-equilibrium domain of the soil system, c^*_{ne} ($kg\,m^{-3}$)
7. Concentration in the liquid phase of the soil system, c_L (($kg\,m^{-3}$)
8. Concentration in the gas phase of the soil system, c_g (($kg\,m^{-3}$)

4.4.3 Importing data in Excel

With the *SelRec* tool, records with the same identifier can be selected from the PEARL output file. *SelRec* is distributed as a part of the PEARL package. These records can be written to a new file, which can be imported in Excel. *SelRec* is called from the command line as follows:

```
SelRec Field_Number Identifier < Pearl_outputfile > SelRec_file
```

where Field_number is the field number with the identifier.

With the following command, for example, all records containing the identifier ConSys_pest are selected:

```
SelRec 3 ConSys_pest < defscen.out > defscen_consys.out
```

Here, defscen.out is the PEARL output file and defscen_consys.out the file with the selected records.

To import the file in Excel, use the following guidelines:
1. From the file menu, chose Open.
2. Select Text Files in the file type box (lower left corner). Type the file name in the file name box
3. In the following window, choose 'delimited'
4. Chose 'space' as delimiter
5. In the following box, you must specify the data format for each column. Column 2 must be set to date (type is DMY), the other columns must be set to general.
6. Then chose Finish.

4.5   Description of the summary output file

The summary output file has extension .sum (e.g. default.sum). It is used for the annual balances (section 4.5.1), FOCUS output (section 4.5.2) and target variables of the Dutch standard scenario (section 4.5.3).

4.5.1   Annual balances

An *annual* summary is written at December 31 of each year. The annual balances are written to records with the following fields:
1. The year
2. The identifier
3. The first data field
…
n. The last data field

The following records are written:
1. Water balance of the FOCUS target layer, with identifier 'BalWatFoc'. The thickness of the FOCUS target layer is controlled by the ZFoc variable in the general input file. Its default value is 1.0 m.
2. Water balance of the entire soil profile, with identifier 'BalWatSol'.
3. Mass balance of pesticide at the crop canopy with identifier 'BalCrp'
4. Mass balance of pesticide in the FOCUS target layer with identifier 'BalFoc'. The thickness of the FOCUS target layer is controlled by the ZFoc variable in the general input file. Its default value is 1.0 m.
5. Mass balance of pesticide in the tillage layer with identifier 'BalSol'.

Compound names are attached to identifiers 3-5, e.g. BalSol_pest.

Annual water balance

The water balance is output for two layers, i.e. the FOCUS target layer and the entire soil profile. Table 10 shows the term of the annual water balance.

Table 10 Terms of the annual water balance

Field	Water balance term	Unit	Acronym
1.	Net storage change of water in the soil profile	$m\ a^{-1}$	DelLiq
2.	Precipitation flux	$m\ a^{-1}$	Prc
3.	Irrigation flux	$m\ a^{-1}$	Irr
4.	Seepage flux at the lower boundary of the system	$m\ a^{-1}$	FlvLea
5.	Evaporation flux of intercepted water	$m\ a^{-1}$	EvpInt
6.	Actual soil evaporation flux	$m\ a^{-1}$	SolAct
7.	Actual transpiration flux	$m\ a^{-1}$	TrpAct
8.	Flux of lateral drainage to field drains and ditches	$m\ a^{-1}$	Dra
9.	Flux of water in run-off	$m\ a^{-1}$	Run
10.	Evaporation of ponded water	$m\ a^{-1}$	EvpPnd
11.	Potential soil soil evaporation flux	$m\ a^{-1}$	SolPot
12.	Actual transpiration flux	$m\ a^{-1}$	TrpPot

Annual mass balance of pesticide at the crop canopy
Table 11 shows the balance terms that are output.

Table 11 Terms of the mass balance of pesticide residing at the crop canopy

Field	Term of mass balance ($kg\ ha^{-1}\ a^{-1}$)	Acronym
1.	Areic mass of pesticide applied to the crop	AmaAppCrp
2.	Storage change of mass of pesticide at the crop canopy	DelAmaCrp
3.	Areic mass of pesticide deposited at the crop canopy	AmaDep
4.	Areic mass of pesticide dissipated at the canopy	AmaDsp
5.	Areic mass of pesticide wash-off	AmaWas
6.	Areic mass of pesticide harvested	AmaHar

Annual mass balance of compounds in the soil system
The mass balance is output for three layers, i.e. the tillage layer, the FOCUS target layer and the entire soil profile. Table 12 shows the balance terms that are output.

Table 12 Terms of the mass balance of compounds in the soil profile. This balance applies to three different layers, i.e. the tillage layer, the FOCUS target layer and the entire soil profile. See further text.

Field	Term of mass balance ($kg\ ha^{-1}\ a^{-1}$)	Acronym
1.	Areic mass of compound applied to the soil	AmaAppSol
2.	Areic mass change of compound in the layer	DelAma
3.	Areic mass change of compound in the equilibrium domain	DelAmaEql
4.	Areic mass change of compound in the non-equilibrium domain	DelAmaNeq
5.	Areic mass of compound transformed	AmaTra
6.	Areic mass of compound formed	AmaFor
7.	Areic mass of compound taken-up by plant roots	AmaUpt
8.	Areic mass of compound discharged laterally	AmaDra
9.	Areic mass of compound deposited	AmaDep
10.	Areic mass of compound volatized	AmaVol
11.	Areic mass of compound leached from the target layer	AmaLea

4.5.2 FOCUS output

FOCUS output is produced at the end of each FOCUS period. The length of the FOCUS period is determined by the variable DelTimEvt (see page 68). The FOCUS Soil Modeling Working Group (2000) has set the following guidelines:

−   The length of the FOCUS period is the same as the application interval, which is one year for annual applications, two years for biennial applications and three years for triennial applications.
−   The first period starts in year 7, so the first 6 years are used for 'warming-up'.
−   The total length of the simulation is 26 years in the case of an annual, 46 years in the case of a biennial and 66 years in the case of a triennial application.

FOCUS output is relevant for the so called FOCUS target layer. The thickness of this layer is set by the ZFoc variable in the general input file. Following the guidelines of the Soil Modeling Working group, its default value is 1.0 m.

4.5.3   Summary variables for the Dutch pesticide registration procedure

Variables that are relevant for the current Dutch pesticide registration procedure are:

−   The maximum average concentration of substance in the upper groundwater (μg L^{-1})
−   The time at which the maximum concentration occurs (d)
−   The areic mass of substance leached to the upper groundwater (kg ha^{-1})
−   The concentration of substance in the top 20 cm at 365 days after the first application, the so-called PEC365 (kg ha^{-1}).

The average concentration in the groundwater is calculated for the 1-2 m soil layer if the groundwater is at a depth less than 1 m and for the upper meter of the groundwater if the groundwater is at a depth greater than 1 m.

5   User's guide for the PEARL user interface

This chapter gives an overview of the PEARL user interface, which is an integrated environment for data storage and data retrieval, model control and viewing the output data (Figure 18). Basically, the user can access the system through the User Interface, which is available for Windows 95/98/NT. The User Interface is linked with a relational database for easy data access. The User Interface generates the input files for the PEARL model and calls the model. Summary outputs are transferred back to the PEARL database where they can be accessed. More comprehensive model outputs (particularly time-series) can be viewed with a separate graphical program, *XYWin*.
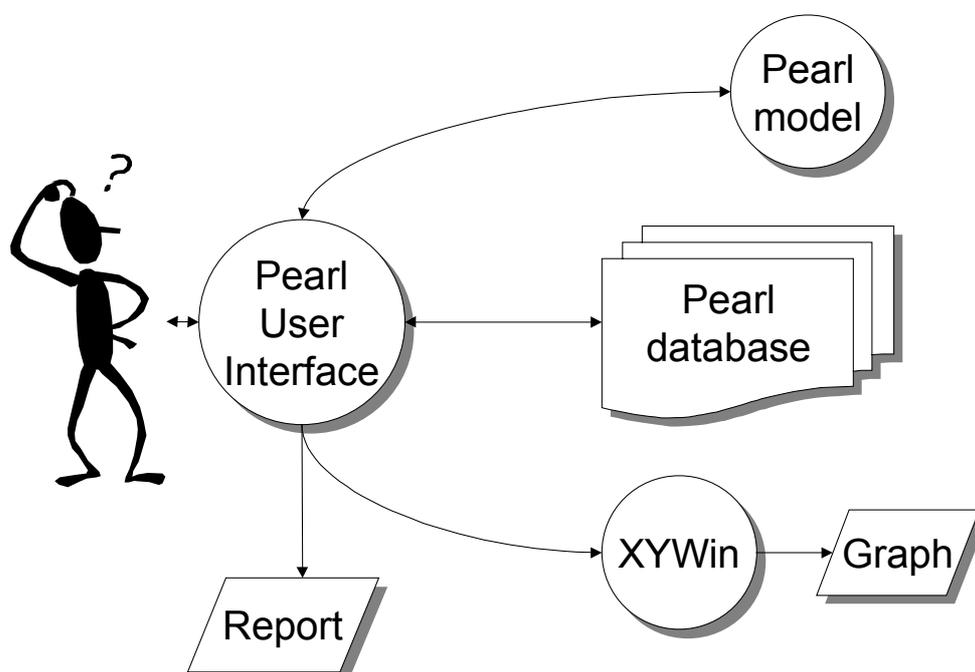

Figure 18 Overview of the PEARL modeling system

It is clear that this system is rather complex. With the PEARL User Interface you don't need to bother about all the relationships. The PEARL User Interface makes it easy to:
–   organize and edit your data in the PEARL database
–   import weather data in the PEARL database
–   access standard scenario's as suggested by the FOCUS modeling working group (2000)
–   select one or more model-runs for execution
–   actually perform one or several model runs
–   display summary reports containing annual water and mass balances, the maximum concentration in the groundwater, and the output suggested by the FOCUS modeling working group (FOCUS, 2000).

–   display model results graphically
–   import graphs in Word processor files, using Enhanced Windows metafile format (.emf).

5.1   Overview of the PEARL database

As described in chapter 3, during first-tier assessments the model will primarily be used in combination with *standardized* scenario's. Standardized scenario's have been developed for 9 locations and approximately 14 crops per location. Different scenario's have further been developed for annual, biennial and triennial applications (FOCUS modeling working group, 2000). Parameter values for these scenario's are distributed in combination with the PEARL model. The large number of scenario's and model inputs required for one model run leads to a considerable amount of data. It is clear that organization of all the data is important to (Vaughan and Corwin, 1994; Tiktak *et al.*, 1996): (i) establish a hierarchy, (ii) minimize data redundancy, and (iii) optimize the data accessibility. An efficient way of handling the data is to use some kind of relational database system. Because of it's widespread availability, we chose to use ACCESS 97 for storing the PEARL data. *This implies that Office 97 must be installed.*

Figure 19 shows the hierarchy within the PEARL database. The highest level of the database (level 1) is the project level. Here, the user can group several model runs, based on a common criterion (e.g. all model runs for one single field-study or all model runs for one single pesticide). The second level is the model-run level. Parameters needed to perform a model-run are
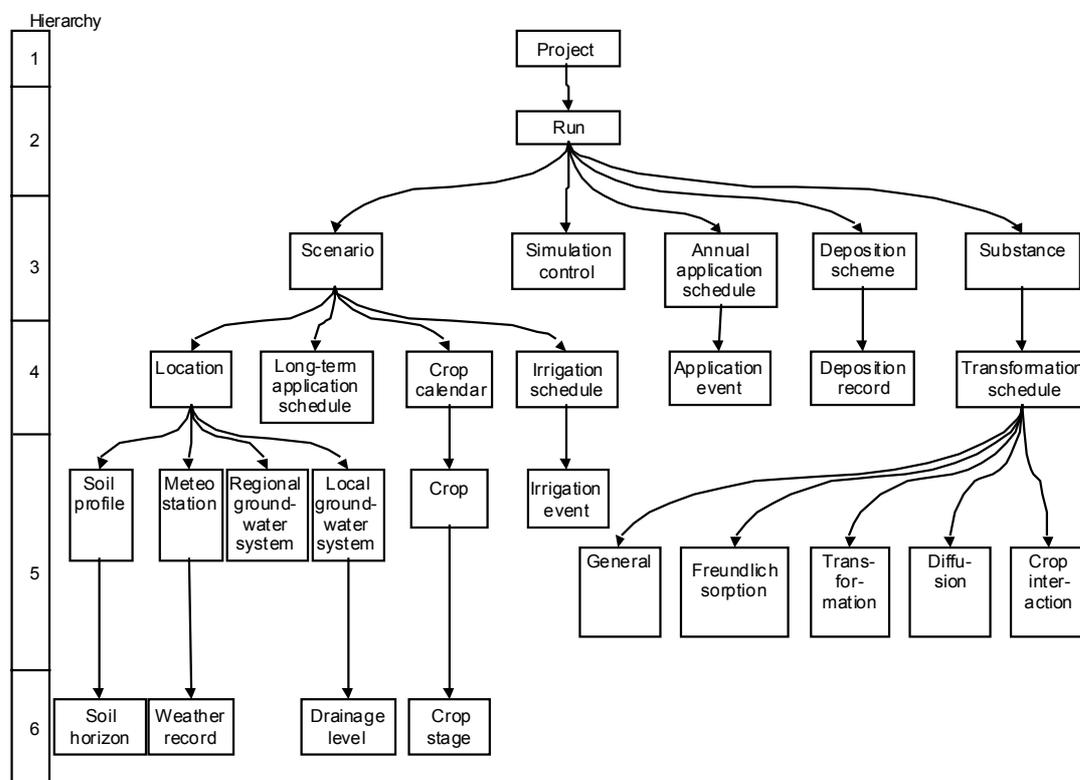

Figure 19 Overview of the PEARL database

scenario data, pesticide data, the annual application schedule and the model-controls, such as the begin and end time of the simulation. These three major building blocks of a model-run are stored at level 3.

The left hand side of the diagram shows the building blocks of the FOCUS scenario's. These are the parameters that one will usually find spatially distributed (see e.g. Vaughan and Corwin, 1994) and that will be used for building mega-plots or unique combinations in regional-scale assessments (Tiktak *et al.,*1996). Also parameter values referring to real locations (fields or lysimeters) can be entered through the scenario entry. Scenario's as defined by the FOCUS modeling working group are a combination of crop, location, the long-term application schedule (i.e. annual, biennial or triennial applications) and agronomic parameters (particularly irrigation data) to be used in the simulation. Parameters referring to a location can be further classified into soil parameters, weather data, parameters describing the regional groundwater system (i.e. the lower boundary of the hydrological model) and parameters describing the local groundwater system (i.e. water flow to ditches and field drains). Notice that in the PEARL context, the crop calendar does not relate to a location. Instead, it is one of the building blocks of a scenario, which is at a higher hierarchical level. As shown in the figure, the crop calendar relates to individual crops. The crop calendar may refer to one single crop (monoculture) or several crops. At the lowest hierarchical level are the basic data, relating to a single crop stage, a single soil horizon, etc.

The right hand side of the diagram contains the pesticide data, *not* including application schedules. The pesticide entry is only used to refer to the name of the compound that has been applied (the parent compound), the actual data are entered in the compound tables, which are at level 5. The pesticide entry relates to a transformation schedule, which gives the relationships between the individual compounds to be simulated (the relevant reaction products, including the parent compound). The compound table relates to tables containing general compounds properties, sorption parameters, diffusion parameters and crop interaction parameters.

The annual application schedule and pesticide deposition data are both pesticide and location dependent. This table relates to the table describing the individual application events, which contains information about such parameters as dosage, application mode, application date, etc. As the annual application schedule cannot be directly linked with the pesticide or location tables, they are directly linked with a model run (level 2). Notice that, contrary to the *annual* application schedule, the *long-term* application schedule (i.e. whether a pesticide is applied annually, biennially or triennially) is part of a scenario. The reason is that we follow the choices made by the FOCUS modeling working group (FOCUS, 2000).

All other parameters can accessed through the 'simulation and output control' entries. Here you will find parameters like start-time of the simulation, minimum time-step, output options, etc.

5.2   Getting started

First install the PEARL user interface. Now start the PEARL user interface (press the start button, followed by programs and PEARL. You will find out that the PEARL user interface is distributed in combination with a comprehensive help-file. The help-file will guide you on-line and contains information about:

* Parameter values including parameter constraints (minimum and maximum values)
* Guidance on model parameters
* Theoretical background

You can always access the help file by pressing F1 on your keyboard (or use the help button). The Help file has, however, a lot more possibilities. You can use the buttons on top of the help window to navigate more efficiently:

* Use the Contents button to get a table of contents.
* Use the Index to search a topic.
* Use the Back button to go to the previous topic.
* Use the Browse buttons of the help system (<< and >>) to browse through the help-file as if it where a printed book.
* Use the Print button to print a topic.
* Use the Get Start button to go to the Get Started topic
* Use the Support button to get information about support.
* Use the Cover page button to jump to the Cover page
* Use the Tree view button to display a tree of the PEARL user interface.
* Use the Theory button to enter the Theory section of the Help file.

Contents	Index	Back	Print	<<	>>	Get started	Support	Cover page	Tree view	Theory

We strongly recommend to read the *Introduction* and *Getting Started* sections of the Help file before proceeding. The Getting Started section gives information on the following three subjects:

* First-tier of the European registration procedure: Generating FOCUS runs
* First-tier of the Dutch registration procedure: Using the Dutch standard scenario
* The FOCUS wizard
* Using PEARL for higher-tier assessments

5.3   Generating FOCUS runs

PEARL supports the target quantities and scenarios set-up by the Forum for International Co-ordination of pesticide fate models and their Use, FOCUS). The model has a special FOCUS wizard, with which you can generate FOCUS runs. To generate FOCUS runs, follow the procedure in the Figure 20.
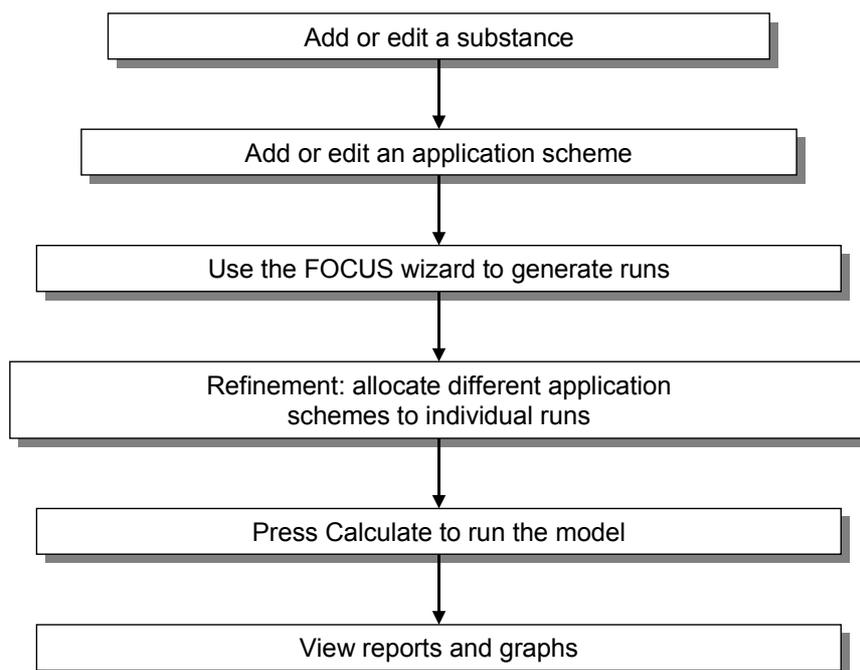
```
┌──────────────────────────────────────────┐
│         Add or edit a substance           │
└──────────────────────────────────────────┘
                    │
                    ▼
┌──────────────────────────────────────────┐
│     Add or edit an application scheme      │
└──────────────────────────────────────────┘
                    │
                    ▼
┌──────────────────────────────────────────┐
│     Use the FOCUS wizard to generate runs  │
└──────────────────────────────────────────┘
                    │
                    ▼
┌──────────────────────────────────────────┐
│   Refinement: allocate different application│
│        schemes to individual runs          │
└──────────────────────────────────────────┘
                    │
                    ▼
┌──────────────────────────────────────────┐
│      Press Calculate to run the model      │
└──────────────────────────────────────────┘
                    │
                    ▼
┌──────────────────────────────────────────┐
│          View reports and graphs           │
└──────────────────────────────────────────┘
```

Figure 20 Procedure for generating FOCUS runs

5.3.1   Create or edit a substance

To Create a new substance do the following:

1. Click the browse button to the right of the substance combo-box in the scenario tab of the main form to go to the Substance form.
2. Click + in the navigator.
3. Fill-in at least the following substance properties:
    3.1. In the General tab, specify a unique code, a name, the molar mass, the saturated vapour pressure and the solubility in water.
    3.2. In the Freundlich tab, specify the coefficient for sorption on organic matter.
    3.3. In the Transformation tab, specify the substance half-life.
4. Click Close when done to return to the main form.

5.3.2   Create or edit one or more application scheme(s)

To Create a new application scheme do the following:

1. Click the browse button to the right of the application schemes combo-box in the scenario tab to go to the Applications form
2. Click + on the navigator in the application schemes box (left-hand side of form)
3. Fill-in a code and a name
4. Click + on the navigator to add an application in the applications box (right-hand side of form)
5. Fill-in the application date, the dosage and application type. It is possible to enter an application date relevative to the emergence date (e.g. 10 days before crop emergence).

6. You can make clones of an existing scheme with the Copy button. This is particularly handy if you want to change the application date only.

7. Click Close when done to return to the main form

5.3.3 Run the FOCUS wizard

Press the FOCUS wizard button to generate one or more standard runs

1. Select one or more crop types and press Next

2. Select one or more locations and press Next

3. Select a substance, an application scheme and a long-term application scheme (repeat interval of application, which can be 1, 2 or 3 years).

4. Note that you can only select one application scheme and one substance for all runs. This can be refined in the next step.

5. Press Finish to go back to the main form. The wizard will ask where to store the new model runs.

5.3.4 Refinement

PEARL has now generated a FOCUS project. You will see that all runs in the project have been selected for execution.

1. You can now choose different application schemes for each individual run. Use the application schemes combo-box for this purpose. When, however, you have specified the application date relative to the crop emergence data, it is often not necessary to specify different application dates.

2. If you want to create user-defined graphs, check 'Detailed Output' in the Output Control tab.

3. You can switch runs on and off by double clicking.

5.3.5 Running PEARL

Press the Calculate button to actually run the model.

1. All selected runs will be carried out.

2. The PEARL User Interface will write the input files and call the simulation kernel.

3. You can follow the course of the simulation.

When all runs are completed, you will see the status bar changing to 'Results there'

1. If errors are encountered, you will see that the Reports and Graphs buttons are disabled.

2. Errors can be reviewed in the Run Status tab of the main form.

5.3.6 Viewing the Results

Press the Reports button to view the summary report. This report contains, amongst others:

1. the water and substance balances.

2. the 80th percentile of the leaching concentration.

Press the Graphs, predefined button to view graphs of

1. The water and substance balances

2. The FOCUS summary

5.4 General properties of the PEARL user interface

All forms of the PEARL user interface have a similar set-up, which will be explained in this chapter. The locations forms will be taken as an example. As you can see, the form consists of two parts: (i) a browse box, and (ii) an edit box.

The browse box

The browse box allows you to scroll through the records of a table (in this case locations). You will notice that the information in the edit box changes when scrolling. All browse boxes are complemented with a navigator:

⏮	Go to the first record in the table
⏭	Go to the last record in the table
+	Add a new (empty) record
−	Delete a record
✓	Confirm changes ('post edit')
✗	Cancel changes
Copy	(not always available): Copy a record

The edit box

In this part of the form you can edit the record which you have selected in the browse box. The PEARL user interface has three categories of data fields:

− ordinary data fields, where you enter a text string, a date string or numerical data. The PEARL user interface will perform range checking after you have entered data.

- option fields or pick lists, where you can make a choice between a number of options. The button to the right of a pick list allows you to edit the underlying tables (i.e. go to a lower hierarchical level).
- check boxes, where you can switch variables on or off.

Most forms are complemented with a comments button, which allows you to add additional information or meta-data.

5.5   The projects form

The projects form can be accessed from the main form (see section 5.6). The projects form allows you to organize your data. Existing projects can be selected in the browse box. The navigator allows you to create or delete projects (see section 5.4). An appropriate description can be added in the edit part. Here, you can also make a choice between one of the two different types of projects that the PEARL user interface has available:

- Fixed substance projects: One substance is used throughout the project. The button to the right of the pick list allows you to create or edit a substance before attaching it to a project.
- Free substance projects: Substances are attached to individual model runs instead of to projects.

5.6   The main form

This form is the central point from where you can access the different tables of the database, run the model and produce graphs from PEARL output. Most of the steps described in section 5.2 will be performed from this screen. You can use buttons, the main menu or shortcut keys to navigate through the user interface.
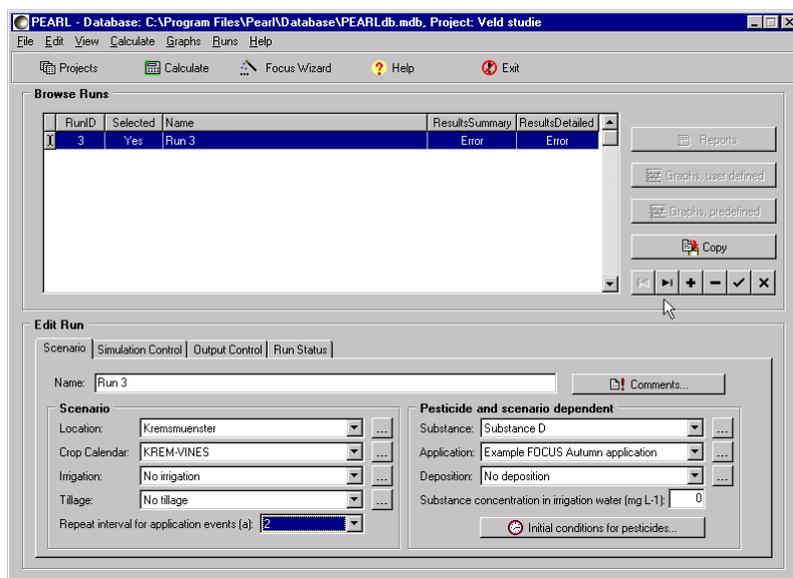

Figure 21 The main form of the PEARL user interface

5.6.1 The main menu

The main menu can be used for quick access to various parts of the PEARL user interface:

− Use File-Exit (ALT-F-X) to quit the application.
− Use the Edit menu (ALT-E) to directly access a table in the database. As an example, use Edit-Substances or ALT-E-S to jump to the substances form.
− Use the View menu (ALT-V) to view the PEARL input and output files.
− Use the Calculate menu (ALT-C) to execute selected runs.
− Use the Graph menu (ALT-G) to jump to the graphs section.
− Use the Help menu (ALT-H) to access the help file.

5.6.2 The tabs of the main form

The main form consists of four tabs, i.e. a scenario tab, a simulation control tab, an output control tab, and a run status tab. The output tab will be described in section 5.12, the control tab in section 5.13.

Edit scenario tab

In this tab, the user has to select the major building blocks of a scenario, i.e. the location, the crop calendar, the irrigation scheme, the (parent) pesticide (substance), the application scheme and the deposition table. The application scheme gives access to tables of application dates. Also the repeat interval of applications (in years) must be specified (DelTimEvt). If set to 2, for example, biennial applications are simulated. If set to NoRepeat, the application table will not be repeated. The initial conditions of pesticide in the equilibrium domain (ConSysEql) and the non-equilibrium domain of the soil system (ConSysNeq) can be specified in the initial conditions form, which is accessible by pressing the 'initial conditions button'.

Notice that you can only chose from *exisitng* building blocks. It may be necessary to add or create new crops, locations, etc. before proceeding. In this case, you can use the button to the right of the pick lists to go to a lower hierarchical level. You can also use the Edit menu of the main menu or use key shortcuts (e.g. ALT-E-C to go directly to the crop calendar).

Simulation control tab

This section contains general options for the simulation run. The time-domain for the simulation is specified in the Start and Stop date fields (TimStart[1] and TimEnd). The date-format specified at page 57 can be used. Please notice that the time-domain is fixed if a FOCUS scenario has been selected. According to guidelines of the FOCUS soil modeling Working group (1997), a FOCUS simulation should start at 1-Jan-1901. The length of the run should be 26 years in the case of annual applications, 46 years in the case of biennial applications and 66 years in the case of triennial applications.

---

[1] Underlined names refer to the variable name in the PEARL input file. You can use the index for easy access to the description of a parameter in the input file.

The simulations may start earlier if the Additional Stop Criterion field has been set unequal to zero (AmaSysEnd). In this case, the simulation will stop if the areic mass of pesticide in the soil system has become less than this criterion.

The minimum and maximum time-steps in the hydrological model SWAP (DelTimSwaMin and DelTimSwaMax). These variables determine the minimum and maximum time-steps in the SWAP model. The model will look for the optimal time step between the preset limits. Making the time-step too large could lead to instability, while making it too small will increase the computation time substantially. The tolerance of the iteration procedure (ThetaTol) defines the accuracy of the simulations. Choosing it too large could introduce a numerical water balance error. The initial groundwater level (GrwLevIni) is also specified in this tab, because it is dependent on the start time of the simulation.

With the hydrology option (OptHyd) you can determine how SWAP is run. The following options are available:

- Run SWAP if there is no existing SWAP output. This option saves computation time.
- Creates input for SWAP only.
- Assumes that SWAP has already been run; a pfo file must be provided.
- Runs SWAP and then PEARL. SWAP will always be run.
- Runs SWAP only (output in PEARL format). This option is interesting when testing or calibrating the hydrological model, without (yet) running the pesticide part.

If the Repeat weather and Irrigation box (RepeatHydrology) is checked, weather and irrigation data of the first year in the weather and irrigation tables will be constantly repeated. *The user should be careful in this using this option, in fact it is meant for the Dutch standard scenario only.*

5.7   Editing locations

From the locations form the user can access data that are usually considered spatially distributed, such as soil data, weather data and information about the local and regional groundwater system. Exceptions are the crop calendar and the irrigation schedules, which are at higher hierarchical levels according to definitions by the Focus Soil Modeling Working group (1997).

5.7.1   The locations form

In the locations form the user will find general information on the site, such as the name and the altitude. The locations form can be accessed from the scenario tab of the main form, but you can also use the edit menu of the main form.

In the locations form the user has to select a soil type and a weather station. Please notice that it may be necessary to create a new soil type and weather station before you can select one. In this case, you have to enter the Soil and MeteoStation forms before proceeding.

An option for the lower boundary condition of the hydrological model must be selected in the Lower Boundary Condition pick list (OptLbo). As described in section 2.3, SWAP offers eight options for the lower boundary condition; parameter values must be introduced in the lower boundary conditions form. A local drainage flux can be defined in addition to the regional seepage flux. The user must first specify whether local drainage has to be simulated by checking the Calculate Lateral Drainage checkbox (OptDra). Parameter values should then be entered in the drainage levels screen (press the drainage levels button for access). See further section 5.7.5.

Figure 22 The Locations form

In the locations form itself, the user must specify a unique code for the location, the location name and the country name. The altitude (Alt), longitude and latitude (Lat) are also required. Positive numbers refer to locations in the Eastern and Northern Hemispheres, respectively. The long-term average soil temperature (^{o}C), which is used to initialize the soil heat flux submodel must also be specified here. The user must further specify the maximum ponding layer depth (ZPndMax), which determines the maximum thickness of the water layer that can be present on the soil profile before surface runoff starts. The thickness of the air boundary layer must be specified in the ThiAirBouLay record. This parameter is relevant in the calculation of surface volatilization of pesticides.

5.7.2 The soil form

The soil form consists of two parts. The upper half of the form (Edit Soil profile) contains parameters that apply to the soil as a whole, in the lower half (Edit Horizon in Soil) you can introduce properties of individual soil horizons.

Edit Soil subform

In this part of the soil form, the user must specify parameters that apply to the soil profile as a whole. First, specify a *unique* code and a name for the soil profile.

Figure 23 The Soil profiles form

In the relative diffusion pick list, the user must chose one of the functions that PEARL has available for the calculation of the relative diffusion coefficient (OptCofDifRel). Three functions can be used, i.e. the functions published by Millington and Quirk (eqn. 32), Currie (eqn. 33), and Troeh *et al.* (eqn. 34). The actual parameters of these functions must be introduced in the 'relative diffusion function', which is accessible with the button to the right of the relative diffusion pick list. See page 62 for more information and page 48 for a discussion on parameterization of the relative diffusion function.

The actual soil evaporation rate is calculated using hydraulic properties and an empirical reduction function (eqn. 13). Parameter β of the Boesten relationship must be provided in the CofRedEvp field. See section 3.1.4 for parameter values. The potential evaporation calculated by eqn. 8 can be corrected by a factor FacEvpSol. This is particularly important in the case of a small soil cover fraction, because eqn. 8 has been derived for situations where the canopy shades the ground. FacEvpSol can be given a value between 0.5 and 1.5.

If the bulk-density is unknown, it can be calculated by the model. In this case, the bulk-density option (OptRho) should be set to calculate. See page 62 for details on the pedo-transfer function which is then used. If observed values are available, the bulk density can be introduced by the user.

The edit soil horizon subform
In this form you have to specify the vertical discretization of the soil profile (i.e. the Soil-Profile table). Soil horizons can be added by using the + button of the navigator.

The user must specify the thickness of each soil horizon and the number of compartments used in the finite-difference scheme (see Figure 3). For each horizon, the user must also specify a soil building block, which contains information on basic soil properties and hydraulic properties (section 5.7.3). If you do not yet have an appropriate soil building block available, enter the soil building blocks form before editing the soil profile. The maximum number of soil horizons is currently set to 10, the maximum number of numerical soil compartments is set to 500. The number of soil compartments is a compromise between accuracy and computation time. Computation time increases approximately with the square of the number of soil layers. On the other hand, predictions may become inaccurate if the layer thickness is taken too large. This is particularly true if the expected concentration in the groundwater is lower than 0.001 μg L^{-1} (Leistra et al., 2000). For most simulations, a layer-thickness of 2.5 cm in the top 30 cm, 5 cm in the 0.3-1 m soil layer and 10 cm in the layer below 1 m is fair compromise.

The dispersion length, $L_{dis,L}$ (eqn. 30) (LenDisLiq) is entered directly in the soils screen (and not in the soil horizon screen), because it is considered a soil property that is not coupled to generic soil horizons. Please notice that the distance between the nodal points, Δz, should be small enough to meet the Peclet condition (eqn. 2). Some information about the dispersion length is given at page 47).

Factors for the effect of depth on transformation (FacZTra) and sorption (FacZSor) are also specified in the soil screen. See section 3.2.9 for further information on transformation parameters. The factor for the effect of depth on sorption is only relevant if the option for the calculation of Freundlich equilibrium sorption in the substance screen is set to CofFre (see section 5.9.1). This factor must be one in the top-soil.

5.7.3   The soil building blocks form
For each soil building block, the basic soil properties (SoilProperties) and soil physical parameters have to be specified.

In the upper part of the form, the textural distribution (FraSand, FraSilt and FraClay), the mass content of organic matter (CntOm), the pH and the bulk-density (Rho) have to be speci-

fied. Notice that the textural distribution refers to the mineral soil only, so the sum of the sand, silt and clay fractions should be one. The mass content of organic matter refers to dry soil. The pH is used for the sorption model of weak acids. As most sorption experiments are being carried out in 0.01 M CaCl$_2$, the pH-CaCl$_2$ is preferred. If the pH-CaCl$_2$ is not available, the user should set the pHCorrection variable in the substance screen unequal to zero (page 99). The bulk density is only required if the option for the calculation of the bulk density in the soils screen (see page 91) was set to Input.

Figure 24 Soil building blocks

In the lower half of the form, you have to introduce the parameters of the Mualem-Van Genuchten functions (eqn. 4 and 5). You have to introduce θ_s (ThetaSat), θ_r (ThetaRes), α (Alpha), n (n), K_s (KSat) and λ (l). See section 3.1.1 for suggestions on parameterization.

5.7.4 The meteo form

In the meteo form, you have to specify information about the weather station. First, you must specify a *unique* code for the weather station (MeteoStation). Please notice that this code may not exceed eight characters. The altitude (Alt), longitude and latitude (Lat) are also required.

The potential evapotranspiration can be obtained in different ways (section 2.3.2). You must specify one of the available methods in the evaporation options field (OptEvp). Three options are available: (i) the potential evapotranspiration is input by the model, (ii) the Penman-Monteith equation is used, and (iii) the Makkink equation is used. If Penman-Monteith is selected, solar radiation, minimum and maximum air temperature, air humidity, wind speed and precipitation are required. If Makkink is selected, only minimum and maximum air temperature, solar radiation and precipitation are necessary.

You can import and export weather data from an ASCII file. The name of this file is the same as the name of the MeteoStation code with the extension .met. If, for example, the name of the meteostation is THIVA-M, the file name would be THIVA-M.met. The format of the file with weather data is described in section 4.2.14.
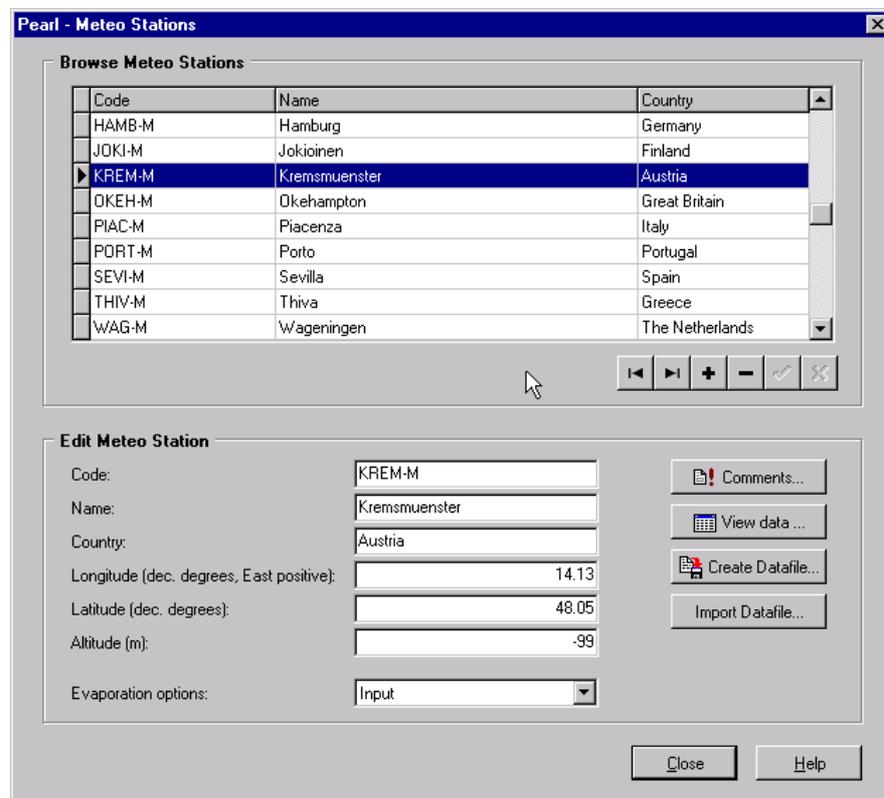
Figure 25 Meteo stations

5.7.5 Boundary conditions of the hydrological model

SWAP makes a distinction between the seepage flux due to regional groundwater flow and the local drainage flux to ditches and field drains (see Figure 5). The seepage flux due to regional groundwater flow is the lower boundary condition of the model, and must be defined in the lower boundary conditons form, the local drainage flux is considered a sink term and must be defined in the drainage levels form.

The lower boundary conditions form

In this section, the lower boundary conditions of the hydrological model are specified.

As described in section 2.3, SWAP offers eight options for the lower boundary condition, which must be specified in the locations form. Most options require additional input, which must be specified in the lower boundary conditions form. Depending on the option chosen, you will see one of eight tabs. The other tabs may be filled, but are not used.

If the lower boundary condition is set to 'time dependent groundwater level', the groundwater level must be specified as a function of time (table GrwLev). Normal data-format can be used.

If the lower boundary condition is set to 'flux boundary condition', a sine function is applied to generate the daily regional bottom flux. The user should specify the mean (FlvLiqLboAvg) and amplitude (FlvLiqLboAmp) of the annual bottom flux. Also the date at which the maximum of the sine wave occurs should be given (DayFlvLiqLboMax). Notice that negative values denote downward fluxes and positive fluxes denote upward values.

If the lower boundary condition is set to 'flux from deep aquifer', the regional bottom flux is calculated using the head difference between the phreatic groundwater and the groundwater in the semi-confining aquifer (see Figure 5 and eqn.15). The average groundwater level in the field, Φ_{avg}, is affected by the drainage base (HeaDraBase) and by the shape of the groundwater table (OptShapeGrwLev), which can be Elliptic, Parabolic, Sinusoidal or NoDrains. The daily value of the hydraulic head in the semi-confining aquifer, Φ_{aqf} is described by a sine-wave. The user must specify its annual average value (HeaAqfAvg), the amplitude (HeaAqfAmp) and the date at which the maximum hydraulic head occurs (TimHeaAqfMax). The bottom flux (eqn.15) is also affected by the vertical resistance of the aquitard (RstAqt, γ_{aqt}).

If the lower boundary condition is set to 'groundwater-level-drainage relationship', the bottom flux is calculated as a function of the groundwater level (eqn. 17). If this option is chosen, the model needs the coefficient (CofFncGrwLev) and the exponent (ExpFncGrwLev). Please realize that this option is only valid for deep, sandy areas. The calculated bottom flux includes local drainage to surface waters and drains, so local drainage should be set to zero if this option is used.

If the lower boundary condition is set to pressure head boundary condition, the pressure head at the lower boundary should be specified as a function of time (table h). Normal data-format can be used.

The FreeDrain, Lysimeter and ZeroFlux options do not require additional input.

The drainage levels form
If the lower boundary condition of the hydrological model is set to 'groundwater level as a function of time', 'flux boundary condition', 'flux from deep aquifer', 'pressure head boundary condition', or 'zero flux', a local drainage flux can be defined in addition to the regional seepage flux. First check the 'calculate local drainage' box, then enter the 'drainage levels screen'. Use the + sign of the navigator to add drainage levels. Up to five local drainage level systems can be specified.

For each local drainage system, a drainage flux is calculated according to eqn. 18. The model needs information about the bottom of the drainage system (ZDra) and the drainage resistance (RstDra) . The procedure that distributes the drainage flux over the individual soil layers additionally requires information about the drainage type (DraTyp) and the distance between the drainage systems (DistDra). You should also specify whether the local drainage system is a field-drain or an open channel.

5.8 Editing crop calendars

From the crop calendar form you can access the crop rotation, parameter values for individual crops and crop stages. The crop calendar is accessed directly from the scenario screen, because it is one of the main building blocks of a FOCUS scenario (Focus Soil Modeling Working group, 1997). PEARL uses a simple crop growth model, i.e. relevant crop parameters such as the Leaf Area Index and rooting depth have to be provided as a function of development stage (see below).

5.8.1 The crop calendar form
The definition of the crop calendar (table Crops) starts in the crop calendar form, which is accessible from the scenario tab of the main form. The crop calendar should be given a unique code and a name. *It is very important that you specify whether the same crop calendar must apply to all years (option RepeatCrops) or that separate crop calendars are used for individual years.*

Figure 26 The crop calendars form

The course of development stage with time can be controlled by the temperature sum, or can be linear with time. One of these two options must be chosen in the Crop cycle pick list (option OptLenCrp), where they are called Variable and Fixed, respectively. The advantage of defining the crop development stage dependent on temperature sum is that regional differentiation of crop growth can be made on the basis of air temperature.

Crops can be added to the crop calendar in the browse crops section. Use the + button of the navigator for this purpose. It may be necessary to add a new crop before proceeding. In this case, first go to the crops screen. The emergence (*not* seeding) date and the harvest date are defined directly in the crop calendar page, all other crop parameters are entered in the crop page. Please notice that a single crop can occur several times in the crop calendar, but a single crop is linked to one crop development stage table (see below). If the user wants the crop to have different development stages over the years, a unique crop name must be specified for each year, e.g. Maize80, Maize81, etc. During periods that no crop is present, the model will use parameter values for bare soil.

5.8.2 The crop and development stage form

In the crop form, all time-independent crop properties are input. Dynamic crop properties are input in the crop stages form.

Figure 27 The crops form

Crop water use
The user must enter the pressure heads defining the root water extraction function (Figure 4). HLim1 is the anaerobiosis point, HLim2 is the reduction point at near-saturation, HLim3U is the reduction point at dry conditions and at low evaporative demand, HLim3L is the reduction point at dry conditions and at high evaporative demand, and HLim4 is the wilting point. If these values are available for pF values instead of pressure heads, they should be converted accoridng to the $h = -10^{pF}$. See section 3.1.3 for parameter values.

If the Penman-Monteith equation is used for the calculation of potential evapotranspiration, SWAP additionally requires the minimum canopy resistance. The minimum canopy resistance ranges from 30 s m^{-1} for arable crops to 150 s m^{-1} for trees in forests. See Allen *et al.* (1989) for parameter values.

Light extinction and interception
PEARL needs the extinction coefficient of global solar radiation, κ, (eqn. 8). Parameter values for some common crops can be found in section 3.1.2. The interception coefficient (CofIntCrp) controls the amount of interception by the crop canopy (parameter *a* in eqn. 14). In case of ordinary agricultural crops, *a* may be set to 0.25 (section 3.1.4). If set to zero, no interception will be calculated (in fact PEARL will substitute a very small value in the SWAP files to prevent division by zero). Please notice that at high precipitation rates, the interception rate asymptotically reaches *a*LAI.

Relative root density distribution
The root density is specified in the relative root density form (press the relative root density button). The user may define up to 11 data pairs to define the relative root density distribution as a function of the relative rooting depth (table RootDensity). Any unit can be used, the model will normalize the root density distribution in such a way that the integral of root density times depth over the root zone equals one.

Temperature sums
If the course of development stage was set to 'Variable', the user must specify the temperature sum at emergence (TemSumSta), the temperature sum from emergence to anthesis (TemSumEmgAnt), and the temperature sum from anthesis to maturity (TemSumAntMat).

Dynamic crop properties
Dynamic crop properties are input in the crop stages screen, which is accessible through the stages button. These properties are input as a function of the development stage. The development stage is 0 at emergence, 0.5 at flowering (anthesis) and 1 at maturity (notice that in the original publication by Van Heemst (1986), the development stage is between 0 and 2. Use the + button of the navigator to add development stages. A maximum number of 36 development stages is allowed for each crop. The development stage is zero at emergence and one at time of harvest.

For each developments stage, the user has to specify the Leaf Area Index (LAI) and the rooting depth (ZRoot). If the potential evapotranspiration is calculated according to the Makkink equation, an empirical crop factors must be introduced (FacCrp). If the potential evapotranspiration is calculated according to Penman-Monteith, the crop height must be specified (HeightCrp).

5.9   Editing substances

The substances form is accessible from the scenario tab of the main form. PEARL can simulate the fate of a parent pesticide and its formation products (metabolites) in soil (see section 3.2.1). This implies that both the properties of the individual compounds, and the transformation scheme have to be parameterized. Both are accessible from the pesticides form. Input must be carried out in the following order:
−   definition of the properties of the individual compounds.
−   definition of the transformation scheme. This step can be ignored if only one compound is simulated.

At least one compound, viz. the parent compound, must be introduced. This compound will be applied, deposited, etc. The user can make a compound a parent compound by checking the 'parent' check box in the general tab of the substances screen (see next section).

5.9.1   Editing individual compounds
The substances form consists of five tabs. These tabs are described below.

Figure 28 The substances form

General tab

In this tab, the user enters the general compound properties. A *unique* code and the compound name must be introduced into the code and name fields. The maximum length of the code is five alphanumerical characters. The following parameter to be introduced is the molar mass. Data on molecular masses of compounds are reported in Tomlin (1994). PEARL then needs the saturated vapor pressure (PreVapRef), the temperature at which this parameter is determined (TemRefVap), the molar enthalpy of vaporization MolEntVap, the solubility of pesticide (SlbWatRef), the temperature at which the water solubility is obtained (TemRefSlb) and the molar enthalpy of dissolution (MolEntSlb). These properties can be taken from a handbook on chemical properties of pesticides (e.g. Tomlin, 1994, Hornsby *et al.*, 1996). See section 3.2.8 for further guidance.

Freundlich sorption tab

The sorption of compounds is described with a Freundlich equation (eqn. 41). See section 3.2.6 for guidance and backgrounds. The Freundlich tab consists of three parts:
−   The first part contains parameters describing the Freundlich coefficient
−   The second part contains the reference concentration and the Freundlich exponent
−   The third part deals with non-equilibrium sorption.

In the first part of the Freundlich tab, the user must make a choice between one of the three options that PEARL has available to calculate the Freundlich coefficient (OptCofFre). The most common approach (OptCofFre is 'Kom, pH-independent') is to calculate the Freundlich coefficient from the organic matter content and the coefficient for sorption on organic matter (eqn. 42). If OptCofFre is set to 'Kom, pH-dependent', the Freundlich coefficient is calculated with eqn. 43. This equation applies to the sorption of weak-acids. In cases that the sorption of pesticides is dependent on other soil properties than the organic matter content (e.g. oxide content or clay content), the Freundlich coefficient can be introduced directly (eqn. 44). In these cases, OptCofFre should be set to 'Kf, user defined'. If OptCofFre is set to 'Kom, pH-independent', only one additional parameter has to be introduced, i.e. the coefficient for sorption on organic matter, $K_{om,eq}$ (KomEql).
If OptCofFre is set to 'Kom, pH-dependent', two coefficients for sorption on organic matter must be specified (section 3.2.6), i.e. KomEqlAcid ($K_{om,eq,ac}$) and KomEqlBase ($K_{om,eq,ba}$). In addition, the negative logarithm of the dissociation constant (pKa) and a pHCorrection are required.

If OptCofFre is set to 'Kf, user defined', the user should specify the Freundlich coefficient measured in the top-soil (CofFre) and the factor to describe the depth dependence of sorption (FacZSor). It is assumed that the depth dependence of sorption is a soil property, which must be introduced into the soil form (page 91). The factor to describe the depth dependence of sorption should be 1 in the top-soil.

The second part of the Freundlich tab contains two parameters. The reference concentration in the liquid phase (ConLiqRef) must be within the concentration range of the simulation study. Its default value is 1 mg L^{-1}. The Freundlich sorption exponent, n (ExpFre) is also required.

Figure 29 The Freundlich tab of the substances menu

Non-equilibrium sorption is described with equation (45). This equation requires two additional parameters, i.e. the desorption rate coefficient, k_d, and the factor describing the ratio $K_{F,ne}/K_{F,eq}$, where $K_{F,ne}$ is the Freundlich coefficient at the non-equilibrium site and $K_{Fe,eq}$ is the Freundlich coefficient at the equilibrium site (FacSorNeqEql).

The desorption rate coefficient should be specified in the CofRatDes record. Please notice that non-equilibrium sorption will not be simulated if CofRatDes is set equal to zero. See further section 3.2.7.

The transformation tab

In this tab, the user has to specify parameters that affect the transformation rate of the compound. The transformation half-life time must be input in the half-life field (DT50Ref). The temperature reflecting the experimental conditions during the incubation study (TemRefTra) must also explicitly be introduced. The user must further specify whether the incubation experiment has been carried out under optimum moisture conditions (OptCntLiqTra). As shown in eqn. 57, optimum moisture conditions are conditions wetter than field capacity (i.e. wetter than pF 2). If the incubation experiments have been carried out at moisture contents dryer than field capacity (i.e. dryer than pF 2), the optimum conditions checkbox must *not* be marked, and the user must additionally specify the moisture content during incubation (CntLiqTraRef). The temperature dependence of transformation is described with eqn. 56; the molar activation energy must be given (MolEntTra). The effect of soil water on the rate coefficient is described with eqn. 57, this equation requires an exponent (ExpLiqTra). The effect of depth on transformation rate is assumed to be a soil property and must be introduced

in the soils form (FacZTra, page 91). See section 3.2.9 for further information on transformation parameters.

The diffusion tab
The diffusion coefficients of pesticides in pure water (CofDifWatRef) and air (CofDifAirRef) are compound properties and must be specified in the diffusion tab. Parameters for the relative diffusion coefficient are specified in the soil form (see page 90). The diffusion coefficients are temperature dependent. The user can specify one reference temperature, which applies to both the diffusion coefficient in air and the diffusion coefficient in pure water (TemRefDif).

The crop tab
PEARL has modules to simulate canopy processes and root uptake. Both modules have to be parameterized in this tab.

As the transformation scheme (Figure 7) applies to products formed in soil, the canopy processes module considers the parent compound only. Processes that occur at the plant canopy are volatilization, penetration into the plant and (photochemical) transformation (page 28). These processes are described with first-order rate reactions. The user can make a choice between a lumped description of the processes at the crop canopy, or a full description of dissipation (canopy processes combo box; OptDspCrp). If set to 'Specified', the user must specify the half-life due to penetration (DT50PenCrp), volatilization (DT50VolCrp) and transformation (DT50TraCrp). If set to 'Lumped'. an overall half-life (DT50DspCrp) is sufficient. The wash-off of pesticides is described with a zero-order equation with one parameter (FacWasCrp).

The only parameter in the equation for uptake of pesticides (eqn. 58) is the coefficient for the uptake by plant roots, FacUpt. See further section 3.2.11.

5.9.2 The transformation scheme form

After the user has defined the properties for all individual compounds (section 5.9.1) to be considered in the simulation, the transformation scheme (table FraPrtDau) can be build. The transformation scheme form can be accessed from the substances form, using the 'transformation scheme' button. Before proceeding, read section 3.2.1 for guidance on deriving transformation fractions and look at Figure 7 for an example of a transformation scheme.

Information about formation products and fractions must be entered *for each compound considered*. If, for example, the user has defined one parent product (PEST) and two metabolites (e.g. MET1 and MET2), the transformation scheme form must be entered three times, i.e. one time from the PEST form, one time from the MET1 form and one time from the MET2 form.

Start with the definition of the transformation scheme of the parent (PEST). Go to the PEST form and press 'transformation scheme'. The left part of the form shows the parent product and some of its main properties. You cannot edit this part of the screen. To the right you will see the metabolites. By default, no metabilites are specified. If you leave these parameters unchanged, PEARL will *not* simulate metabolites. Extra metabolites can be added using the + button in the browse toolbar. Pick a metabolite from the 'to substance' list. If you want to add more metabolites, repeat the preceeding two steps. After you have selected all metabolites, enter the transformation fractions.

Figure 30 The transformation scheme form

Repeat the steps in the last paragraph for the two other metabolites. To achieve this, first go to the MET1 and MET2 forms, then press 'transformation scheme'.

5.10 Editing application schemes

5.10.1 Application schemes

The event scheme form is accessible from the scenario tab of the main form, because it is considered a major building block of a FOCUS scenario (Events table). The entire events scheme can be repeated annually, biennially or triennially using the 'repeat interval for events' option (see section 5.6.2).

Event schemes can be added with the + button of the navigator. You can also copy an existing event scheme. Event schemes should be given a *unique* code for reference and a description. Use the 'Events' button to define the individual events.

5.10.2 Applications

Add a new event with the + button of the navigator or copy an existing event. In the lower half of the screen, the event has to be further defined. First define the application type: 'application to the soil surface' (AppSolSur), 'injection' (AppSolInj), 'incorporation' (AppSolTil),

'application to the crop canopy, interception fraction calculated by the model' (AppCrpLAI) or 'application to the crop canopy, interception fraction supplied by the user' (AppCrpUsr). Then enter the date (can be relative to the emergence date!) and the dosage. Normal date format can be used. You have to enter a year number, but the year will not be used if the repeat interval of applications is set to 1, 2 or 3 (see section 5.6.2). In the case of injection or incorporation, you must additionally supply the incorporation or injection depth.

Figure 31 The application schemes form

5.11 Editing irrigation schemes

The irrigation scheme form is accessible from the scenario tab of the main form, because it is considered a major building block of a FOCUS. Please remember that the irrigation scheme will be repeated annually if the 'repeat weather and irrigation box' in the control tab of the main form is checked.

Add a new irrigation scheme with the + button of the navigator or copy an existing scheme. The irrigation scheme must then be given a *unique* code and a description.

Two types of irrigation can be specified in PEARL, i.e. sprinkler irrigation and surface irrigation. In the case of sprinkler irrigation, interception at the crop canopy will be calculated. The choice between both types of irrigation has to be specified in the 'type' pick list (OptIrr).

The actual irrigation data (IrrTab) must be specified in the irrigations part of the form. Use the navigator to add a new irrigation event. Both the date (column 1) and the irrigation depth

(column 2) should be given. You can import irrigation schemes from an ASCII file using the import button. See Figure 16 for a description of the format of the file.

5.12 Defining the output of the model

Before running the model, you have to define the output that you want to create with PEARL. However, te default settings of the PEARL user interface have been set so that you usually don't need to bother about output control. Output is controlled in the output tab of the main form. This tab contains three fields that affect all variables in the output file.

5.12.1 The output control tab of the main form

You can set the print interval (DelTimPrn). The default value for the print interval is one day. You can reduce the size of the output file by setting the print interval to higher values. *Notice that the output of PEARL is averaged over the print interval* and that the time printed is in the middle of the print interval.

The format of the time column in the output file can be chanced using the pick list (DateFormat). It can be set to 'days since the start of the simulation', 'days since 1-1-1900' or 'years'. The first is the default option. Finally, the precision of the output can be set in the 'format for reals' field (RealFormat). The following FORTRAN specifiers can be used. In these specifiers, w represents an integer specifying the width and d represents the number of digits to be displayed:

– F<w.d>: Fixed format. Using F14.3, printing the number 1.23 will result in: 1.230
– E<w.d>: Exponent format. Using E14.3, printing 1.23 will result in: 0.123E+01
– G<w.d>: General format. Using G14.3, printing 1.23 will result in: 1.23

You can set the thickness of the FOCUS target layer (ZFoc). You can further set the following switches:

– You can specify whether you want to suppress the detailed output file
– You can specify whether fluxes must be printed cumulative or not.

With the 'detailed output options' button you go to the form where you can switch variables on and off.

5.12.2 The detailed output options form

The detailed output options form is accessible from the output control tab of the main form. This form consists of three parts:

– In the upper part you can browse the categories of available variables.
– In the lower-left part of the form you can browse the individual variables within a category
– In the lower-right part of the form you can select and browse the intended output depths.
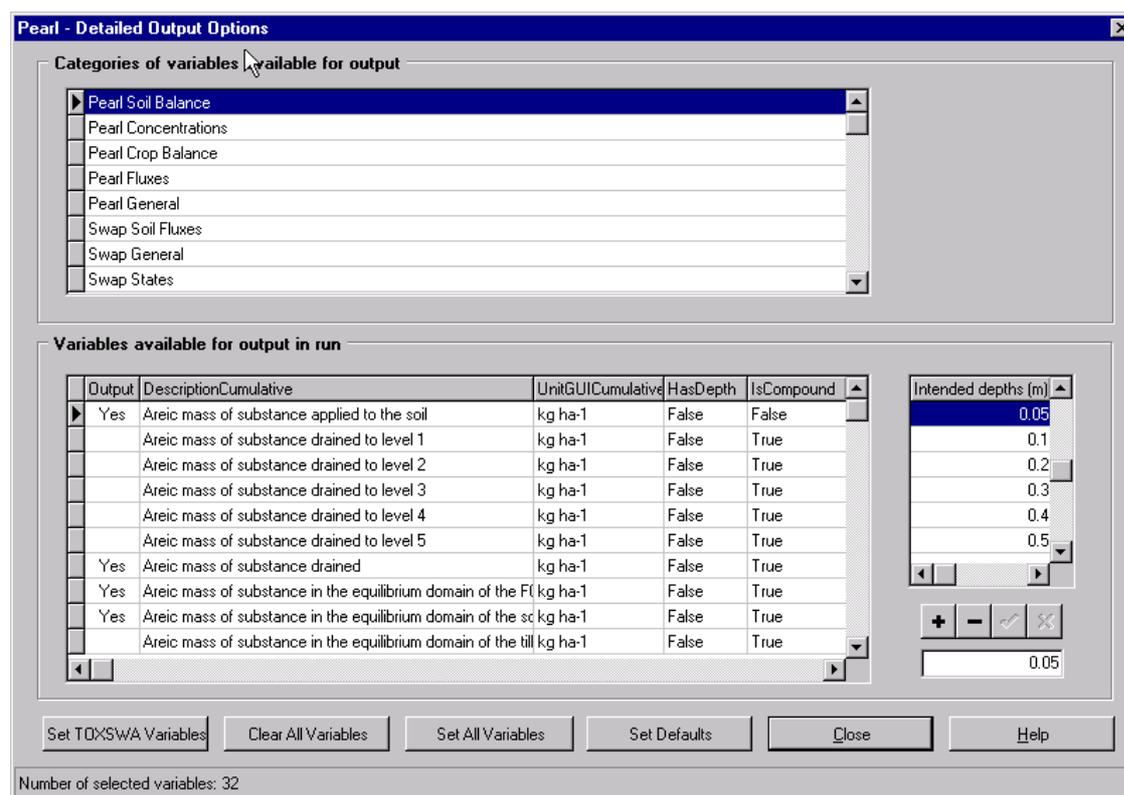
Figure 32 Output control

The available categories

PEARL has the following categories of output variables available:

– Pearl balance: Mass balance of the soil system, which includes variables like the areic mass of transformation and the areic mass of pesticide in the soil system

– Pearl contents: Concentration of pesticide in the various phases of the soil system, such as the total mass content and the concentration in the liquid phase

– Pearl crops: Mass balance of pesticide at the crop canopy

– Pearl fluxes: Mass fluxes of pesticides, such as the total mass flux of pesticide

– Pearl general: Miscellaneous variables, such as the time-step.

– Swap fluxes: Volume fluxes of water, such as the soil water flux

– Swap states: State variables of the hydrological model, such as the soil water content

– Swap general: Miscellaneous variables, such as the groundwater level.

Variables available for output

In this part of the form, you can select variables for output. Variables can be switched on and off by double-clicking. You can also use the buttons at bottom of the form:

– Pressing the 'ToxSwa' button selects all variables wanted by the TOXSWA model (Adriaanse *et al.*, 2000).

– Presssing the 'Clear all variables' button disables all variables.

– Pressing the 'Set all variables' enables all variables.

– Pressing 'Set defaults' enables the most important model outputs.

Intended depths
Use the + button of the navigator key to add additional output depths, use the − key to delete depths. By default, the model will produce output at 5, 10, 20, 30, 40, 50, 75, 100 and 200 cm. Notice that the output depths form applies to all selected variables. Be critical in selecting output depths: More output depths will result in larger output files.

5.13 Running the model

When ready with editing the model input and defining the output variables wanted, you can proceed with running the model. A powerful feature of the PEARL user interface is that you can execute multiple runs, so that you don't need to wait with starting the second run until the first is ready.

To execute the model, first go to the main form. If you are not in the appropriate project, first go to the projects form and select the wanted project. *Now double click all runs you want to execute.* You will see the 'Selected' indicator changing to 'Yes'. When all runs are selected, you can press the 'Calculate' button to actually run the model.

The first time that you select a run for execution, the PEARL user interface will generate the weather and irrigation data files. This can take some take. The PEARL input file will always be generated.

After a while, you will see a console window with the logo of the PEARL simulation kernel. You can follow the course of the simulation in this window. You can enter CNTRL-C to interrupt model execution. The actual computation time depends upon the number of numerical compartments in the soil profile (Leistra *et al.*, 2000). As a guide, execution of the 26 years FOCUS scenario for maize in Hambourg took 11 minutes on a computer with a Pentium™ 330 MHz computer. Computation time can be reduced by reducing the number of output variables selected for output or reducing the number of output depths (section 5.12.1).

When a model run is completed, you will see the ResultsDetailed, ResultsSummary and Modified columns changing. Possible values for the Results columns are:
− NotThere: the model has not (yet) been run or the user has removed the output files
− Error: an error has occurred. Details can be seen in run status tab of the main form.
− There: the model has succesfully been run, and the model output is available for further processing (e.g. graphing).

5.14 Creating graphs

After a model run has been completed, the output can be analyzed via the graphical function of the PEARL model interface. PEARL comes with a number of predifined graphs, but you can also create your own graphs. The predifined graphs provide easy access to the most commonly used model outputs, such as the concentration of pesticide in the groundwater, the

areic mass of pesticide, etc. With user-defined graphs, you can view the data in several different ways, which is an extremely powerful feature for those users who want to analyze several aspects of the leaching study.

5.14.1 Working with predefined graphs

Predefined graphs can be accessed with the 'predefined graph' button in the main form. The following graphs are available:

−   Annual mass balance of the compound in the soil system and the FOCUS target layer, which shows the annual mass balance terms (i.e. annual application, transformation, lateral drainage, leaching, uptake and volatilization)

−   Annual water balance of the soil profile and the FOCUS target layer (i.e. annual precipitation, irrigation, seepage, soil evaporation, transpiration and evaporation of intercepted water)

−   FOCUS summary graph. The FOCUS summary graphs shows the frequency distribution of the leaching concentration, the 80th percentile of the leaching concentration, etc. (see Figure 33).

Frequency distribution of the concentration in leaching water (%)

Concentration of pest in leaching water (µg L^{-1})

Mass of pest leached from the upper meter of the soil (kg ha^{-1})

Water leached from the upper meter of the soil (mm)
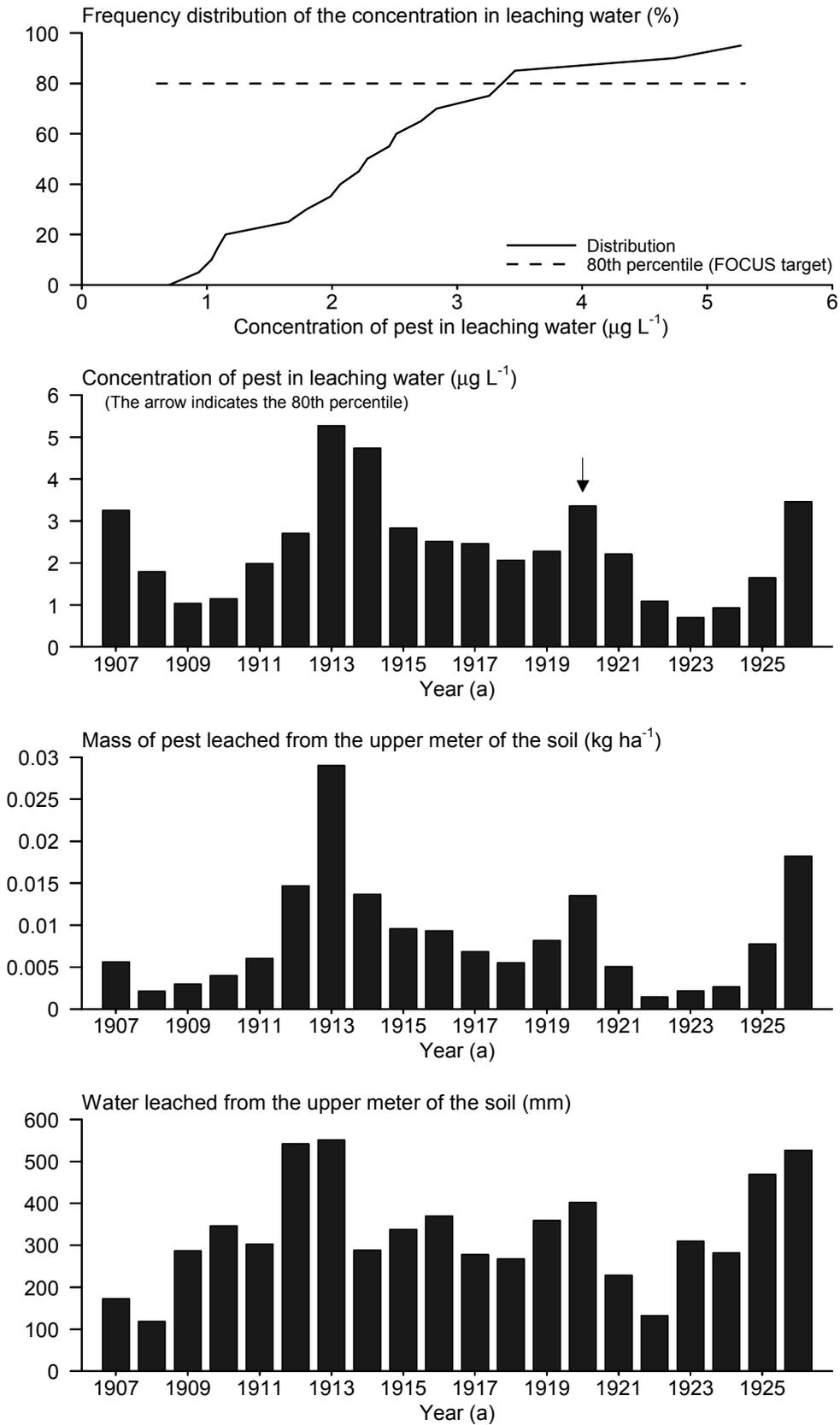
Figure 33 Example of a FOCUS *summary graph*

5.14.2 Working with user-defined graphs

PEARL can create graphs of all selected model outputs (section 5.12.2). The custom graphs form is accessed from the main form. To create a graph perform the following actions:

−   Select one of the categories in the upper box
−   Select one or more variables by double-clicking the variable name in the lower box
−   If the selected variables are depth dependent, you can select one or more depths by clicking in the output dephts box (refer to the HasDepth column)
−   If the selected variables are substance properties, you can select one or more substances in the substances box (refer to the IsCompound column)

You can plot multiple variables in one graph, but a variable that is depth dependent cannot be mixed with another variable that is depth independent. Press 'Graph' when ready.

5.14.3 The XYWIN program

PEARL uses the graphical program XYWIN (Van Heerden and Tiktak, 1994). After you have pressed the 'graph' button, you will see a message box that will show the number of selected data-pairs. After a while, the selected graph will be displayed. You can zoom in with the *left* mouse button and zoom out to the original size (Edit menu or press F8). This function is *not* available in predefined graphs.
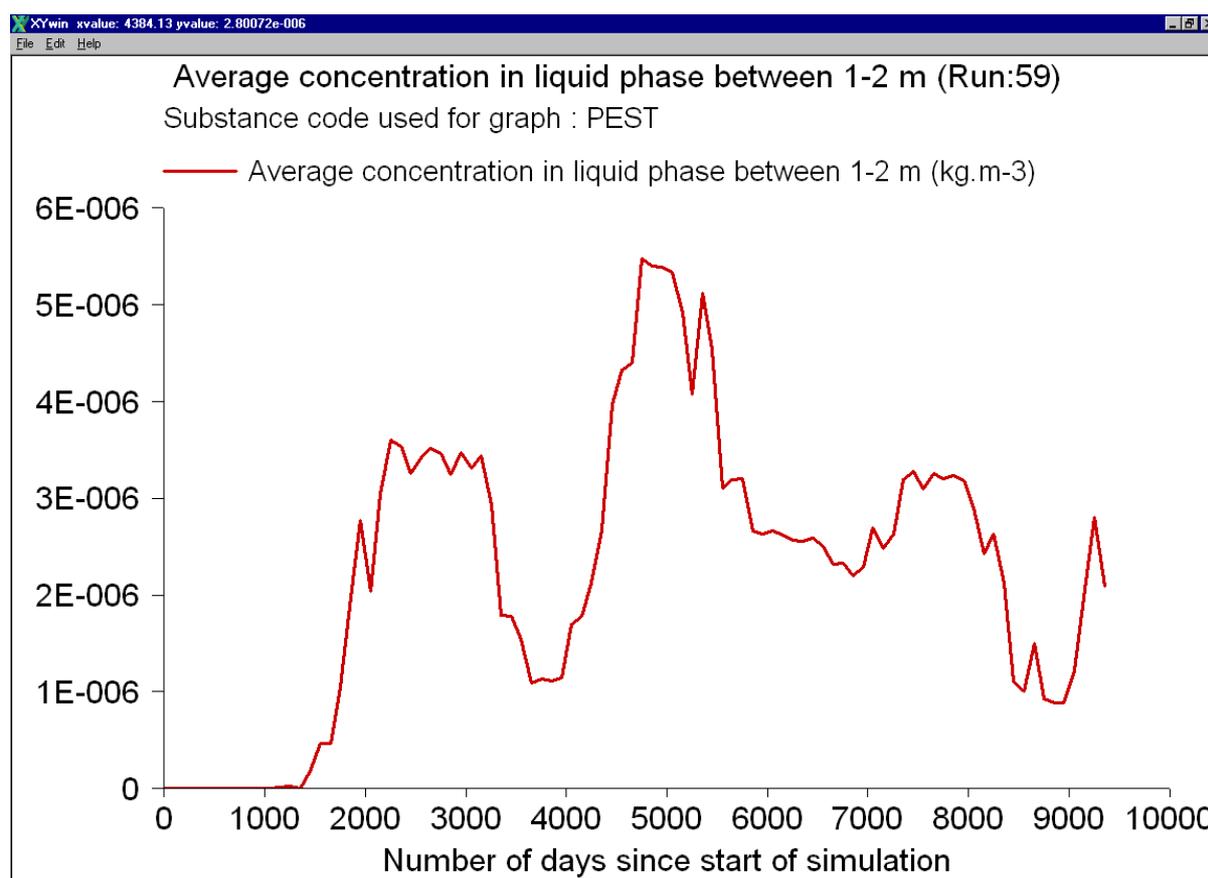
Graphs can be printed from the XYWIN menu (select Print from the File menu or press Cntrl+P). XYWIN can also create a Windows Enhanced MetaFile, which can be imported into a report or into a publication. Select Create Enhanced MetaFile from the File menu or press

F6. To import the picture into WORD 97, select Picture from the Insert menu, then select From File. Both the print function and the MetaFile function ask for the orientation of the graph. For best results, select the orientation according to the actual graph (in the above example, best results are obtained when printing the graph landscape).

5.15 The FOCUS wizard

As mentioned in chapter 3, the pesticide registration procedure starts with using the model in combination with standardized scenario's (FOCUS Modeling Working Group, 2000. These scenario's can be build with the FOCUS wizard, which can be accessed by pressing the FOCUS wizard button in the main form. The FOCUS wizard guides you through the following steps:

1. Selection of crop(s)
2. Selection of location(s)
3. Selection of repeat interval of the application schem (annual, biennial or triennial)
4. Section of application scheme
5. Selection of substance. Here, you can select parent substances only.

Notice that in the FOCUS wizard, you can select from exististing building blocks only. If you want to use PEARL in combination with new building blocks (e.g. a new substance or a new application scheme), you have to add this substance to the database first (sections 5.9 and 5.10).

According to requirements set by the FOCUS Soil Modeling Working Group, you cannot edit crops and locations. Also, the time-domain for the simulations is fixed, depending on the repeat interval of the application scheme.

After running the FOCUS wizard, the user interface has created a new project. You will see that combinations that are not allowed (e.g. vines in Jokioinen) will not appear in the project. The newly created project is a so called 'fixed substance project', which implies that all runs refer to the same substance. Editing this substance affects all selected runs. As it may be desirable to run the model with different application schemes, each run has got its own application scheme (a pesticide may be applied at different times in Greece than it is in Finland). The application schemes of the individual runs are clones of the application scheme that you have specified in the wizard.

All runs in the newly created project have already been selected for execution – you can press the Calculate button to run the model (section 5.13). When done, you can make graphs (section 5.14) and view the summary reports.

If you made a mistake during the creation of a project, you can always remove it from the database. The original components will always be there – it is very easy to create a new FOCUS project.
In the example below, we will create a project with maize runs.

Step 1: Start the FOCUS wizard

Step 2: Select maize and press the > button.
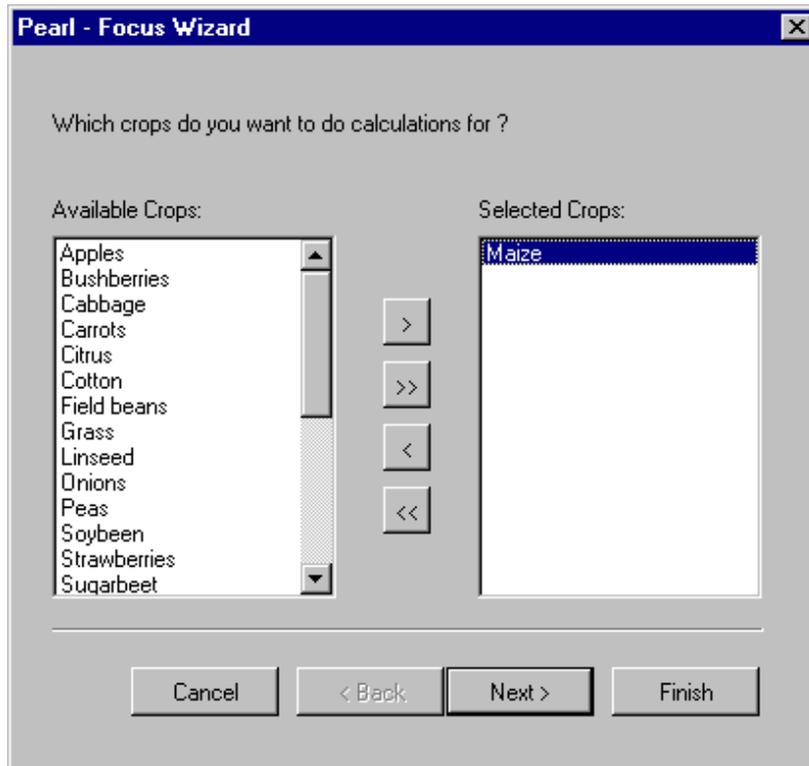
Step 3: Select all locations using the >> button
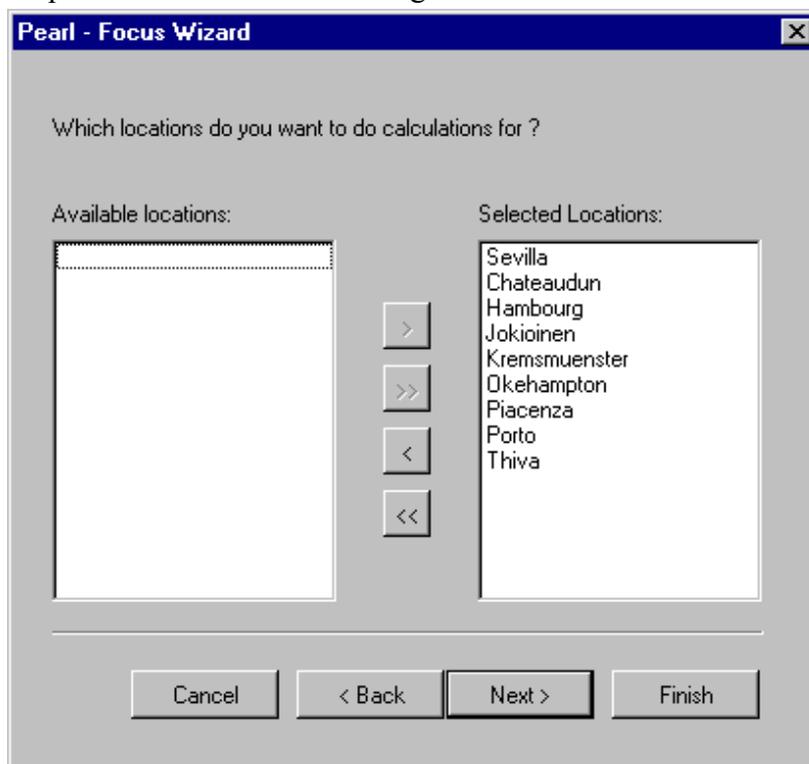
Step 4: Select the substance, the application scheme, and the repeat interval. You can only select from existing substances and application schemes.
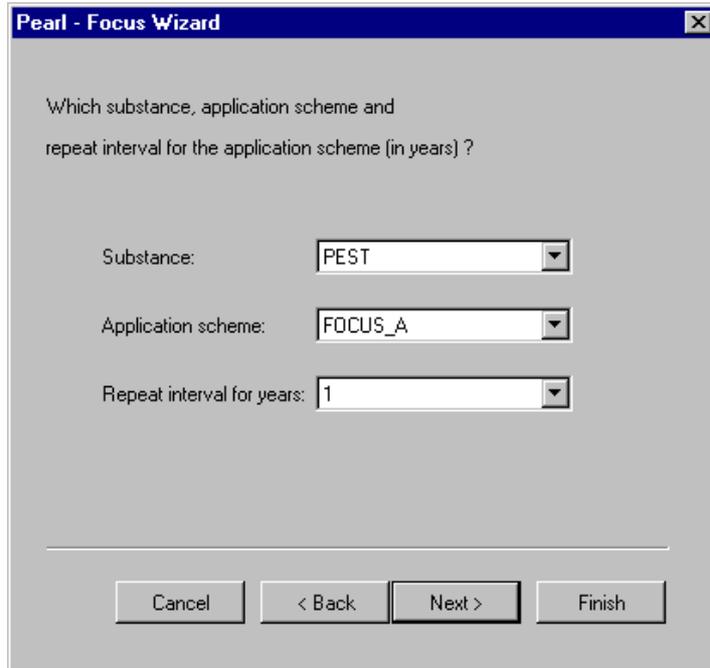
Step 5: PEARL created a new project. Notice that Joikionen is not added to the list of available runs, because it is an invalid combination.
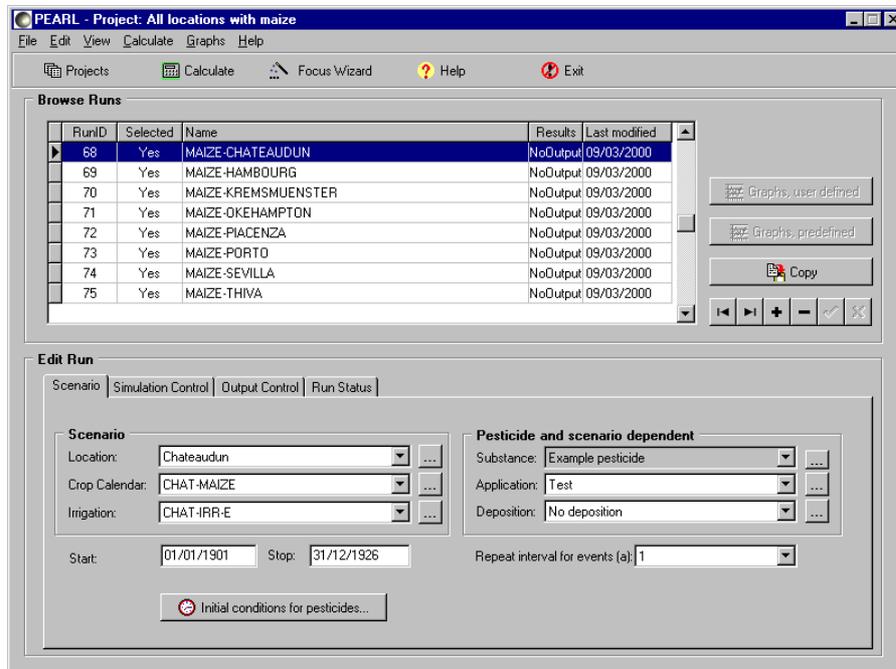
Step 6: If wanted, you can now edit the application scheme for the individuals runs. You can also edit the substance.

Step 7: Press Calculate to execute the model.

5.16 Installation, support and registration

Official FOCUS PEARL versions can be downloaded from the website of the Joint Research Centre in Ispra, Italy (www.jrc.it; you can sent an e-mail to lbg-pearl@rivm.nl to obtain the correct address). You can also download a version of PEARL from the following address: www.alterra.nl/models/pearl. Notice, however, that the FOCUS working group for version control will only accept versions downloaded from the JRC website in the EU registration procedure. If you have downloaded PEARL from the JRC website, you are not yet registered as a PEARL user. We strongly recommend to register. Registered users have some benefits over non-registered users:

− If you do not yet have these manuals, you will obtain the manuals and latest updates.
− You will receive the full version of the PEARL package, including the program PEARLNEQ.
− You can get the source code upon request.
− You will be put on the PEARL mailing list. Through the mailing list, we will inform you about updates, bugs and reports.

To get support, you must register. You can use either the JRC website or the Alterra website for registration. Without registration, we cannot support you efficiently.

Installing the model is simply a question of running the wizard – the system will guide you through the installation process.

If you encounter problems, contact us at lbg-pearl@rivm.nl. Please remember: We need **you** to improve the model, so do not hesitate to mail comments and bugs. And don't forget: Positive comments are also welcome!

6   The Dutch standard scenario

For the first tier of the Dutch pesticide registration, a standard scenario has been developed. The Dutch standard scenario is described in detail by van der Linden and Boesten (1989) and Boesten and van der Linden (1991). Contrary to the FOCUS scenario's, in the Dutch standard scenario, a pesticide is applied only one time in an initially pesticide free soil. Also, one year of weather data is used. These data are constantly repeated. Target variable for the Dutch registration procedure is the maximum in time of the average substance concentration in the upper meter of the groundwater. The PEARL user interface provides direct acces to the Dutch standard scenario. A meta-model of the Dutch standard scenario is included in Uses 3.0 (Linders *et al.*, 2000). This meta-model is, however, not suitable for the calculation of volatile compounds.

6.1   Parameterization

As there have been some adaptations in the parameterization of the Dutch standard scenario, a summary is given here.

6.1.1   Soil properties

The soil selected was a sandy soil based on a soil profile situated near Landhorst, Province of North Brabant (STIBOKA, 1976). The soil profile should represent a realistic worst case situation and should be representative for a large agricultural area. Major soil properties are listed in Table 13.

Table 13. Soil profile used in the Dutch standard scenario. Properties are derived from STIBOKA (1976).

Depth (cm)	Horizon	Bulk density (kg m^{-3})	Organic matter (%)	pH(KCl)	Clay (%)	Silt (%)	M_{50} (µm)
0-30	Ap	1310	4.7	4.7	3	5	200
30-50	B3	1540	0.8	4.4	2	2	200
50-59	C11	1650	0.2	4.6	2	3	200
110-120	C12	1650	0.1	4.6	2	5	200

The soil hydraulic properties were selected from the data given by Wösten *et al.* (1994). Based on the textural distribution, the soil profile was classified as loam-poor fine sand (B1 and O1; Table 4). Corresponding parameter values of the Mualem-Van Genuchten functions (1980) are listed in (Table 4). The parameter describing the reduction of evaporation due to drying of the top layer was estimated to be 2 mm$^{1/2}$ (based on a review by Boesten, 1986). The dispersion length was set to 5 cm, which is in the range of values found by van Ommen *et al.* (1989) in a field experiment with maize on a Dutch sandy soil. The relative diffusion coefficient was described with the functions proposed by Millington and Quirk (1960).

In the original Dutch standard scenario, the groundwater level was fixed at 1 m. In the new scenario, the groundwater level is simulated as a function of time. The boundary condition for

the hydrological model was a Cauchy conditions (bottom boundary flux calculated from an exponential groundwater level-flux relationship). Parameter values of this relationship were obtained by inverse modelling with the PEST program (Doherty *et al.*, 1994). The average groundwater level was 1 m. Optimized parameter values were –0.0112 m d^{-1} for the coefficient and –2.5 m^{-1} for the exponent.

6.1.2 Meteorological conditions

Meteorological conditions were those recorded by the Royal Netherlands Meteorological Institute (KNMI) in de Bilt (near Utrecht) in 1980 (KNMI, 1980). The 1980 was selected because it was a comparatively wet year for Dutch conditions; total rainfall was 860 mm (in the Netherlands only 28% of the years since 1911 had higher annual rainfall). Daily averages of rainfall were used as input in the model. For the rate of evaporation from a hypothetical shallow water surface, only decade averages were available and used. In the original Dutch standard scenario, measured soil temperatures were used. In the adapted standard scenario, soil temperatures are simulated.

6.1.3 Crop properties

The empirical crop factor for transpiration, f_c, was estimated to be equal to 1.0. This is the value given by Feddes (1978) for a fully grown maize crop and this value is also in the range of values found for bare soil (Penman, 1948; McIlroy and Angus, 1964). The emergence and harvest dates were set to May, 16th and October 4th, respecitvely. The Leaf Area Index and rooting depth were based on field observations on a sandy soil (J. Elbers, 1988, personal communication). See 14 for details. The relative root density as a function of depth was set to 1 throughout the rooting zone.

Table 14 Leaf Area Index and rooting depth as a function of crop development stage

Crop stage	*LAI* (m^2 m^2)	rooting depth (m)
0.000	0.0	0.0
0.099	0.2	0.1
0.241	0.95	0.2
0.383	1.9	0.3
0.525	2.95	0.4
0.596	3.4	0.41
0.667	3.6	0.44
0.738	3.7	0.40
0.879	3.6	0.4
1.000	3.5	0.3

The critical pressure heads h_1, h_2, h_3 and h_4 for the reduction of water uptake were set to -10, -30, -1000 and -8000 cm, respectively. The extinction coefficient for global solar radiation was set to 0.5325 based on Van Diepen (personal communication, 1999).

6.1.4 Compound properties

The PEARL database contains a default parameterization for pesticide properties. This default parameterization has been used for deriving the PEARL meta-model as included in Uses 3.0. However, in PEARL, these parameter values can be changed by the user. In the Dutch standard

scenario, by default a single pesticide dosage of 1 kg ha^{-1} is used. The default application dates were set to May, 25th in the case of a spring application and November 1st in the case of an autumn application. By default, a surface application is simulated. For other compound parameters and default values, please follow the guidelines given in chapter 3.2.

6.2   Running the Dutch standard scenario

Running the Dutch standard scenario comes down to the following five steps:

−   Editing a substance. Refer to section 5.9 for details.
−   Selection of an application scheme. In the Dutch standard scenario, the user can chose between a spring (May 25th) or an autumn (November 1st) application of 1 kg ha^{-1}. Substances are always surface applied.
−   Run the Standard scenario wizard to create model run(s).
−   Press the Calculate to run the model.
−   View reports and graphs.

The procedure for running the Dutch standard scenario is described in detail in the help file of the Pearl User Interface. To access this information quickly, press the 'Getting Started' button for guidance.

6.3   Results

Figure 34 shows the simulated groundwater level as a function of time. In the first four months after application, the groundwater level was deeper than 1 m, which was the fixed groundwater level in the former standard scenario. The total actual evapotranspiration was calculated to be 460 mm (Figure 35), which is slightly lower than the 480 mm calculated by Boesten and van der Linden (1991). This implies that the net downward volume flux of water is slightly higher (400 instead of 380 mm).

The results of the calculations on leaching are shown in Figure 37. The countour lines are based on calculations for about 150 combinations of Kom and $DT_{50,ref}$ regularly distributed in the Kom-$DT_{50,ref}$ plane. From the results of these 150 combinations, the contour lines were estimated by spline interpolation. The figure shows both the maximum in time of the average concentration in the upper meter of the groundwater (upper part of figure), and the fraction of the dosage leached into the upper groundwater (lower part of figure). The figure shows the results of the new standard scenario and the results of the old standard scenario. Results of the old standard scenario were discussed in detail by Boesten and van der Linden (1991), here we will discuss the differences only.

At high concentration levels (maximum concentration > 1 µg L^{-1}), the differences between the former and new standard scenarios are negligible. At low concentration levels (< 0.1 µg L^{-1}), the new standard scenario predicts slightly higher concentration levels. Compared with the previous Dutch standard scenario, three major groups of model inputs and processes have been changed: (i) The hydrological boundary condition resulting in a variable ground-

water level (Figure 34) and a somewhat higher precipitation surplus (Figure 35), (ii) process formulations of the transformation process have been slightly adapted, and (iii) soil temperatures are simulated, whereas soil temperatures measured under gras were used in the former standard scenario.

Groundwater level in the Dutch standard scenario (m)
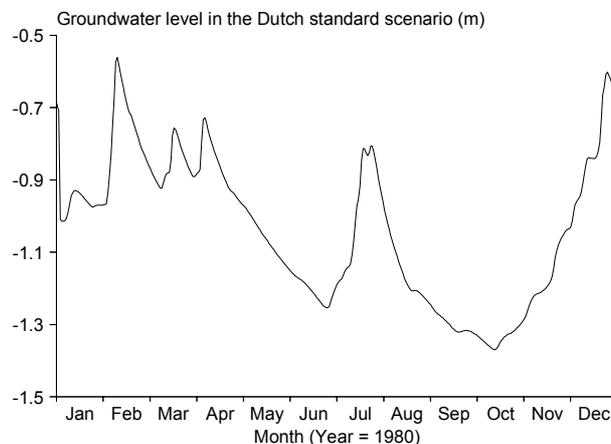
Figure 34 Groundwater level as a function of time during a one-year period starting at Januari 1, 1980.

Earlier sensitivity analyses with the previous models (Boesten and van der Linden, 1991; Tiktak *et al*, 1994) have shown that the hydrology is particularly important for mobile substances. Figure 37 shows, however, that for mobile substances the differences are negligible, so this cannot be the cause of the differences. The differences are most likely due to adaptations in the process formulations for transformation and the use of simulated soil temperatures. The simulated soil temperatures in the period after application are slightly lower than the soil temperatures used in the former standard scenario (i.e. those introduced into PESTLA 1.1; Figure 36). It should be noted that the tempeatures introduced into PESTLA 1.1 do not

Cumulative precipitation and (evapo)transpiration in the Dutch standard scenario
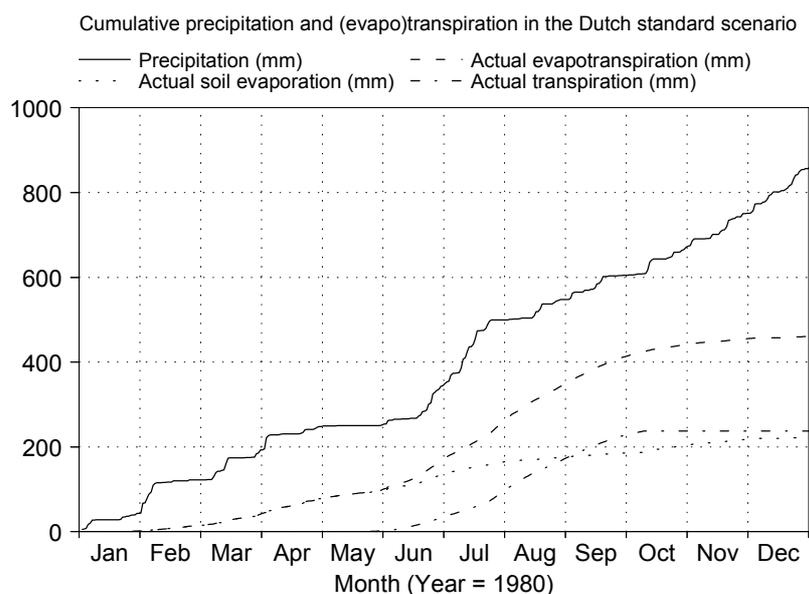
Figure 35 Cumulative rainfall and (evapo)transpiration as a function of time during a one-year period, starting at Januari 1, 1980.

apply to a soil cropped with maize, rather they were taken from the weather station De Bilt where soil temperatures were measured under gras (Van der Linden, personal communication). It is to be expected that the attenuation under gras is different than the attenuation under maize, particularly in the beginning of the growing season when the canopy does not yet shade the ground. Higher leaching rates can also be explained by the fact that PEARL assumes no degradation at temperatures below zero, whereas in PESTLA and PESTRAS the Arrhenius equation was also used at temperatures below zero. During the first 25 days of 1980, soil temperatures were below zero. Finally, the depth dependence of degradation in PEARL is described as a function of soil horizon. For each soil horizon, we introduced the average of the continous function used in the former models. The net effect is also a slightly reduced degradation rate.
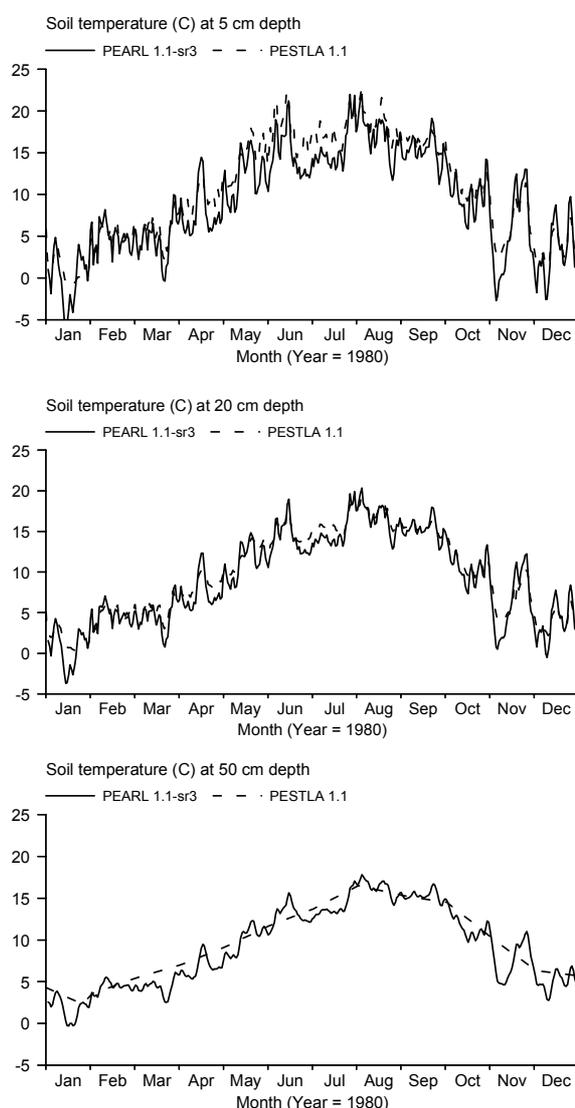
Figure 36 Soil temperatures (deg C) in the former (PESTLA 1.1) and new (PEARL) Dutch standard scenarios as a function of time during a one-year period starting at Januari 1, 1980.

Maximum average concentration (µg L⁻¹) of pesticide in the upper groundwater. Lines are contour lines. Calculations for a spring application (i.e. one application on 25 May 1980).

Mass percentage of pesticide leached below 1 m depth. The lines are contour lines. Calculations for a spring application (i.e. one application on 25 May 1980).
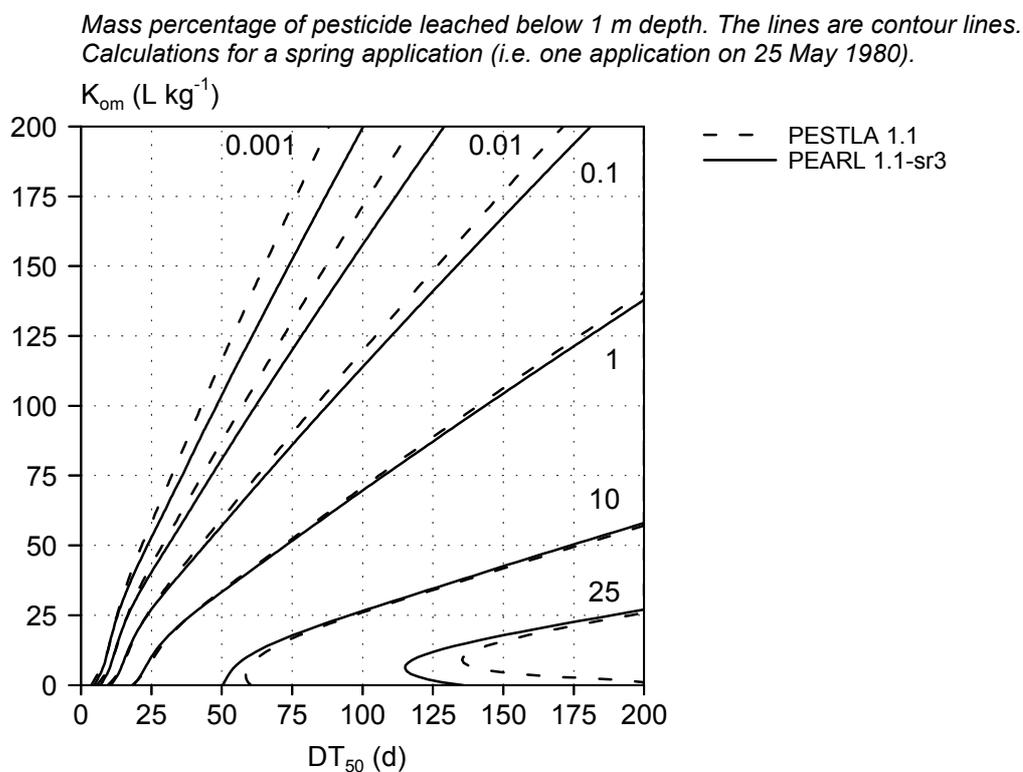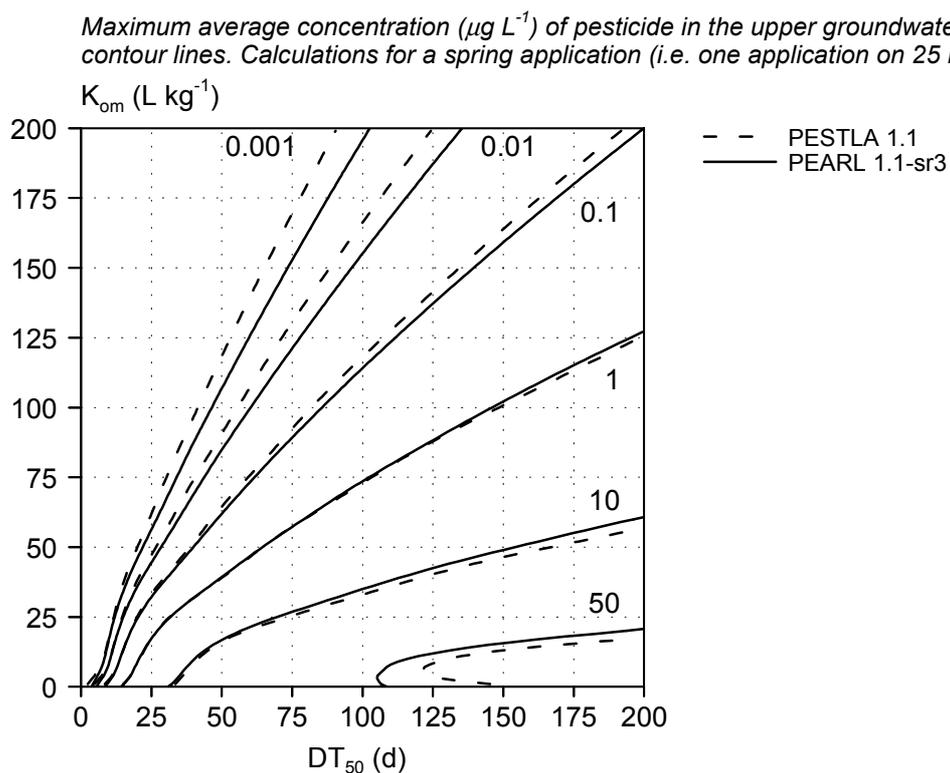
Figure 37 Maximum in time of average pesticide concentration in the upper meter of the groundwater (upper part) and fraction of pesticide dosage leached into the upper groundwater (lower part). Calculations with PESTLA 1.1 and PEARL 1.1-sr3 and for one single application on May 25th 1980.

References

Allen, R.G., M.E. Wright and R.D. Burman. 1989. Operational estimates of evapotranspiration. *Agron. J.* (81):650-662.

Ashby, M., A.J. Dolman, P. Kabat, E.J. Moors and M.J. Ogink-Hendriks. 1996. SWAP *S version 1.0. Technical Reference Manual.* Technical Document 42. SC-DLO, Wageningen, The Netherlands.

Bakker, J.W., F.R. Boone and P. Boekel. 1987. *Diffusie van gassen in grond en zuurstofdiffusiecoëfficiënten in Nederlandse akkerbouwgronden.*ICW Rapport 20. Wageningen, The Netherlands, pp. 44.

Boekhold, A.E., H. van den Bosch, J.J.T.I. Boesten, M. Leistra, F.A. Swartjes and A.M.A. van der Linden. 1993. *Validation of the PESTLA model: Definitions, objectives and procedure.* RIVM report no. 715802001, RIVM, Bilthoven, the Netherlands.

Boesten, J.J.T.I. 1986. *Behavior of pesticides in soil: Simulation and experimental assessment.* Ph.D. thesis, Wageningen Agricultural University, Wageningen, the Netherlands.

Boesten, J.J.T.I. 1991. Sensitivity analysis of a mathematical model for pesticide leaching to groundwater. *Pestic. Sci.* (31):375-388.

Boesten, J.J.T.I. 2000. Modeler subjectivity in estimating pesticide parameters for leaching models using the same laboratory data set. *Agric. Water Mgmt*, (44):389-409.

Boesten, J.J.T.I. and B. Gottesbüren. 2000. Testing PESTLA by two modelers for bentazone and ethoprophos in a sandy soil. *Agric. Water Mgmt* (44):283-305.

Boesten, J.J.T.I., and A.M.A. van der Linden. 1991. Modeling the influence of sorption and transformation on pesticide leaching and persistence. *J. Environ. Qual.* (20):425-435.

Boesten, J.J.T.I., and L.J.T. van der Pas. 1983. Test of some aspects of a model for the adsorption/desorption of herbicides in field soil. *Aspects of Applied Biology* (4):495-501.

Boesten, J.J.T.I., and L.J.T. van der Pas. 1997. *Movement of water, bromide ion and the pesticides ethoprophos and bentazone measured in a sandy soil in Vredepeel (the Netherlands).* SC-DLO report no. 122, Wageningen, the Netherlands.

Boesten, J.J.T.I., and L.J.T. van der Pas. 2000. Movement of water, bromide ion and the pesticides ethoprophos and bentazone in a sandy soil: Description of the Vredepeel data set. *Agric. Water Mgmt* (44):21-42.

Boesten, J.J.T.I. and L. Stroosnijder. 1986. Simple model for daily evaporation from fallow tilled soil under spring conditions in a temperate climate. *Neth. J. Agric. Sci.* (34):75-90.

Bollen, M.J.S., F.H.W.M. Bekhuis, R. Reiling, and E. Scheper. 1995. *Towards a spatial pattern of the vulnerability of soil and groundwater.* RIVM report no. 711901012, Bilthoven, the Netherlands. (In Dutch.)

Bowman, B.T. and W.W. Sans. 1985. Effect of temperature on the water solubility of insecticides. *J. Environ. Sci. and Health.* (B20):625-631.

Bouten, W. 1992. *Monitoring and modeling forest hydrological processes in support of acidification research.* Ph.D. thesis, University of Amsterdam, the Netherlands, p.218.

Braden, H. 1985. Ein Energiehaushalts- und Verdunstungsmodell für Wasser und Stoffhaushaltunguntersuchungen landwirtschaftlich genutzer Einzugsgebiete. *Mitteilungen Deutsche Bodenkundliche Geselschaft* (42):294-299.

Briggs, G.G., R.H. Bromilow, and A.A. Evans. 1982. Relationships between lipophilicity and root uptake and translocation of non-ionized chemicals by barley. *Pestic. Sci.* (13):495-504.

Brouwer, W.W.M., J.J.T.I. Boesten, J.B.H.J. Linders and A.M.A. van der Linden. 1994. *The behavior of pesticides in soil: Dutch guidelines for laboratory studies and their evaluation.* Pesticide Outlook (5):23-28.

Calvet, R., M. Tercé, and J.C. Arvieu. 1980. Adsorption des pesticides par les sols et leurs constituents. III. Charactéristiques générales de l'adsorption des pesticides. *Ann. Agron.* (31):239-257.

Carsel, R.F. and R.S. Parrish. 1988. Developing joint probability distributions of soil water characteristics. Water Resour. Res. (22):211-227.

Currie, J.A. 1965. Diffusion within soil microstructure: A structural parameter for soils. *J. Soil Sci.* (16):279-289.

De Vries, D.A. 1963. Thermal properties of soils. *In:* W.R. Van Wijk (ed). *Physics of the Plant environment.* North-Holland Publ. Company, Amsterdam, The Netherlands, p. 210-235.

Feddes, R.A. 1987. Crop factors in relation to Makkink reference-crop evapotranspiration. In: *Evapotranspiration and weather.* Proceedings and Information (39):33-45. TNO Committee on Hydrological Research, The Hague, the Netherlands.

Feddes, R.A., P.J. Kowalik and H. Zaradny. 1978. *Simulation of field water use and crop yield.* Simulation Nomographs. Pudoc. Wageningen, The Netherlands. pp. 189.

FOCUS Soil Modeling Working Group. 1997. *Soil Persistence models and EU registration.* DG VI. European Commission, Doc. 7617/VI/96, Brussels, pp. 74.

FOCUS. 2000. *Focus groundwater scenarios in the EU pesticide registration process.* Report of the FOCUS Groundwater Scenarios Working Group, EC document.

Fontaine, D.D., R.G. Lehmann, and J.R. Miller, J.R. 1991. *Soil Adsorption of Neutral and Anionic Forms of a Sulfonamide Herbicide, Flumetsulam.* J. Environ. Qual. (20):759-762.

Freijer, J.I. 1994. *Mineralization of hydrocarbons and gas dynamics in oil-contaminated soils.* Ph.D. Thesis, University of Amsterdam, the Netherlands.

Freijer, J.I., A. Tiktak, S.M. Hassanizadeh, and A.M.A. van der Linden. 1996. *PESTRASv3.1.: A one dimensional model for assessing leaching, accumulation and volatilization of pesticides in soil.* RIVM Report no. 715501007, Bilthoven, the Netherlands.

Goudriaan, J. 1977. *Crop Meteorology: A simulation study.* Simulation Nomographs, Pudoc, Wageningen, The Netherlands.

Hallberg, G.R. 1989. Pesticide pollution of groundwater in the humid United States. *Agric. Ecosyst. Environ.* (26):299-367.

Herkelrath, W.N., E.E. Miller, and W.E. Gardner, W.E. 1977. Water uptake by plants: II. The root contact model. *Soil Sci. Soc. Am. J.*, (41):1039-1043.

Hornsby, G.H., R.D. Wauchope and A.E. Herner. 1996. *Pesticide properties in the Environment.* Springer Verlag, New York.

Jarvis, N. 1991. *MACRO - A model of water movement and solute transport in macroporous soil.* Monograph, Reports and dissertations, 9. Dept. of Soil Sci., Swedish Univ. Agric. Sci., Uppsala, Sweden, 58pp.

Jin, Y. and W.A. Jury. 1996. Characterizing the dependence of gas diffusion coefficient on soil properties. *J. Environ Qual.* (60):66-71.

Jury, W.A., D. Russo, G. Streile and H.E. Abd. 1990. Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resour. Res.* (26):13-20.

Jury, W.A., W.F. Spencer and W.J. Farmer. 1983. Behavior Assessment Model for trace organics in soil. I. Model description. *J. Environ. Qual.* (12):558-564.

Kroes, J.G., J.C. van Dam, J. Huygen, and R.W. Vervoort. 1999. *User's Guide of SWAP version 2.0 Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment.* SC-DLO technical document 53, Wageningen, The Netherlands, pp. 127.

Leij, F.J., W.J. Alves, M.Th. van Genuchten and J.R. Williams. 196. The UNSODA Unsaturated Soil Hydraulic Database. User's manual Version 1.0. Soil Salinity Laboratory, Riverside, CA.

Leistra, M., and J.J.T.I. Boesten. 1989. Pesticide contamination of groundwater in western Europe. *Agric. Ecosyst. Environ.* (26):369-389.

Leistra, M., and W.A. Dekkers. 1976. Computed leaching of pesticides from soil under field conditions. *Water Air Soil Pollut.* (5):491-500.

Leistra, M., A.M.A. van der Linden, J.J.T.I. Boesten, A. Tiktak and F. van den Berg. 2000. PEARL model for pesticide behaviour and emissions in soil-plant systems. Description of processes. Alterra report 013, Alterra, Wageningen, the Netherlands.

Linders, J.B.H.J. J.W. Jansma, B.J.W.G. Mensink, and K. Otermann. 1994. *Pesticides: Benefaction or Pandora's Box? A synopsis of the environmental aspects of 243 pesticides*. RIVM Report no. 679101014, Bilthoven, the Netherlands.

Makkink, G.F. 1957. Testing the Penman formula by means of lysimeters. *J. Inst. Water Eng.* (11):277-288.

Millington, R.J. and J.P. Quirk. 1960. Transport in porous media. *In:* F.A. van Beren *et al. Trans. Int. Congress Soil Sci Soc.* 7th. Volume 1. Madison, WI. Elsevier, Amsterdam. p. 97-106.

Monteith, J.L. 1965. Evaporation and environment. *Proc. Symp. Soc. Exp. Biol.*, (19):205-234.

Reid, R.S. and T.K. Sherwood. 1966. *The properties of gases and liquids*. McGraw-Hill, London, 646pp.

Shone, M.G.T. and A.V. Wood. 1974. A comparison of the uptake and translocation of some organic herbicides and a systematic fungicide by barley. *J. Experimental Botany* (25):390-400.

Smit, A.A.M.F., F. van den Berg and M. Leistra. 1997. *Estimation method for the volatilization of pesticides from shallow soil*. Env. Planning Bureau Series 2. Agricultural Research Department, Wageningen, The Netherlands, pp. 108.

Tiktak, A. 1999. *Modeling Non-Point Source Pollutants in Soils. Applications to the Leaching and Accumulation of Pesticides and Cadmium*. Ph.D. Thesis, University of Amsterdam, Amsterdam, The Netherlands, pp. 224.

Tiktak, A. 2000. Application of pesticide leaching models to the Vredepeel dataset. II. Pesticide fate. *Agric. Water Mgmt* (44):119-134.

Tiktak, A., and W. Bouten. 1992. Modeling soil water dynamics in a forested ecosystem. III: Model description and evaluation of discretization. *Hydrol. Proc.* (6):455-465.

Tiktak, A., A.M.A. van der Linden, and F.A. Swartjes. 1994. *PESTRAS: A one dimensional model for assessing leaching and accumulation of pesticides in soil*. RIVM report no. 715501003, Bilthoven, the Netherlands.

Tiktak, A., A.M.A. van der Linden, and I. Leine. 1996a. Application of GIS to the Modeling of Pesticide Leaching on a Regional Scale in the Netherlands. In: D.L. Corwin and K. Loague (Ed.). *Application of GIS to the Modeling of Non-Point Source Pollutants in the Vadose Zone*. SSSA-Special Publication number 48, pp. 259-281.

Tiktak, A., A.M.A. van der Linden and R.C.M. Merkelbach. 1996b. *Modeling pesticide leaching at a regional scale in the Netherlands*. RIVM report no. 715801008, Bilthoven, the Netherlands.

Tiktak, A., A.M.A. van der Linden, and L.J.T. van der Pas. 1998. Application of the Pesticide Transport Assessment Model to a field-study in a humic sandy soil in Vredepeel, the Netherlands. *Pestic. Sci* (52):321-336.

Tomlin, C. (Ed.). 1994. *The Pesticide Manual*. 10th Edition. Crop Protection Publications, Royal Soc. Chemistry, Cambridge, UK.

Troeh, F.R., J.D. Jabro and D. Kirkham. 1982. Gaseous diffusion equations for porous materials. *Geoderma* (27):239-253.

Vanclooster, M. and J.J.T.I. Boesten. 2000. Application of nine pesticide leaching models to the Vredepeel dataset. I. Water. solute and heat transport. *Agric. Water Mgmt.* (44):105-117.

Vanclooster, M., J.J.T.I. Boesten, M. Trevisan, C.D. Brown, Capri, Vacek, Eklo, B. Gottesbürren, Gouy and A.M.A. van der Linden. 2000. A European test of pesticide-leaching models: Methodology and major recommendations. *Agric. Water Mgmt* (44):1-3.

Van Dam, J.C., J. Huygen, J.G. Wesseling, R.A. Feddes, P. Kabat, P.E.V. van Walsum, P. Groenendijk and C.A. van Diepen. 1997. *Theory of SWAP version 2.0. Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment*. SC-DLO technical document 45, Wageningen, The Netherlands, pp. 167.

Van den Berg, F. 1992. *Emission of fumigants from soil and dispersion in air.* Ph.D. Thesis, Wageningen Agricultural University, Wageningen, The Netherlands.

Van den Berg, F. and J.J.T.I. Boesten. 1998. *Pesticide Leaching and Accumulation model (PESTLA) version 3.4. Description and User's guide.* SC-DLO technical document 43, Wageningen, The Netherlands, pp. 150.

Van den Bosch, H., and J.J.T.I. Boesten. 1994. *Validation of the PESTLA model: Field test for leaching of two pesticides in a humic sandy soil in Vredepeel (the Netherlands).* SC-DLO report no. 82, Winand Staring Center, Wageningen, the Netherlands.

Van der Linden, A.M.A. and J.J.T.I. Boesten. 1989. *Berekening van de mate van uitspoeling en accumulatie van bestrijdingsmiddelen als functie van hun sorptiecoëfficiënt en omzettingssnelheid in bouwvoormateriaal.* RIVM report no. 728800003, Bilthoven, The Netherlands (in Dutch).

Van Genuchten, M.Th. 1980. A closed form for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* (44):892-898.

Van Genuchten, M.Th., F.J. Leij and S.R. Yates. 1991. *The RETC code for quantifying the hydraulic functions of unsaturated soil.* U.S. Salinity Laboratory, Riverside, CA.

Van Heemst, H.D.J. 1986. Crop phenology and dry matter distribution. *In:* H. van Keulen and J. Wolf (Ed). Modeling of Agricultural Production: Soil, Weather and Crops. p. 13-60.

Van Ommen, H.C., M.Th. van Genuchten, W.H. van der Molen, R. Dijksma, and J. Hulshof. 1989. Experimental and theoretical analysis of solute transport from a diffuse source of pollution. *J. Hydrol.* (105):225-251.

Walker, A. 1974. A simulation model for prediction of herbicide persistence. *J. Environ. Qual.* (3):396-401.

Wesseling, J.G. 1991. Meerjarige simulaties van grondwateronttrekking voor verschillende bodemprofielen, grondwatertrappen en gewassen met het model SWATRE. SC-DLO report 152, Wageningen, the Netherlands (*In Dutch*).

Wesseling, J.G., J.A. Elbers, P. Kabat and B.J. van den Broek. 1990. *SWACROP – Instructions for input.* Internal Communication 80, SC-DLO, Wageningen, The Netherlands, pp. 56.

Wösten, J.H.M., G.H. Veerman and J. Stolte. 1994. Water retention and hydraulic conductivity functions of top- and subsoils in the Netherlands: The Staring Series. SC-DLO Technical document no. 18, Wageningen, the Netherlands (*In Dutch*).

Yates, S.R., M.Th. van Genuchten, A.W. Warrick and F.J. Leij. 1992. Analysis of measured, predicted and estimated hydraulic conductivity using the RETC computer program. Soil Sci. Soc. Am. J. (56):347-354.

Appendix 1   Mailing list

1.   J.A. Suurland, DGM/BWL, Den Haag, the Netherlands
2.   Directie RIVM
3.   Directie Alterra Green World Research
4.   H. Merkus, DGM/BWL, Den Haag, the Netherlands
5.   H. de Heer, LNV/DL, Den Haag, the Netherlands
6.   N. de Man, LNV/DL, Den Haag, the Netherlands
7.   P.I. Adriaanse, Alterra Green World Research, Wageningen, the Netherlands
8.   K. Aden, BBA, Braunschweig, Germany
9.   T.M. Addiscott, IACR-Rothamsted Experimental Station, Harpenden, UK
10.   G. Arnolds, RIZA, Lelystad, the Netherlands
11.   A. Armstrong, ADAS, Mansfield, UK
12.   M. van Assen, Nefyto, The Hague, the Netherlands
13.   M. Bach, University Giessen, Institut für Landeskultur, Giessen, Germany
14.   P.J.T. van Bakel, Alterra Green World Research, Wageningen, the Netherlands
15.   D. Bakker, Provincie Flevoland, Lelystad, the Netherlands
16.   A. Bontoux, EU-Commision DG XII, Brussels, Belgium
17.   I. Bärlund, Finnish Environmental Agency, Helsinki, Finland
18.   S. Beernaerts, CERVA, Tervuren, Belgium
19.   C. Beigel, BASF, Princeton, New Jersey, USA
20.   S. Beulke, SSLRC, Silsoe, UK
21.   G. Bidoglio, EC-Joint Research Centre, Ispra (VA), Italy
22.   J.S.M. Boleij, CTB, Wageningen, the Netherlands
23.   J. Bouma, WAU, the Netherlands
24.   W. Bouten, University of Amsterdam, the Netherlands
25.   W.W.M. Brouwer, PD, The Hague, the Netherlands
26.   C. Brown, SSLRC, Silsoe, UK
27.   P. Burauel, Forschungszentrum Jülich Gmbh, Jülich, Germany
28.   P.A. Burrough, University of Utrecht, Utrecht, the Netherlands
29.   M. Businelli, Istituto di Chimica Agraria, Perugia, Italy
30.   E. Capri, Universita Cattolica del Sacro Cuore, Piacenza, Italy
31.   R. Carsel, US-EPA, Athens, Georgia
32.   F. Claessen, RIZA, Lelystad, the Netherlands
33.   Y. Coquet, INRA, France
34.   J. Cornejo, IRNASE, Instituto de Recursos Naturales y Agrobiologica de Sevilla, Sevilla, Spain
35.   D.L. Corwin, USSL, Riverside, CA
36.   A. Delmas, INRA, Versailles, France
37.   B. Diekkrüger, University of Braunschweig, Braunschweig, Germany
38.   A. Dieses, University of Heidelberg, Heidelberg, Germany
39.   I. Dubus, SSLRC, Silsoe, UK
40.   M. Dust, DuPont France, France
41.   O.M. Eklo, Norwegian Crop Research Institue, Ås, Norway
42.   B. Erzgräber, AVENTIS, Germany
43.   R.A. Feddes, WAU, Wageningen, the Netherlands
44.   E. Fernandez, Instituto de Recursos Naturales y Agrobiologica de Sevilla, Sevilla, Spain
45.   J. Feijen, Universiteit van Leuven, Leuven, België
46.   P. Flori, Centro di Fitofarmacia, Bologna, Italy
47.   R. Francaviglia, Istituto Sperimentale per la Nutrizione delle Piante, Roma, Italy

48.   V. Gouy, CEMAGREF, Lyon, France
49.   C. Guyot, AVENTIS, Lyon, France
50.   B. Gottesbüren, BASF AG, Limburgerhof, Germany
51.   K.P. Groen, RIZA, Lelystad, the Netherlands
52.   P. Groenendijk, Alterra Green World Research, Wageningen, the Netherlands
53.   C.D. Hansen, EPA, Roskilde, Denmark
54.   K. Hanze, National Chemicals Inspectorate, Solna, Sweden
55.   G. Hecquet, UCL, Louvaine la Neuve, Belgium
56.   C. van Heerden, Caseware, Wijk bij Duursted, the Netherlands
57.   G.B.M. Heuvelink, University of Amsterdam, Amsterdam, the Netherlands
58.   T.J. Heimovaara, IWACO, Rotterdam, the Netherlands
59.   G. Hoogeweg, ESRI, Redlands, CA.
60.   A. Hornsby, University of Florida, Gainesville, FL, USA.
61.   J. Hosang, FH Wädenswill, Switzerland
62.   A. Huber, NOVARTIS, Switzerland
63.   P. Hucorne, Min. van Middenstand en Landbouw, Brussel, België
64.   J.L. Hutson, Cornell University, Cornell, New York
65.   N.J. Jarvis, Swedish University of Agricultural Sciences, Uppsala, Sweden
66.   T. Jarvis, JSC International, Harrogate, United Kingdom
67.   D. Jacques, ILWM, Leuven, Belgium
68.   H. Johanssen, Swedish University of Agricultural Sciences, Uppsala, Sweden
69.   A. Jones, EC-Joint Research Centre, Ispra (VA), Italy
70.   R. Jones, Rhône-Poulenc Ag. Company, Research Triangle Park, USA
71.   G. A-N. Khalil. Dept. of Crop and Soil Science, Washington State University, Pullman, WA
72.   M. Klein, Fraunhofer Gesellschaft, Schmallenberg, Germany
73.   T. Kroon, RIZA, Lelystad, the Netherlands
74.   J.G. Kroes, Alterra Green World Research, Wageningen, the Netherlands
75.   R. Kruijne, Alterra Green World Research, Wageningen, the Netherlands
76.   M.H. Larsson, Swedish University of Agricultural Sciences, Uppsala, Sweden
77.   P.A. Leffelaar, WAU, Wageningen, the Netherlands
78.   F. Leus, RIZA, Lelystad, the Netherlands
79.   A. Leijnse, TNO-NITG, Delft, the Netherlands
80.   M. van Liedekerke, EC-Joint Research Centre, Ispra (VA), Italy
81.   V. Linneman, Forschungszentrum Jülich Gmbh, Jülich, Germany
82.   K. Loague, Stanford University, Stanford, CA.
83.   W-M Maier, EU-Commision DG SANCO, Brussels, Belgium
84.   A. Massey, PSD, York, UK
85.   C. Mouvet, BRGM, Orléans, France
86.   Nolting, BBA, Braunschweig, Germany
87.   P. Nicholls, Rothamsted, UK
88.   L. Padovani, Universita Cattolica del Sacro Cuore, Piacenza, Italy
89.   J.D. Piñeros Garcet, UCL, Louvaine la Neuve, Belgium
90.   J.W. Pol, CTB, Wageningen, the Netherlands
91.   L. Pussemier, CERVA, Tervuren, Belgium
92.   S. Rekolainen, Finnish Environmental Institute, Helsinki, Finland
93.   G. Reinken, AVENTIS, Ongar, Essex, UK
94.   H. Resseler, Novartis Agro, Frankfurt, Germany
95.   W.H. van Riemsdijk, WAU, Wageningen, the Netherlands
96.   C. Riparbelli, ERSAL Lombardia, xxx, Italy
97.   C.J. Ritsema, Alterra Green World Research, Wageningen, the Netherlands

98.   C. Roest, Alterra Green World Research, Wageningen, the Netherlands
99.   C. Roquero, Universidad Politechnica de Madrid, Madrid, Spain
100.   M.H. Russel, DuPont, DE
101.   M.G. Schaap, USSL, Riverside, CA
102.   J. Schlöder, University of Heidelberg, Heidelberg, Germany
103.   H. Schäfer, BAYER AG, Leverkusen, Germany
104.   L. Smeets, EU-DG SANCO, Brussel, België
105.   J.H. Smelt, Alterra Green World Research, Wageningen, the Netherlands
106.   J. Steenvoorden, Alterra Green World Research, Wageningen, the Netherlands
107.   B. Stein, UBA, Berlin, Germany
108.   M. Styczen, Danish Hydraulic Institute, Hørsholm, Denmark
109.   P. Sweeney, ZENECA, Bracknell, UK
110.   J.W. Tas, DGM/BWL, Den Haag, the Netherlands
111.   M. Thorsen, Danish Hydraulic Institute, Hørsholm, Denmark
112.   K. Travis, ZENECA Agrochemicals, Bracknell, United Kingdom
113.   M. Trevisan, Istituto di Chimica Agraria e Ambientale, Piacenza, Italy
114.   M. Vanclooster, UCL, Louvaine la Neuve, Belgium
115.   M.Th.. van Genuchten, USSL, Riverside, CA
116.   H. Vereecken, FZ Jülich, Jülich, Germany
117.   J.M. Verstraten, University of Amsterdam, the Netherlands
118.   J.P.M. Vink, RIZA, Lelystad, the Netherlands
119.   P.J.M. van Vliet, CTB, Wageningen, the Netherlands
120.   A. Walker, Wellesbourn, Warwick, UK
121.   A. van Vossel, EU-Commision DG VI, Brussels, Belgium
122.   A. Wadley, ZENECA Agrochemicals, Bracknell, United Kingdom
123.   A. Wolters, Forschungszentrum Jülich Gmbh, Jülich, Germany
124.   J.H.M. Wösten, Alterra Green World Research, Wageningen, the Netherlands
125.   J.C. van Dam, WAU, Wageningen, the Netherlands
126.   S.E.A.T.M. van der Zee, WAU, Wageningen, the Netherlands
127.   Bibliotheek Alterra Green World Research, Wageingen, the Netherlands
128.   Bibliotheek RIZA, Lelystad, the Netherlands
129.   Depot Nederlandse Publikaties en Nederlandse Bibliografie, Den Haag, the Netherlands
130.   N.D. van Egmond
131.   F. Langeweg
132.   R. van den Berg
133.   A.H.M. Bresser
134.   J.J.B. Bronswijk
135.   J.C.H. van Eijkeren
136.   A. van der Giessen
137.   J.J.J.M. van Grinsven
138.   B. de Haan
139.   H. van den Heiligenberg
140.   A. Bakema
141.   A.M. Breure
142.   A.A. Cornelese
143.   G. van Drecht
144.   J. Freijer
145.   P.H.M. Janssen
146.   J.B.H.J. Linders
147.   R. Luttik

148.   H. Könemann
149.   K. Kovar
150.   G. de Mik
151.   M. Montforts
152.   B. Overbeek
153.   M.J.M. Pastoors
154.   F.A. Swartjes
155.   G.J.M. Uffink
156.   T. Vermeire
157.   A. Verschoor
158-162 Authors
163.   SBD/Voorlichting & Public Relations
164.   Bureau Rapportenregistratie
165.   Bibliotheek RIVM
166-170 Bureau Rapportenbeheer
171-200 Reserve exemplaren

Appendix 2   The PEARL input file – Expert users

This appendix gives a listing of the extended PEARL input file. This file is intended to be used by expert users. Users who want to run PEARL for the Dutch standard scenario can use the file 'default.prl'.

```
*--------------------------------------------------------------------------------------
* STANDARD FILE for Pearl version 1.1 sr3 (01-Aug-2000).
*
* This file is intented for use with the Dutch standard scenario as described by
* Van der Linden and Boesten (1989), Boesten and van der Linden (1991) and
* and Tiktak et al. (2000).
*
* Van der Linden, A.M.A. and J.J.T.I. Boesten, 1989. Berekening van de mate van
* uitspoeling en accumulatie van bestrijdingsmiddelen als functie van hun
* sorptiecoefficient en omzettingssnelheid in bouwvoormateriaal. RIVM rapport
* nr. 728800003, Bilthoven, the Netherlands, pp. 52 (In Dutch).
*
* Boesten, J.J.T.I. and A.M.A. van der Linden. 1991. Modeling the influence of sorption
* and transformation on pesticide leaching and persistence.
* J. Environ. Qual. (20):425-435.
*
* Tiktak, A., F. van den Berg, J.J.T.I. Boesten, M. Leistra, A.M.A. van der Linden and
* D. van Kraalingen. 2000. Pearl: Pesticide Emission Assessment for Regional and Local
* Scales. User Manual of Pearl 1.1. RIVM report no. 711401008, Bilthoven, The Netherlands.
*
* This file is intended to be used by expert users.
* Figures between brackets refer to constraints (maximum and minimum values).
*
* Pearl e-mail address: lbg-pearl@rivm.nl
*
* (c) RIVM/Alterra 01-Aug-2000
*--------------------------------------------------------------------------------------


*--------------------------------------------------------------------------------------
* Sector 0: Run identification
*--------------------------------------------------------------------------------------

DutchRegistration       OptReport               Type of report (FOCUS, DutchRegistration)
Dutch_Location          Location                Location identification
Dutch_Soil              SoilTypeID              Soil identification
Monoculture_Maize       CropCalendar            Crop calendar
A                       SubstanceName           Substance name
One_Spring_Application  ApplicationScheme       Appplication scheme
No                      DepositionScheme        Deposition scheme
No                      IrrigationScheme        Irrigation scheme


*--------------------------------------------------------------------------------------
* Section 1: Control section
*--------------------------------------------------------------------------------------

No              AcceptDefaults          Accept values from Dutch standard scenario?

* Time domain
01-Jan-1980     TimStart                Begin time of simulation [01-Jan-1900|-]
31-Dec-2000     TimEnd                  End time of simulation [TimStart|-]
1.d-4           AmaSysEnd     (kg.ha-1)  Stop criterion - ignored if zero [0|-]
0               DelTimPrn     (d)        Print timestep [0|-] - zero is automatic

* SWAP control
Yes             RepeatHydrology         Repeat weather data: Yes or No
Automatic       OptHyd                  OnLine, OffLine, Stationary, Only, Automatic
1.d-5           DelTimSwaMin  (d)        Minimum time step in SWAP [1d-8|0.1]
0.2             DelTimSwaMax  (d)        Maximum time step in SWAP [0.01|0.5]
0.001           ThetaTol      (m3.m-3)   Tolerance in SWAP [1e-5|0.01]


*--------------------------------------------------------------------------------------
* Section 2: Soil section
```

```
*-------------------------------------------------------------------------------


* The soil profile
* Specify for each horizon:
* Horizon thickness (m)
* The number of soil compartments [1|500]
* Nodes are distributed evenly over each horizon
table SoilProfile
ThiHor NumLay
(m)
0.3      12
0.2       8
0.2       4
0.3       6
2        20
end_table


* Basic soil parameters
* Specify for each soil horizon:
* Mass content of sand, expressed as a fraction of the mineral soil  (kg.kg-1)  [0|1]
* Mass content of silt, expressed as a fraction of the mineral soil  (kg.kg-1)  [0|1]
* Mass content of clay, expressed as a fraction of the mineral soil  (kg.kg-1)  [0|1]
* Organic matter mass content                                        (kg.kg-1)  [0|1]
* pH. pH measured in 0.01 M CaCl2 is preferred (see theory document) (-)        [1|13]
table  horizon SoilProperties
Nr     FraSand    FraSilt    FraClay    CntOm       pH
       (kg.kg-1)  (kg.kg-1)  (kg.kg-1)  (kg.kg-1)   (-)
1      0.92       0.05       0.03       0.0470      4.7
2      0.96       0.02       0.02       0.0080      4.4
3      0.95       0.03       0.02       0.0019      4.6
4      0.94       0.04       0.02       0.0014      4.6
5      0.93       0.05       0.02       0.0000      4.6
end_table


* Parameters of the Van Genuchten-Mualem relationships (B1 + O1)
* Specify for each soil horizon:
* The saturated water content   (m3.m-3)  [0|0.95]
* The residual water content    (m3.m-3)  [0|0.04]
* Parameter alpha               (cm-1)    [1.d-3|1]
* Parameter n                   (-)       [1|5]
* The saturated conductivity    (m.d-1)   [1.d-4|10]
* Parameter lambda (l)          (-)       [-25|25]
* New Staring Series - not used for standard scenario
table  horizon VanGenuchtenPar
Nr     ThetaSat   ThetaRes   Alpha      n         KSat      l
       (m3.m-3)   (m3.m-3)   (cm-1)     (-)       (m.d-1)   (-)
1      0.43       0.01       0.0249     1.507     0.1746    -0.140
2      0.43       0.01       0.0249     1.507     0.1746    -0.140
3      0.36       0.01       0.0224     2.167     0.1321     0.000
4      0.36       0.01       0.0224     2.167     0.1321     0.000
5      0.36       0.01       0.0224     2.167     0.1321     0.000
end_table

Input              OptRho                       Calculate or Input
* If RhoOpt = Input:
table horizon    Rho            (kg.m-3)   [100|2000]
1    1310.0
2    1540.0
3    1640.0
4    1650.0
5    1650.0
end_table


* End If


* Maximum ponding depth and boundary air layer thickness (both location properties)
0.01            ZPndMax        (m)        Maximum ponding depth [0|1]
0.01            ThiAirBouLay   (m)        Boundary air layer thickness [1e-6|1]

* Soil evaporation parameters
1.0             FacEvpSol      (-)        "Crop factor" for bare soil [0.5|1.5]
0.63            CofRedEvp      (cm1/2)    Parameter in Boesten equation [0|1]
```

```
* Parameter values of the functions describing the relative diffusion coefficients
MillingtonQuirk   OptCofDifRel              MillingtionQuirk, Troeh or Currie


* If MillingtonQuirk:
2.0               ExpDifLiqMilNom (-)       Exponent in nominator of equation [0.1|5]
0.67              ExpDifLiqMilDen (-)       Exponent in denominator of eqn    [0.1|2]
2.0               ExpDifGasMilNom (-)       Exponent in nominator of equation [0.1|5]
0.67              ExpDifGasMilDen (-)       Exponent in denominator of eqn    [0.1|2]


* If Troeh:
0.05              CofDifLiqTro    (-)       Coefficient in Troeh equation     [0|1]
1.4               ExpDifLiqTro    (-)       Exponent in Troeh equation        [1|2]
0.05              CofDifGasTro    (-)       Coefficient in Troeh equation     [0|1]
1.4               ExpDifGasTro    (-)       Exponent in Troeh equation        [1|2]


* If Currie:
2.5               CofDifLiqCur    (-)       Coefficient in Currie equation    [0|-]
3.0               ExpDifLiqCur    (-)       Exponent in Currie equation       [1|-]
2.5               CofDifGasCur    (-)       Coefficient in Currie equation    [0|-]
3.0               ExpDifGasCur    (-)       Exponent in Currie equation       [1|-]


* End If

* Dispersion length of solute in liquid phase [0.5Delz|1]
Table horizon LenDisLiq (m)
1  0.05
2  0.05
3  0.05
4  0.05
5  0.05
end_table



*-------------------------------------------------------------------------------------
* Section 3: Weather and irrigation data
*-------------------------------------------------------------------------------------

defscen           MeteoStation             Maximum 7 (!!) characters.
Input             OptEvp                   Evapotranspiration: Input, Penman or Makkink
52.0              Lat                      Latitude of meteo station [-60|60]
10.0              Alt             (m)      Altitude of meteo station [-400|3000]

* Initial lower boundary soil temperature [-20|40]
* Upper boundary temperature is read from meteo file
9.97              TemLboSta       (C)

* Irrigation section
No                OptIrr                   No, Surface or Sprinkler irrigation
defscen           IrrigationData           Maximum 7 (!!) characters.
* Irrigation data have to be provided in a file Station.irr (e.g. debilt.irr)
* If RepeatHydrology is set to Yes, the first year is required only
* Format of the file should be as below:
* table IrrTab (mm)
* 01-Aug-1980 10.0
* end_table


*-------------------------------------------------------------------------------------
* Section 4:  Boundary and initial conditions of hydrological model
* Section 4a: Lower boundary flux conditions
*-------------------------------------------------------------------------------------

* Initial condition
1.00              ZGrwLevSta      (m)      Initial groundwater level [0|50]

* Choose one of the following options:
* GrwLev Flux Head FncGrwLev Dirichlet ZeroFlux FreeDrain Lysimeter
FncGrwLev         OptLbo                   Lower boundary option

* LboOpt = GrwLev (groundwater level boundary condition)
table   GrwLev    (m)                      Groundwater level [0|-]
01-Jan  1.00
31-Dec  1.00
end_table

* LboOpt = Flux (flux lower boundary condition)
-0.250            FlvLiqLboAvg    (m.a-1)  Average annual lower boundary flux [-1|1]
0.10              FlvLiqLboAmp    (m)      Amplitude of lower-boundary flux [0|0.5]
```

```
01-Oct              DayFlvLiqLboMax             Day of maximum flux [01-Jan|31-Dec]

* LboOpt = Head (head lower boundary condition)
Elliptic            OptShapeGrwLev             Elliptic, Parabolic, Sinusoidal, NoDrains
-1.1                HeaDraBase      (m)        Drainage base to correct GrwLev [-100|0]
500.0               RstAqt          (d)        Resistance of aquitard [0|1e4]
-1.4                HeaAqfAvg       (m)        Mean hydraulic head of aquifer [-10|10]
0.2                 HeaAqfAmp       (m)        Amplitude of aquifer hydraulic head [0|10]
01-Apr              TimHeaAqfMax    (d)        Day with maximum head [01-Jan|31-Dec]

* LboOpt = FncGrwLev (flux boundary condition - flux is a function of groundwater level)
-0.0112             CofFncGrwLev    (m.d-1)    Coefficient in Q(h) relationship [-1|1]
-2.5                ExpFncGrwLev    (m-1)      Exponent in Q(h) relationship [-100|100]

* LboOpt = Dirichlet (pressure head boundary condition)
table    h  (m)                                Pressure head [-1e4|1e4]
01-Jan  -1.0
31-Dec  -1.0
end_table


*-------------------------------------------------------------------------------------------
* Section 4b: Local drainage fluxes to ditches and drains
*-------------------------------------------------------------------------------------------

0                   NumDraLev                  Number of drainage levels (0|5)

* Parameters below should be specified for each drainage level:
100.0               RstDra_1        (d)        Drainage resistance (10|1e5)
20.0                DistDra_1       (m)        Distance between drains or channels [1|1000]
1.5                 ZDra_1          (m)        Bottom of drain system [0|10]
Drain               TypDra_1                   Type of drain system: Drain or Channel


*-------------------------------------------------------------------------------------------
* Section 5: Compound section
*-------------------------------------------------------------------------------------------

* Compounds. First compound is the parent pesticide, the others are metabolites.
table compounds
pest
end_table
200.0               MolMas_pest     (g.mol-1)   Molar mass [10|10000]

* Transformation table (parent-daughter relationships)
* The "end" substance is the final transformation product
* Condition: Sum of rows should be 1 (see theory document)

table FraPrtDau (mol.mol-1)
pest    end
0.00    1.00   pest
end_table

* Example for a pesticide with two daughters, named "met1" and "met2":
* Line 1: pest is transformed into met1 (25%), met2 (70%) and undefined end products (5%)
* Line 2: met1 is transformed into met2 (16%) and undefined end products (84%)
* Line 3: met2 is transformed into undefined end products only (100%)
* table FraPrtDau (mol.mol-1)
* pest    met1   met2    end
* 0.00    0.25   0.70    0.05    pest
* 0.00    0.00   0.16    0.84    met1
* 0.00    0.00   0.00    1.00    met2
* end_table

* Transformation rate parameters
50.0                DT50Ref_pest    (d)        Half-life time [1|1e6]
20.0                TemRefTra_pest  (C)        Temperature at which DT50 is measured [5|30]
0.70                ExpLiqTra_pest  (-)        Exponent for the effect of liquid [0|5]
OptimumConditions OptCntLiqTraRef_pest         OptimumConditions or NonOptimumConditions
1.0                 CntLiqTraRef_pest (kg.kg-1) Liq. content at which DT50 is measured [0|1]
54.0                MolEntTra_pest  (kJ.mol-1) Molar activation energy [0|200]

*                                              Factor for the effect of depth [0|1]
table horizon FacZTra       (-)
1  1.00
2  0.95
3  0.74
4  0.33
5  0.00
```

```
end_table

* Freundlich equilibrium sorption
pH-independent     OptCofFre_pest              pH-dependent, pH-independent, CofFre
1.0                ConLiqRef_pest (mg.L-1)     Reference conc. in liquid phase [0.1|-]
0.9                ExpFre_pest    (-)          Freundlich sorption exponent [0.1|1.3]

* If pH-independent (use the coefficient for sorption on organic matter):
70.00              KomEql_pest    (L.kg-1)     Coef. eql. sorption on org. matter [0|1e9]

* If pH-dependent (use pKa value and coefficient for sorption on organic matter):
374.7              KomEqlAcid_pest (L.kg-1)    Coef. for eql. sorption on om - acid [0|1e9]
7.46               KomEqlBase_pest (L.kg-1)    Coef. for eql. sorption on om - base [0|1e9]
4.6                pKa_pest       (-)          Coef. for influence of pH on sorption [0|14]
0.0                pHCorrection   (-)          pH correction [-2|1]

* If CofFre (specify the depth dependence and the coefficient for equilibrium sorption):
1.0                KSorEql_pest   (L.kg-1)     Coef. for equilibrium sorption [0|1e9]
table horizon FacZSor        (-)              Factor for the effect of depth [0|1]
1   1.00
2   0.17
3   0.04
4   0.03
5   0.00
end_table

* End If

* Gas/liquid partitioning
0.0                PreVapRef_pest  (Pa)        Saturated vapour pressure [0|2e5]
20.0               TemRefVap_pest  (C)         .. measured at [0|40]
100.0              MolEntVap_pest  (kJ.mol-1)  Molar enthalpy of vaporisation [-200|200]
33.0               SlbWatRef_pest  (mg.L-1)    Solubility in water [1e-9|1e6]
20.0               TemRefSlb_pest  (C)         .. measured at [0|40]
40.0               MolEntSlb_pest  (kJ.mol-1)  Molar enthalpy of dissolution [-200|200]

* Non-equilibrium sorption
0.00               CofDesRat_pest  (d-1)       Desorption rate coefficient [0|0.5]
0.5                FacSorNeqEql_pest (-)       CofFreNeq/CofFreEql [0|-]

* Uptake
0.5                FacUpt_pest    (-)          Coefficient for uptake by plant [0|10]

* Canopy processes
Lumped             OptDspCrp                   Lumped or Specified

* If Lumped:
1.d6               DT50DspCrp     (d)          Half-life at crop surface [1|1e6]

* If Specified:
1.d6               DT50PenCrp     (d)          Half-life due to penetration [1|1e6]
1.d6               DT50VolCrp     (d)          Half-life due to volatilization [1|1e6]
1.d6               DT50TraCrp     (d)          Half-life due to transformation [1|1e6]

* End If

1.d-4              FacWasCrp      (m-1)        Wash-off factor [1e-6|0.1]

* Diffusion of solute in liquid and gas phases
4.3d-5             CofDifWatRef_pest (m2.d-1)  Reference diff. coeff. in water [10e-5|3e-4]
0.43               CofDifAirRef_pest (m2.d-1)  Reference diff. coeff. in air [0.1|3]
20.0               TemRefDif_pest  (C)         Diff. coeff measured at temperature [10|30]

*-------------------------------------------------------------------------------------
* Section 6: Management section
*-------------------------------------------------------------------------------------
1.0                ZFoc           (m)          Depth of Focus target layer [0.1|Z(N)-1]
NoRepeat           DelTimEvt      (a)          Repeat interval of events [NoRepeat|1|2|3]

* Event table:
* If AnnualEventSameDay is set to Yes, the year is not used.

* Column 1: Date
* Column 2: Event type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr, AppCrpLAI

* If Event = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]
```

```
* If EventType = AppCrp (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Optional: Fraction of dosage applied to the crop canopy (-) [0|1]

* If EventType = AppIrr (application in irrigation water):
* Column 3: Concentration (mg/L) - checked for compatability of Irrigation table (IrrTab)

* End If

table Applications
26-May-1980  AppSolSur 1
end_table

* Tillage table - can be empty
table TillageDates
end_table

*-------------------------------------------------------------------------------------------
* Section 7: Initial and boundary conditions of pesticide fate model
*-------------------------------------------------------------------------------------------
* Initial conditions                         Concentration in equilibrium domain [0|-]

* If using metabolites, ConSysEql should be specified for all metabolites
table interpolate CntSysEql      (mg.kg-1)
z       pest
0.0000   0.000
5.0000   0.000
end_table

* Initial conditions                         Concentration in non-equil. domain [0|-]
* If using metabolites, ConSysNeq should be specified for all metabolites
table interpolate CntSysNeq      (mg.kg-1)
z       pest
0.0000   0.000
5.0000   0.000
end_table

* Upper boundary flux                   [0|-]
table    FlmDep   (kg.ha-1.d-1)
01-Jan-1980  0.0
31-Dec-1989  0.0
end_table

* Concentration in irrigation water
0.0             ConIrr          (mg.L-1)   Concentration in irrigation water [0|-]

*-------------------------------------------------------------------------------------------
* Section 8: Crop section
*-------------------------------------------------------------------------------------------

Yes             RepeatCrops             Repeat crop table: Yes or No

* Emergence and harvest date of crop.
* Note: Length of growing season must be constant for one crop
* If reapeat crops: Specification of year not required
table  Crops
16-May-1980      04-Oct-1980   Maize
end_table

* Crop cycle fixed or variable (calculated from temperature sum)
Fixed   OptLenCrp                        Fixed or Variable

* If OptLenCrp = Variable:
0.0             TemSumSta_Maize     (C)   Start value of temperature sum [-10|20]
1050.0          TemSumEmgAnt_Maize  (C)   Sum from emergence to anthesis [0|1e4]
1000.0          TemSumAntMat_Maize  (C)   Sum from anthesis to maturity [0|1e4]

* End If

* Crop parameters as a function of development stage
* Column 1: Development stage: 0 = emergence; 1 = harvest (-)          [0|1]
* Column 2: LAI: Leaf Area Index                          (m2.m-2)     [0|12]
* Column 3: FacCrp: Crop factor                           (-)          [0|2]
* Column 4: ZRoot: Rooting depth                          (m)          [0|10]
* Column 5: HeightCrp:  Crop height                       (m)          [0|10]
*      LAI   FacCrp ZRoot  HeightCrp
```

```
table  CrpPar_Maize
0.000  0.00  1.00   0.00    0.01
0.099  0.20  1.00   0.10    0.05
0.241  0.95  1.00   0.20    0.20
0.383  1.90  1.00   0.30    1.00
0.525  2.95  1.00   0.40    1.70
0.596  3.40  1.00   0.41    1.70
0.667  3.60  1.00   0.44    1.75
0.738  3.70  1.00   0.40    1.80
0.879  3.60  1.00   0.40    1.80
1.000  3.50  1.00   0.30    1.80
end_table


* Root density table (first column is relative depth)
* Column 1: Relative depth 0 = soil surface; 1 = DepRoot  (-)          [0|1]
* Column 2: Root density distribution                     (-)          [0|1]
Table RootDensity_Maize
0.00        1.00
1.00        1.00
end_table


* Crop water use
-10.0           HLim1_Maize     (cm)     Anaerobiosis point  [-100|0]
 25.0           HLim2_Maize     (cm)     Wet reduction point [-1000|0]
-1000.0         HLim3L_Maize    (cm)     Dry reduction point [-10000|0]
-1000.0         HLim3U_Maize    (cm)     Dry reduction point [-10000|0]
-8000.0         HLim4_Maize     (cm)     Wilting point       [-16000|0]

70.0            RstEvpCrp_Maize (s.m-1)  Min. canopy resistance [0|1000]
0.5325          CofExtRad_Maize (-)      Extinction coef. for solar radiation [0|2]
1.d-4           CofIntCrp_Maize (cm)     Constant in Braden eq for interception [0|1]


*-------------------------------------------------------------------------------------
* Section 9: Output control
*-------------------------------------------------------------------------------------

* First, specify the time format in the output file:
* DaysFromSta  : Print number of days since start of simulation
* DaysFrom1900 : Print number of days since 1900
* Years        : Print years
DaysFromSta     DateFormat                      Format of time column in output file
No              OptDelOutput
Yes             PrintCumulatives


table VerticalProfiles
end_table


* Format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g = general is general notation
* Then follow the number of positions
* Then the number of digits
g12.4           RealFormat                      Format of ordinary output


* Second, specify the nodal heights for which output is requested
table OutputDepths (m)
0.05
0.10
0.15
0.20
0.25
0.50
1.00
1.50
2.00
3.00
end_table


* Finally, specify for all variables whether output is wanted (Yes or No)
* As Pearl can potentially generate large output files, it is recommended to minimise
* the number of output variables


* Section I : Output from the SWAP model, version 2.0.7c

* General variables
No              print_GrwLev            Groundwater level (m)
No              print_LAI               Leaf Area Index (m2.m-2)
No              print_ZRoot             Rooting depth (m)
```

```
No              print_FacCrpEvp     Crop factor (-)
No              print_FraCovCrp     Soil cover (-)
No              print_AvoLiqErr     Water balance error (m)


* State variables
No              print_Tem           Soil temperature (C)
No              print_Eps           Volumic air content (m3.m-3)
No              print_Theta         Volumic soil water content (m3.m-3)
No              print_PreHea        Soil water pressure head (m)

* Volumic volume rates (m3.m-3.d-1)
Yes             print_VvrLiqDra     Volumic volume rate of drainage
Yes             print_VvrLiqUpt     Volume flux of water uptake

* Volume fluxes (m3.m-2.d-1)
No              print_FlvLiq        Volume flux of vertical soil water flow
No              print_FlvLiqPrc     Volume flux of precipitation
No              print_FlvLiqIrr     Volume flux of water in irrigation
No              print_FlvLiqLbo     Volume flux of water leaching from the soil system
No              print_FlvLiqEvpIntPrc Evaporation flux of intercepted rainfall
No              print_FlvLiqEvpIntIrr Evaporation flux of intercepted irrigation
No              print_FlvLiqEvpSol  Volume flux of evaporation from the soil surface
No              print_FlvLiqEvpSolPot Idem, potential
No              print_FlvLiqTrp     Volume flux of transpiration by plant roots
No              print_FlvLiqTrpPot  Idem, potential
No              print_FlvLiqDra_1   Volume flux of drainage to level 1
No              print_FlvLiqDra_2   Volume flux of drainage to level 2
No              print_FlvLiqDra_3   Volume flux of drainage to level 3
No              print_FlvLiqDra_4   Volume flux of drainage to level 4
No              print_FlvLiqDra_5   Volume flux of drainage to level 5

* Section II : Output from the PEARL model
* Remark: All fluxes are averages over the print interval
*------------------------------------------------------

* Time step
No              print_DelTimPrl     Average time-step during the print interval (d)

* Mass balance (kg.m-2)
Yes             print_AmaEqlPro     Areic mass in equilibrium domain of profile
Yes             print_AmaEqlTil     Areic mass in equilibrium domain of tillage layer
Yes             print_AmaEqlFoc     Areic mass in equilibrium domain of focus layer
Yes             print_AmaNeqPro     Areic mass in non-eql. domain of profile
Yes             print_AmaNeqTil     Areic mass in non-eql. domain of tillage layer
Yes             print_AmaNeqFoc     Areic mass in non-eql. domain of focus layer
Yes             print_AmaSysPro     Areic mass of pesticide in the system
Yes             print_AmaSysTil     Areic mass of pesticide in the tillage layer
Yes             print_AmaSysFoc     Areic mass of pesticide in the focus layer
Yes             print_AmaAppSol     Areic mass applied to the soil system
Yes             print_AmaDraPro     Areic mass of lateral discharge
Yes             print_AmaForPro     Areic mass of formation
Yes             print_AmaTraPro     Areic mass of pesticide transformation
Yes             print_AmaUptPro     Areic mass of pesticide uptake
Yes             print_AmaDra_1      Areic mass of drainage to level 1
Yes             print_AmaDra_2      Areic mass of drainage to level 2
Yes             print_AmaDra_3      Areic mass of drainage to level 3
Yes             print_AmaDra_4      Areic mass of drainage to level 4
Yes             print_AmaDra_5      Areic mass of drainage to level 5
Yes             print_AmaErrPro     Areic numerical mass error

* Pesticide concentrations (kg.m-3) and contents (kg.kg-1)
No              print_ConLiq        Concentration in liquid phase
No              print_ConGas        Concentration in gas phase
No              print_ConSysEql     Concentration in equilibrium domain
No              print_ConSysNeq     Concentration in non-equilibrium domain
No              print_ConSys        Concentration in the soil system
No              print_CntSorEql     Mass content at soil solid phase
No              print_ConLiqSatAvg  Avg. conc.in liq. phase between 1-2 m

* Pesticide mass fluxes (kg.m-2.d-1)
No              print_FlmLiq        Pesticide mass flux in liquid phase
No              print_FlmGas        Pesticide mass flux in gas phase
No              print_FlmSys        Total pesticide mass flux (FlmLig+FlmGas)
No              print_FlmLiqLbo     Accumulated mass flux at the lower boundary
No              print_FlmLiqInf     Accumulated mass flux of pesticide infiltration
No              print_FlmGasVol     Accumulated mass flux of pesticide volatilisation
```

```
* Canopy interaction
*-------------------
No              print_AmaCrp        Areic mass of pesticide at the canopy
No              print_AmaAppCrp     Areic mass of pesticide applied to the canopy
No              print_AmrDspCrp     Areic mass rate of pesticide dissipation
No              print_AmaHarCrp     Areic mass rate of pesticide removal by harvest
No              print_AmrWasCrp     Areic mass rate of pesticide wash-off
No              print_FlmDepCrp     Areic mass rate of pesticide deposited on canopy
*----------------------------------------------------------------------------------------
* End of Pearl input file
*----------------------------------------------------------------------------------------
```

Appendix 3   Manual of PEARLNEQ

This appendix describes the PEARLNEQ-PEST combination, that can be used to obtain the half-life at reference temperature (DT50Ref), the desorption rate coefficient (CofRatDes), and the non-equilibrium sorption coefficient (FacSorNeqEql) in the case of sorption/desorption kinetics.. If the incubation experiment has been carried out at multiple temperatures, the molar activation energy (MolEntTra) can be optimized simultaneously.

The following steps must be followed.

1. Installation of PEST and it's components. To obtain PEST, please check the internet for appropriate addresses. Type 'pest+optimization' in the search engine box. You will find plenty of addresses were PEST can be ordered. You can start working immediately with PEST by downloading a light version of PEST, which is called PESTLITE. This version can be used if the total number of observations to be fitted does not exceed 80.

2. Before using the PEARLNEQ-PEST combination, you have to follow the additional installation instructions.

3. After a successful download of PEST, you have to install PEST. Unpack the file that you have downloaded or obtained; the installation program will give you the opportunity to specify a directory name (e.g. c:\pest). After unpacking, this directory must be added to your path statement; you must also assign this directory name to an environment variable called PESTDIR. Tip: If you add the PEST executables to the directory where you have already installed the PEARL executables, you don't need to extend your path again.

4. You can now start the optimization exercise, provided that appropriate incubation experiments have been carried out (see section 3.2.10). The first step of the optimization procedure consists of editing the file default.mkn, which can be found in the NEQ subdirectory of the PEARL package. *Please make a copy of this file before editing.* An example of this input file is listed at the end of this appendix.The following parameters must be provided:

   - TimEnd (d): The duration of the incubation experiment.
   - MasIni (µg): The initial total mass of pesticide in each jar.
   - MasSol (g): The total mass of soil incubated in each jar.
   - VolLiqSol (mL): Volume of liquid in the moist soil *before* incubation.
   - VolLiqAdd (mL): Volume of liquid added to the soil *after* incubation (i.e. the amount of liquid added to perform the conventional equilibrium experiment).
   - CntOm (kg.kg^{-1}): Mass fraction of organic matter in the soil.
   - ConLiqRef (mg L^{-1}): Reference concentration in the liquid phase (see page 66).
   - ExpFre (-): Freundlich exponent (see page 66).
   - KomEql (L kg^{-1}): coefficient of equilibrium sorption on organic matter (see page 66).
   - FacSorNeqEql (-): factor describing the ratio $K_{F,ne}/K_{F,eq}$ (page 67). *This parameter will be optimized,* but you have to specify an initial guess here. The default value is 0.5.

- CofRatDes (d^{-1}): the desorption rate coefficient. *This parameter will be optimized*, but you have to specify an initial guess here. The default value is 0.01 d^{-1}.
- DT50Ref (d): the transformation half-life under reference conditions. applying to the equilibrium domain. *This parameter will be optimized*, but you have to specify an initial guess here. As a default value, you can use the 'classical' half-life, which applies to the total soil system (i.e. the equilibrium domain + the non-equilibrium domain).
- TemRefTra (C): The reference temperature, at which the half-life should be known. The default values is 20 ^{o}C.
- MolEntTra (kJ mol^{-1}): the molar enthalpy of transformation. *This parameter will be optimized if you have carried out the experiment at multiple temperatures; otherwise it is a model-input*. If optimised, you have to specify an initial guess here. The default value is 54 kJ mol^{-1}.
- table Tem (C): List of temperatures at which the incubation experiment has been carried out. At least two temperatures must be specified.
- table Observations: List of observations. The first column contains the time (d), the second column the temperature, column 3 contains the total mass of pesticide in the system (μg), and column 4 should contain the concentration of pesticide in the suspension (μg L^{-1}).

5. After completing the input file, type the command MKNEQ default to prepare the input files for the PEST-PEARLNEQ combination (see figure).
6. MKNEQ will create the files default.pst, default.tpl and default.ins. These file are required by PEST.
7. If you are using PESTLITE, type wspestlt default to start the optimization. If using other PEST versions, please check your PEST manual.
8. After a successful optimization, read the results from the file default.rec. The relevant results, including parameter values, 95% ocnfidence intervals and corrllation matrices can be found at the end of this file.
9. If you encounter errors, you can try running PEARLNEQ directly. MKNEQ has created a file default.neq, which is the input file for PEARLNEQ. Type PEARLNEQ. pearlneq will create an output file (default.out) and a log file (default.log). The output files are self-explaining.
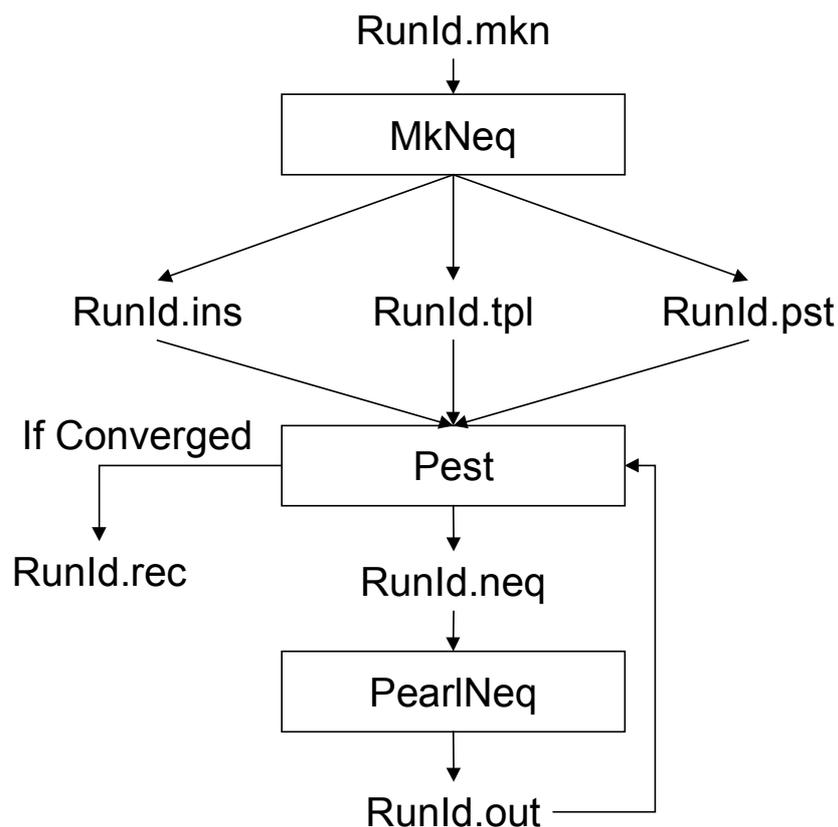
Figure 38 Dataflow diagram for the PEARLNEQ-PEST combination.

```
*------------------------------------------------------------------------------------------
* STANDARD FILE for MkNeq version 1.1.0.
* Program to fit the half-life, activation energy and desorption rate in the case of
* pesticide that show kinetic sorption behaviour
*
* This file is intented for use with the PEST program (Doherty et al., 1991).
*
* (c) RIVM/Alterra 15-Feb-2000
*------------------------------------------------------------------------------------------

* Model control
No              AcceptDefaults
500.0           TimEnd          (d)           Duration of the incubation experiment

* System characterization
45.36           MasSol          (g)           Mass of soil in the icubation jars
54.64           MasIni          (ug)          Initial mass of pesticide in the incubation jars
6.64            VolLiqSol       (mL)          Volume of liquid in the moist soil
0.0             VolLiqAdd       (mL)          Volume of liquid ADDED for equilibrium experiment
0.047           CntOm           (kg.kg-1)     Organic matter content

* Sorption parameter
1.0             ConLiqRef       (mg.L-1)      Reference liquid content
0.87            ExpFre          (-)           Freundlich exponent
2.1             KomEql          (L.kg-1)      Coefficient of equilibrium sorption on org. matter
0.5             FacSorNeqEql    (-)           Initial guess of ratio Kfneq/Kfeql
0.01            CofRatDes       (d-1)         Initial guess of desorption rate coefficient

* Transformation parameters
10.00           DT50Ref         (d)           Initial guess of half-life at reference temperature
20.0            TemRefTra       (C)           Reference temperature
54.0            MolEntTra       (kJ.mol-1)    Initial guess of molar activation energy

* Temperature at which the incubation experiments are being carried out
table Tem (C)
```

```
1  5.0
2  15.0
end_table

* Measured mass and concentration of pesticide as a funciton of time and temperature
* Tim  Tem  Mas       Con
* (d)  (C)  (ug)      (ug/L)
table Observations
2      5    51.6300   5.7285    OBS
10     5    50.5900   5.0560    OBS
42     5    46.0200   3.6635    OBS
87     5    38.6100   2.9320    OBS
157    5    32.8150   1.9280    OBS
244    5    25.8700   1.4650    OBS
358    5    20.3150   0.8820    OBS
451    5     9.4250   0.6015    OBS
2      15   51.3300   5.8955    OBS
6      15   47.3950   4.4425    OBS
10     15   45.0650   3.9510    OBS
42     15   23.1400   1.6470    OBS
87     15   10.8950   0.6710    OBS
157    15    3.1350   0.1525    OBS
244    15    1.4400   0.0305    OBS
358    15    0.4500   0.0000    OBS
451    15    0.1500   0.0000    OBS
end_table
```