SMASS - a simulation model of physical and chemical processes in acid sulphate soils

Version 2.1

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ABSTRACT

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The Simulation Model for Acid Sulphate Soils (SMASS) was developed to predict the effects of water management strategies in areas with potential or actual acid sulphate soils on acidification and de-acidification. The model is a combination of a solute transport submodel (TRANSOL), a chemical submodel (including EPIDIM) and a oxygen transport and pyrite oxidation submodel. The model can only be used in combination with the water transport model SWACROP. It combines physical processes like transport of water and solutes in unsaturated soil, and chemical processes like oxidation and reduction, complexation, adsorption/desorption and precipitation/dissolution of chemical compounds. The output data include the acidity and the chemical quality of soil and (ground) water, with special attention to the presence of toxic compounds.

The report is a users manual and presents a detailed outline of input and output files, guidelines for installation of the software on a VAX-VMS computer and the description of an application of the model, where the effects of drainage of an initially submerged soil are calculated over a period of 770 days.

Keywords: acid sulphate soils, modelling, drainage, leaching, oxidation, reduction, water management, reclamation, acidification, soil physics, soil chemistry,

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Contents

pag.

Preface 7

Summary 9

1 Introduction 11

2 Program description 15
2.1 Main chemical processes in acid sulphate soils 15
2.2 Model structure 16
2.3 Short description of the models and the main subroutines 19
2.4 Model input and output 21
2.4.1 Model input for SWACROP 21
2.4.2 Model output from SWACROP 22
2.4.3 Model input for SMASS 22
2.4.4 Model output from SMASS 22
2.5 Subroutine description 23

3 Program use 25
3.1 Input files for SWACROP and SMASS 25
3.2 Output files from SMASS 39

4 Program evaluation 49
4.1 Validation and application 49
4.2 Example of application 49

5 Installation 57

6 References 59

Figures
1 Structure of SMASS - a Simulation Model for Acid Sulphate Soils and relation to SWACROP 17
2 Schematization of a soil profile, as applied in the SMASS model. Arrows indicate water and solute fluxes. 18
3 The pyrite content of the soil at various times 50
4a The calculated course of the pH during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 51
4b The calculated course of the Fe^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 52

4c The calculated course of the Ca^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 53
4d The calculated course of the Mg^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 54
4e The calculated course of the Al^{3+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 55
4f The calculated course of the SO_4^{2-} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770) 56

Appendixes 63
1 Example of a complete set of input files and output files for SWACROP and SMASS 67
2 Description of required format for input files for SWACROP 5 105
3 Description of required format for input file for TRANSOL 157

Preface

The present simulation model was developed during the Research Program on Acid Sulphate Soils in the humid Tropics, an multi-disciplinary collaboration between the Indonesian Agency for Agricultural Research and Development (AARD) and the Dutch Land and Water Research Group (LAWOO). The AARD institutes involved are the Centre for Soil and Agroclimate Research (CSAR) and the Banjarbaru Research Institute for Food Crops (BARIF). The institutes participating in LAWOO are: the International Institute for Land Reclamation and Improvement (ILRI), the DLO Winand Staring Centre for Integrated Land, Soil and Water Research (SC-DLO), the Institute for Soil Fertility Research (AB-DLO) and the Institute for Forest and nature Management (IBN-DLO). Euroconsult BV provides the logistics of the Research Program. The research was done at both Banjarbaru and Wageningen.

The execution of the Program was made possible by financial contributions from The Netherlands Directorate-General for International Development Cooperation (DGIS), the Indonesian Ministry of Agriculture and The Netherlands Ministry of Agriculture, Nature Management and Fisheries. The Program started in the autumn of 1987; it was concluded mid 1992.

Field and laboratory experiments to study the main physical and chemical processes in acid sulphate soils, and to collect data for calibration and validation of the simulation model, were conducted in Delta Pulau Petak, Southern Kalimantan, Indonesia, a coastal plain with vast areas of potential and actual acid sulphate soils. The objectives, execution and results of this project have been reported in AARD (1992).

Summary

Reclamation, and in particular drainage, of potential acid sulphate soils initiates a number of physical and chemical processes. Physical ripening and structure formation upon drainage allow for penetration of oxygen into the soil leading to oxidation of pyrite and release of acidity. When oxidized, the soil may have a pH as low as 2.0. Under these conditions the diversity of crops that can be grown is restricted and yields are low. Moreover, the produced acid and toxic elements released, adversely affect groundwater and surface water quality inside and outside the reclaimed area. Subsequent submergence of already oxidized acid sulphate soils leads to various other problems, like H_2S and CO_2 toxicity and is only feasible when intensive leaching is applied as well.

The Simulation Model for Acid Sulphate Soils (SMASS) was developed to predict the effects of water management strategies in areas with potential or actual acid sulphate soils on acidification and de-acidification. The model is a combination of a solute transport submodel (TRANSOL), a chemical submodel (including EPIDIM) and a oxygen transport and pyrite oxidation submodel. The model can only be used in combination with the watertransport model SWACROP, and it combines physical processes like transport of water and solutes in unsaturated soil, and chemical processes like oxidation and reduction, complexation, adsorption/desorption and precipitation/dissolution of chemical compounds. The output data include the acidity and the chemical quality of soil and (ground) water, with special attention to the presence of toxic compounds.

The model was validated successfully by comparing model computations with measurements from lysimeter experiments and field experiments on various plots in South Kalimantan, Indonesia (AARD/LAWOO, 1993; Van Wijk et al., 1993; Ritsema and Groenenberg, 1993 and Bronswijk et al, 1994).

The report presents a detailed outline of input and output files, guidelines for installation of the software on a VAX-VMS computer and a description of an application of the model, where the effects of drainage of an initially submerged soil are calculated over a period of 770 days.

1 Introduction

There are in the world an estimated 12 million ha of acid sulphate soils. Acid sulphate soils are problem soils (Beek et al., 1980; Dost and Van Breemen, 1982; Dent, 1986). These soils contain pyrite (FeS_2), which upon exposure to oxygen oxidizes to sulphuric acid causing severe acidification. Because of their occurrence in coastal plains, acid sulphate soil areas have a favourable topography which appears to make them suited to (irrigated) agriculture. In addition they generally occur near densely populated areas where a continuous pressure on land resources exists.

Potential acid sulphate soils are waterlogged soils which are rich in pyrite that has not yet been oxidized and acidified. Main problem of the potential acid sulphate soils is waterlogging, resulting in unripeness of the topsoil, low bearing capacity and poor accessibility. To improve these conditions, large areas of potential acid sulphate soils were drained in the past. In a number of cases, this disastrously affected soil productive potential, resulting in abandonment of the area.

Reclamation, and in particular drainage, of potential acid sulphate soils initiates a number of physical and chemical processes. Physical ripening and structure formation upon drainage allow for penetration of oxygen into the soil leading to oxidation of pyrite and release of acidity. When oxidized, the soil may have a pH as low as 2. In connection to this acidification a number of chemical, biological and physical problems arise: aluminum and ferric iron toxicities, decreased availability of phosphate, nutrient deficiencies, arrested soil ripening, hampered root growth, blockage of drains by ochre and corrosion of metal and concrete structures (Dent, 1986). Under these conditions the diversity of crops that can be grown is restricted and yields are low. Moreover, the produced acid and toxic elements released, adversely affect groundwater and surface water quality inside and outside the reclaimed area. Subsequent submergence of already oxidized acid sulphate soils leads to various other problems, like H_2S and CO_2 toxicity and is only feasible when intensive leaching is applied as well.

The high degree of acidity (or potential acidity) of acid sulphate soils makes liming to neutralize the acid impracticable in most cases. The only practical way to manage these soils is by adequate soil and water management (Dent, 1986; Le Ngoc Sen, 1988). Maintaining high water tables controls the oxidation of pyrite and the rate of acid production. Drainage and leaching can be applied to remove acidity. Adequate water management and controlled drainage could minimize the acid production and maximize the leaching of oxidation products (Dost and Van Breemen, 1982).

Development of sound water management strategies for new land reclamation projects, or for rehabilitation of existing projects in coastal plains with (potential)

acid sulphate soils, would strongly benefit from the possibility to predict at forehand the (long-term) consequences of the various possible strategies. In this process a computer simulation model capable to forecast effects of water management on (de-)acidification and release of toxic compounds is a valuable tool, because it describes the complete sequence of soil physical and chemical processes taking place in specific situations in an integrated approach. By using long term climatic records as input data, a simulation model is especially suitable to predict the future long-term effects of various water management options.

Development of a simulation model is attractive not only for planning, design and engineering purposes but also from a scientific point of view. A model integrates knowledge on single processes, often from different disciplines (in case of acid sulphate soils from soil physics, soil chemistry and hydrology) in a coherent system based on the most recent state of knowledge. Making a model, the scientist has to understand and to make an inventory of all relevant single physical and chemical processes and next to understand the coherence between these processes. This requires system-thinking by the modeller. Building a model is also a mean to identify which relevant knowledge is missing, so which additional theoretical or experimental work is needed to arrive to an operational system. In this way model development may play an important role in research planning.

Therefore the model Simulation Model for Acid Sulphate Soils (SMASS) was developed. The objective of this model is to predict effects of water management strategies, like drainage, irrigation and leaching, on acidification and de-acidification of potential and actual acid sulphate soils under different conditions of soil and climate. The model was developed for evaluation of water management strategies and for scenario analysis on behalf of land reclamation or project rehabilitation studies. The model combines physical processes like transport of water and solutes in unsaturated soil, and chemical processes like oxidation and reduction, complexation, adsorption/desorption and precipitation/dissolution of chemical compounds. The output data include the acidity and the chemical quality of soil and (ground) water, with special attention to the presence of toxic compounds.

SMASS is a combination of a solute transport submodel (TRANSOL, see Kroes, 1991), a chemical submodel (including the chemical equilibria model EPIDIM, see Groenendijk, 1993) and a oxygen transport and pyrite oxidation submodel (see Bronswijk et al., 1993). SMASS can only be used in combination with the water transport model SWACROP (see Wesseling et al., 1991, included in this report in Annex 2). As the model is based on a so called quasi two dimensional water transport model; water and solute fluxes within the soil profile can be calculated as well as the cumulative fluxes of water and solutes to the surface water. This makes the model multi applicable. Firstly the chemical properties of the soil profile are predicted for agricultural purposes. Secondly the total load of acidifying components, transported to the surface water, can be calculated,

linking water management strategies in acid sulphate soil areas to possible negative environmental effects.

This report is a manual for the computer simulation model SMASS. In chapter 2 a short description is given of the main chemical processes in acid sulphate soils addressed to in the model, of the models structure and its subroutines and of the model input and output. Chapter 3 gives a detailed description of the input and output files that are specific files for SMASS. Chapter 4 elaborates on the validation of the model and gives an example for the application possibilities of the model. Chapter 5 gives the outline for the installation and use of the model in a VAX-VMS environment. The main text elaborates on SMASS model only. For detailed information on the water transport model SWACROP and the solute transport model TRANSOL the reader is referred to appendix 2 and appendix 3 of this manual.

2 Program description

2.1 Main chemical processes in acid sulphate soils

In this section we will give a brief summary of the chemical processes occurring in acid sulphate soils. For more details, refer to e.g. Dent (1986) or Van Breemen (1976).

Oxidation
If a pyrite containing soil layer is drained, oxidation will occur, according to the reaction (Van Breemen, 1976):

$$FeS_2 + 15/4O_2 + 1/2H_2O \rightarrow Fe^{3+} + 2SO_4^{2-} + H^+ \quad (1)$$

The ferric iron released in this reaction may precipitate as amorphous hydroxide, which is ultimately transformed into goethite and hematite. Under acid and oxidized conditions, jarosite is usually formed:

$$FeS_2 + 15/4O_2 + 5/2H_2O + 1/3K^+ \rightarrow 1/3KFe_3(SO_4)_2(OH)_6 + 4/3SO_4^{2-} + 3H^+ \quad (2)$$

Jarosite is stable under oxidized and acid conditions.

The acid released by these reactions will be partly neutralized by various buffer mechanisms. If present, calcite and/or dolomite, or sometimes siderite, will neutralize the produced acidity. In non calcareous soils or if the amount of produced sulphuric acid exceeds the content of these minerals, exchange of hydrogen ions against basic cations at the exchange complex will buffer the pH. In most acid sulphate soils the pH will drop below 4. At this pH aluminum minerals will buffer the pH and dissolve into the soil solution. Al^{3+} may reach concentrations which are toxic to plants (Cate and Sukhai, 1964; Moorman and Van Breemen, 1978).

High iron and aluminum concentrations will reduce the availability of phosphate. Also, aluminum will replace basic cations on the cation exchange complex, upon which these basic cations will be leached from the soil. Not only will the K^+ supply for plant growth become restricted, but also Mg^{2+} and Ca^{2+} deficiencies may be the result (Moore and Patrick, 1989). Low concentrations of basic cations also increase the plants susceptibility to iron toxicity (Van Mensvoort et al., 1985).

Finally, at very low pH (around 3) iron oxides will dissolve and buffer the pH of the soil solution.

Reduction
Flooding of an already acidified acid sulphate soil may alleviate the high concentrations of acid substances and their related toxicities, but some new problems are introduced.

Upon flooding, the supply of oxygen to the soil is stopped. After the present oxygen has been consumed, other compounds will act as the electron acceptor in the oxidation of organic matter. After oxygen nitrate is the strongest oxidator found in soils and is the first to be reduced. Thereafter, manganese oxides, iron (hydr)oxides and sulphate are reduced successively although some overlap may occur (Turner and Patrick, 1968). With the reduction of ferric (hydr)oxides the concentration of ferrous iron increases and hydrogen ions are consumed:

$$Fe(OH)_3 + 1/4CH_2O + 3H^+ \rightarrow Fe^{2+} + 1/4CO_2 + 11/4H_2O \quad (3)$$

The reduction of iron may lead to toxic concentrations of ferrous iron (Moorman and Van Breemen, 1978; Van Mensvoort et al., 1985). After the reduction of iron has stopped, sulphate reduction may start during which the sulphate concentration decreases and H^+ is consumed. H_2S, which accompanies sulphate reduction, is highly toxic to plants.

2.2 Model structure

The structure of SMASS is pictured in figure 1. Because the computations of SMASS are closely related to the computations of the watertransport model SWACROP, the position of this latter model in the calculation scheme is also given. In order to solve numerically the water, oxygen and solute transport equations the soil profile is divided into compartments of variable size (figure 2).

The computations are conducted in two steps. Firstly, the water transport is computed with the SWACROP model for the full simulation period. Secondly, the SWACROP output is used as input for the SMASS model and solute transport and chemcial reactions are computed.

At the beginning of a simulation run with SWACROP, the initial physical conditions of each compartment should be given as model input. For the complete simulation period, values for the boundary conditions, as given in figure 1, are required as input as well. At the end of a simulation run, the physical conditions in each compartment are output of the model, together with the water fluxes between the compratments and at the boundaries of the soil system.

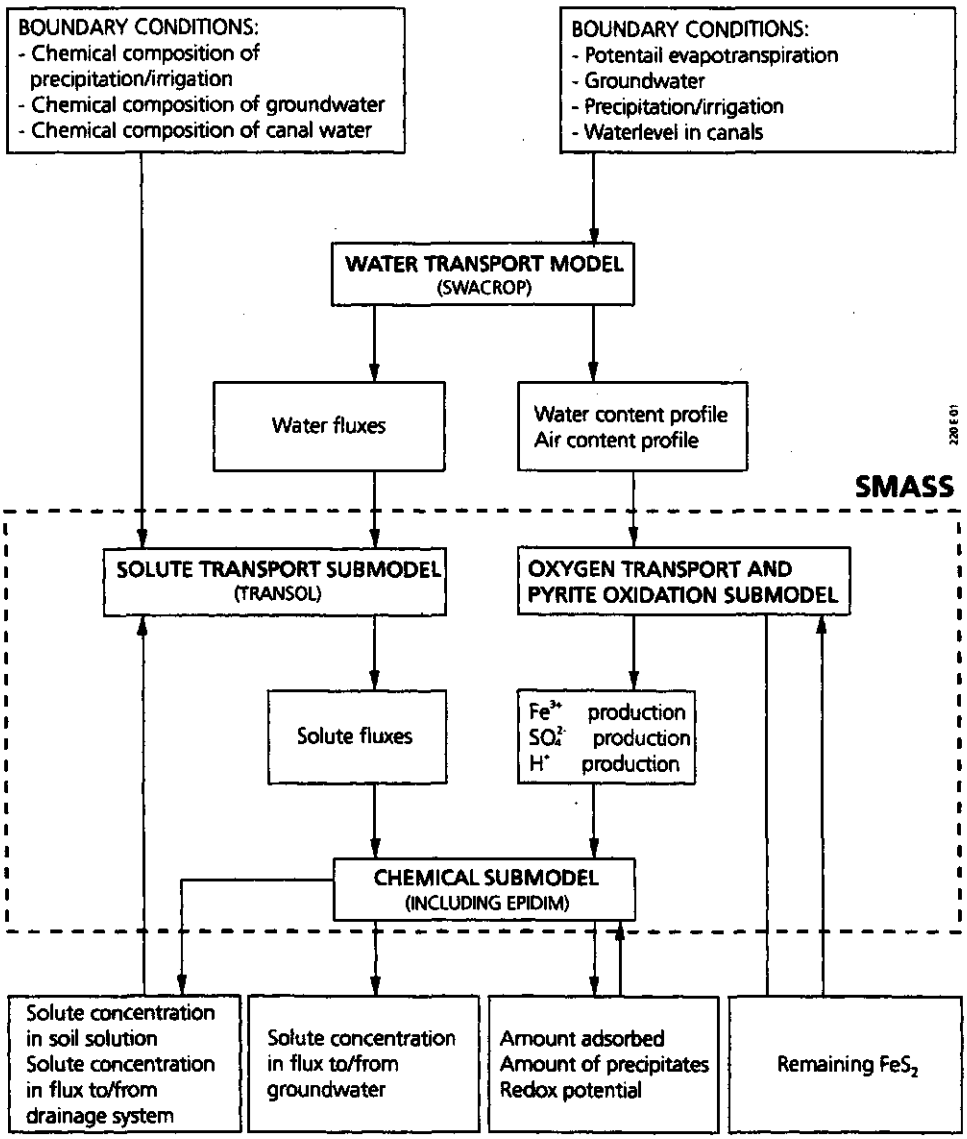

Fig. 1 Structure of SMASS - a Simulation Model for Acid Sulphate Soils and relation to SWACROP

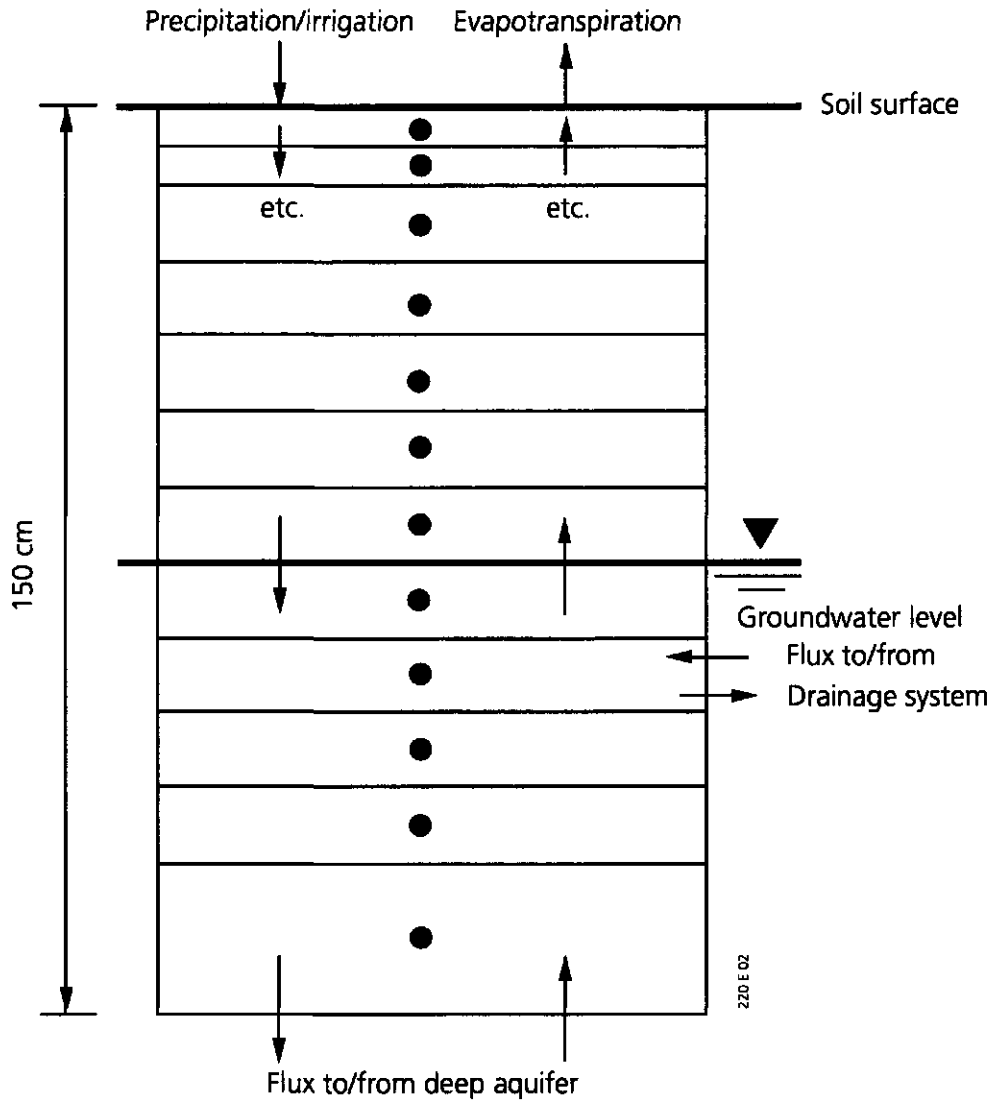

Fig. 2 Schematization of a soil profile, as applied in the SMASS model. Arrows indicate water and solute fluxes.

At the beginning of the subsequent run with SMASS, the initial physical and chemical conditions of each compartment should be given as model input. For the complete simulation period, values for the boundary conditions, as given in figure 1, are required as input as well. At the end of a simulation run, the physical and chemical conditions in each compartment are output of the model, together with the water and solute fluxes at the boundaries of the soil system.

figure 1 illustrates the sequence in which the various physical and chemical processes are computed:

1) Depending on the initial conditions in the various compartments, and the

boundary conditions, the vertical water transport in the soil profile is computed within the water transport model SWACROP. This yields for each day of the considered simulation period the water content profile in the soil. The air contents in the soil are complementary to the water contents. Furthermore, for each day of the simulation period, the fluxes between the compartments and at the boundaries of the soil system are given as output. All these data, that are required by SMASS, are stored in one output file.

2) SMASS reads the data from the SWACROP output file for the whole simulation period. Furthermore, the initial chemical conditions (e.g. mineral content, initial solute concentrations, etc.) and the chemical boundary conditions (e.g. composition of irrigation water) are read by SMASS.

For each day of the simulation period, steps 3) to 6) are now executed in SMASS:

3) First, from the air content profile, oxygen diffusion coefficients are calculated within the oxygen transport and pyrite oxidation submodel. From the pyrite and organic matter contents, oxygen consumption is calculated. Together, oxygen diffusion and oxygen consumption determine the oxygen profile in the soil.
4) Depending on the oxygen concentration at a given depth, the rate of pyrite oxidation at that depth is calculated within the oxygen transport and pyrite oxidation submodel. The oxidized amount of pyrite is converted into amounts of produced H^+, Fe^{3+}, SO_4^{2-}. The remaining amount of pyrite in the soil is used for calculations in the next time step.
5) The solute transport submodel computes solute fluxes between soil layers, depending on the water fluxes and the solute concentrations.
6) For each soil layer, the in- and outflow (step 5) and production (step 4) of chemical compounds is now calculated. As a result, a number of chemical processes will occur in each soil layer: complexation, precipitation/dissolution, oxidation/reduction, adsorption/desorption. These processes are all computed within the chemical submodel, resulting in computed concentrations of chemical compounds in the soil solution, composition of the exchange complex, amount of precipitates, and the concentration of elements in the flux to the groundwater and the surface water. Computations now start again for the next day with step 3).

Time steps used for the calculations of the water transport in SWACROP are in the order of minutes to hours. The output of SWACROP is given on a daily basis. This means that calculations with SMASS should also be carried out on a daily basis. The output frequency of the SMASS-model and its sub-models is optional, but minimally one day.

At present, model predictions can be carried out over a period of maximally ten years. In this way, long term effects of various water management strategies can be evaluated quantitatively.

2.3 Short description of the models and the main subroutines

SMASS requires water contents and water fluxes at the end of each day for each compartment as model input. The SWACROP (Wesseling et al., 1991) model has been used to computed this SMASS input. SWACROP is a recent version of the well-known water transport simulation model SWATRE (Belmans et al., 1983). In its original form, SWACROP is designed to read input files for a one-year period. If more (succesive) years need to be calculated, seperate input files with for example crop data or meteorological data need to be prepared. However, for irrigation data, it was not yet possible to read different irrigation gifts over a period of more than one year. Therefore, the used SWACROP model is slightly adapted, with the result that all input files may now contain as much as 4000 data's. In this way, periods of up to 10 years can be simulated in one run. For example, in section 4.2 one meteo file with 770 values is used for a two years simulation period. The same aplies to the irrigation data, the groundwater levels etc.

SWACROP simulates the water balance of a cropped soil with the possibility to chose between different types of boundary conditions. Simulation of irrigation, drainage to surface water and crop yield is optional.

Water transport is calculated for an average profile, assumed to be representative for the area in question. For calculations this one-dimensional profile is divided in compartments. For each time step the following parameters are calculated:
- vertical fluxes between the compartments, including the flux through the top of the profile at the soil surface and the bottom of the profile (either upwards or downwards);
- lateral drainage fluxes between each compartment and the drainage canals (both directions);
- moisture content for each compartment.

The crop production option of SWACROPis based on sole limitation of the production by water stress. Because in acid sulphate soils crop production is merely inhibited by toxic stress of acid, iron and aluminum, the crop production option is not suitable for application in SMASS.

In SMASS, solute transport is computed with the solute transport simulation model TRANSOL (Kroes, 1991). Because solute transport cannot be separated from chemical reactions, the TRANSOL model is incorporated as an integral part op SMASS. TRANSOL simulates the transport by mass flow, adsorption/desorption and transformation of solutes in soils. The model should be used in connection with a water transport model.

TRANSOL calculates solute transport, retardation and transformation by analytically solving a general transport and conservation equation for each layer.

For calculations in SMASS the adsorption option of TRANSOL is not used, because these processes are handled in EPIDIM. The transformation option is not used either, as the chemical species of interest in acid sulphate soils are not subject to transformation processes, meaning that in SMASS TRANSOL is used to calculate mass flow and dispersion only.

Chemical equilibria in SMASS are computed with the simulation model for chemical equilibria in soils, EPIDIM (Groenendijk, 1993). This model simulates equilibria in the aqueous phase, adsorption/desorption equilibria in relation to the solid phase and the kinetics of dissolution and precipitation of minerals.

EPIDIM assumes instantaneous equilibration within the aqueous phase and for adsorption to the solid phase. Equilibrium with precipitates may be rate-limited. The calculations are made for a set of aqueous species, adsorbing species and kinetic species, of interest for the studied problem. This set defines the chemical environment, within witch the processes occur. An example of such a set for acid sulphate soils is given in the appendix 1 (file COMPON.TAB).

Oxygen transport and pyrite oxidation in acid sulphate soils are computed with various subroutines in SMASS. SMASS simulates oxygen diffusion through the unsaturated soil, consumption of oxygen by the oxidation of organic matter and pyrite and the change of organic matter and pyrite content as a result of these processes.

Iron reduction is also a very important process in acid sulphate soils, because potentially reduction reduces acidity and increase the soil's pH. Iron reduction is computed in the subroutine IRON. The rate of iron reduction is assumed to be constant. Reduction only occurs if the oxygen content of a compartment is zero. Furthermore, freshly precipitated $Fe(OH)_3$ is easily reducable, while older crystaline forms (goethiet) are much more difficult to reduce. Therefore, in the model two forms of $Fe(OH)_3$ are distinguished: easily reducable $Fe(OH)_3$ and non-reducable $Fe(OH)_3$. Subroutine IRON calculates the amount easily reducable $Fe(OH)_3$ transformed into non-reducable $Fe(OH)_3$ according to a first order differential equation, where the rate depends on the soil pH (Schwertmann and Murad, 1983). For more details, refer to Bronswijk and Groenenberg (1993).

2.4 Model input and output

2.4.1 Model input for SWACROP

Top boundary conditions
Top boundary conditions for SWACROP are daily precipitation, actual evaporation, actual transpiration and irrigation. Actual evaporation and actual transpiration may be computed with various equations.

Bottom boundary conditions
Several bottom boundary conditions are optional in SWACROP (e.g. daily ground water level input, daily pressure head input in the bottom compartment, zero flux at bottom of the profile, free drainage).

Additional boundary condition
The water level in one to four levels of drainage systems is a daily varying boundary condition.

Initial conditions
For each layer: initial moisture conditions (either moisture content or pressure head) and initial groundwater level.

2.4.2 Model output from SWACROP

For each layer: moisture conditions (moisture content and pressure head), groundwater level (computed or echo from input), water fluxes between compartments and at the top and bottom boundary of the soil system, drainage fluxes, root extraction.

2.4.3 Model input for SMASS

Top boundary conditions
Top boundary conditions are precipitation (quantitative, from SWACROP output) plus chemical composition of precipitation, actual evaporation and transpiration (from SWACROP output), irrigation (quantitative and qualitative).

Bottom boundary conditions
Several bottom boundary conditions are optional in SMASS, corresponding with the SWACROP options (e.g. daily ground water level input, daily pressure head input in the bottom compartment, zero flux at bottom of the profile, free drainage). In al cases the quality of the water below the defined profile is a bottom boundary condition.

Additional boundary condition
Flux of water from one to four levels of drainage systems (from SWACROP output) is a daily varying boundary condition. The quality of the water should be given as model input.

Initial conditions
For each layer: initial moisture conditions (either moisture content or pressure head, from SWACROP output), initial composition of the soil moisture, CEC

(occupation of the adsorption complex is computed), initial pyrite content, initial organic matter content and initial content of precipitates.

2.4.4 Model output from SMASS

For each layer, per day: Moisture conditions (moisture content and pressure head, echo from input), chemical composition of the soil moisture, occupation of the adsorption complex, pyrite content, oxygen concentration in soil air, groundwater level (echo from input), produced amounts of H^+, SO_4^{2-} and Fe^{3+} by pyrite oxidation, content of precipitates, produced amounts of OH^-, HCO_3^- and Fe^{2+} by $Fe(OH)_3$ reduction, saturation indices for the considered precipitates, flux of all chemical components to the surface water.

2.5 Subroutine description

In this section the various SMASS-subroutines are described in alphabetical order. For description of the SWACROP, TRANSOL and EPIDIM subroutines the reader is referred to Kroes (1991) and Groenendijk (1993) and appendices 2 and 3.

SUBROUTINE:	FUNCTION:
ANAEROBIC:	calculates anaerobic volume of soil matrix and reduced oxygen consumption values
ASSIGN:	is an intermediar between SMASS and TRANSOL. As TRANSOL is made for calculations with one chemical component only and calculations with SMASS handle more chemical components, TRANSOL needs to be run for each separate component. ASSIGN copies values of one component to the input arrays of TRANSOL and stores the calculated values of each component.
CHEM:	intermediair between EPIDIM and SMASS
CHEMCHECK:	(optional) produces (1) output of input after initialization and (2) output of H^+-concentrations, OH^--concentrations, H^+-balance, Fe^{2+}-concentrations, Fe^{3+}-concentrations, Fe-balance and e-balance.
EPICHECK:	(optional) writes input and output of EPIDIM to output files.

INIDAT:	reads general input data.
INPOUT:	produces echo of the input.
IRON:	calculates (1) the transformation of freshly precipitated reducable $Fe(OH)_3$ into non-reducable $Fe(OH)_3$ (goethite) and (2) the reduction of reducable $Fe(OH)_3$, and the corresponding production of OH^-, Fe^{2+} and HCO_3^-.
IRRIG:	reads amount of irrigation and chemical composition for each day.
MIX:	calculates the new concentration in the ponding water as a result of a mixing process of ponding water, precipitation and irrigation.
OUTPSMASS:	produces output.
OXCO:	reads inputdata for calculation of oxygen concentrations
OXCONC:	calculates vertical oxygen concentration in macropore-air using values of diffusion coefficient and oxygen consumption
OXOUT:	writes pyrite contents, oxygen concentrations, etc. to the output file
OXYGEN:	calculates steady state oxygen profiles
PYRITE:	calculates amount of pyrite oxidized, remaining pyrite and produced H^+,Fe^{3+},SO_4^{2-}
SELECT:	selects wether or not (1) output is generated and (2) chemical calculations are carried out during the present time step.

3 Program use

3.1 Input files for SWACROP and SMASS

In order to run SMASS in combination with SWACROP, the 16 input files listed below should be prepared. The files 1 to 6 are SWACROP input files. The format description of these files is given in Appendix 2.

The files 7 and 8 are original TRANSOL files. The format description of these files is given in Appendix 3.

The files 9 to 14 and 16 are files newly created for this version of the SMASS. The format description of these files is given in this chapter. File 15 is an original EPIDIM input file. A format description of this file is given in this chapter as well. The description is based on Groenendijk (1993).

Input files for SWACROP

1. General input SWACROP (SWADAT.INP)
2. Input top boundary
3. Input of crop data
4. Input of soil physical data
5. Input bottom boundary data
6. Input of drainage data

Input files for SMASS

7. General input file for TRANSOL (GENERAL.INP)
8. Input of additions to the soil system (ADDIT.INP)

9. General input file for SMASS (GENFIL)
10. Input of initial soil properties (INIFIL)
11. Input of chemical soil data (CHEMFIL)
12. Input of oxygen regime parameters (OXFIL)
13. Input of irrigation data (quantity and quality) (IRRFIL)
14. Input of chemical composition of surface water (INFILFIL)
15. Input for EPIDIM with chemical components (COMTAB)
16. Additional information about the configuration of COMPTAB (HELPTAB)

SWACROP creates un unformatted output file with water balance data. The name of this file can be chosen in the input file SWADAT.INP. After running SWACROP this unformatted output file should be renamed to SWATRE.UNF and is input for further calculations with SMASS.

Each of the input files described below consists of a number of groups. Each group corresponds with one record in the input files. Groups are separated by a dotted line.

Input file 9: The file containing the general input data for SMASS (GENFIL)

Type	Symbol	GENFIL Description
C80	GENDSC	desired heading to be printed in output file
I	IRPAR	switch for irrigation (1=yes; 0=no)
I	INFILPAR	switch for input of surface water quality on a daily base (1) or constant in time (2)
C10	INIFIL	name of file containing initial concentrations of solutes
C10	CHEMFIL	name of file containing CEC, bulkdensity en initial concentrations of kinetic species.
C10	COMTAB	name of file containing the component table for chemical calculations
C10	OXFIL	name of input file with oxygen regime parameters
C10	(only if IRPAR=1) IRRFIL	name of input file with irrigation data
C10	(only if INFILPAR=1) INFILFIL	name of input file with surface water quality
R	COPRECIP(I)	chemical composition of precipitation water i = 1,NRCOMP If NRCOMP = 11 then: COPRECIP(1) pH COPRECIP(2) concentration of Na^+ (meq.l^{-1}). COPRECIP(3) concentration of K^+ (meq.l^{-1}). COPRECIP(4) concentration of Ca^{2+} (meq.l^{-1}). COPRECIP(5) concentration of Mg^{2+} (meq.l^{-1}). COPRECIP(6) concentration of Fe^{2+} (meq.l^{-1}). COPRECIP(7) concentration of Al^{3+} (meq.l^{-1}). COPRECIP(8) concentration of HCO_3^- (meq.l^{-1}). COPRECIP(9) concentration of SO_4^{2-} (meq.l^{-1}). COPRECIP(10) concentration of Cl^- (meq.l^{-1}). COPRECIPECIP (11) pE (= - log (59.2)*Eh (in mVolt))

R	COAQUIF(i)	chemical composition of aquifer water below the soil profile i = 1,NRCOMP If NRCOMP = 11 then: COAQUIF(1) pH COAQUIF(2) concentration of Na^+ ($meq.l^{-1}$). COAQUIF(3) concentration of K^+ ($meq.l^{-1}$). COAQUIF(4) concentration of Ca^{2+} ($meq.l^{-1}$). COAQUIF(5) concentration of Mg^{2+} ($meq.l^{-1}$). COAQUIF(6) concentration of Fe^{2+} ($meq.l^{-1}$). COAQUIF(7) concentration of Al^{3+} ($meq.l^{-1}$). COAQUIF(8) concentration of HCO_3^- ($meq.l^{-1}$). COAQUIF(9) concentration of SO_4^{2-} ($meq.l^{-1}$). COAQUIF(10) concentration of Cl^- ($meq.l^{-1}$). COAQUIF(11) pE (= - log (59.2)*Eh (in mVolt))
	(only if INFILPAR = 2, if INFILPAR = 1 or 0, give dummy values)	
R	COINFIL(i)	chemical composition of the lateral infiltrating surface water i = 1,NRCOMP If NRCOMP = 11 then: COPRECIP(1) pH COINFIL(2) concentration of Na^+ ($meq.l^{-1}$) COINFIL(3) concentration of K^+ ($meq.l^{-1}$) COINFIL(4) concentration of Ca^{2+} ($meq.l^{-1}$) COINFIL(5) concentration of Mg^{2+} ($meq.l^{-1}$) COINFIL(6) concentration of Fe^{2+} ($meq.l^{-1}$) COINFIL(7) concentration of Al^{3+} ($meq.l^{-1}$) COINFIL(8) concentration of HCO_3^- ($meq.l^{-1}$) COINFIL(9) concentration of SO_4^{2-} ($meq.l^{-1}$) COINFIL(10) concentration of Cl^- ($meq.l^{-1}$) COINFIL(11) pE (= - log (59.2)*Eh (in mVolt))
I	DTCHEM	time step for execution of chemical calculations (d). (we advise DTCHEM = 1)
I	DTOUTP	time interval for production of output (d).
I	FLAG_CHEM	flag for execution of subroutine CHEMCHECK
I	FLAG_EPI	flag for execution of subroutine EPICHECK
C10	OUTFIL1	name of output file to contain the calculated pH, pE and solute concentrations in all compartments

C10	OUTFIL2	name of output file to contain the calculated amounts of adsorbed components in all compartments
C10	OUTFIL3	name of output file to contain the calculated amounts of precipitates in all compartments
C10	OUTFIL4	name of output file with echo of the (general) input for water and solute data
C10	OUTFIL5	name of output file to contain the calculated saturation indices.
C10	OUTFIL6	name of output file to contain the calculated amounts of produced Fe^{2+}, H^-, OH^-, HCO_3^-, and SO_4^{2-} by pyrite oxidation and $Fe(OH)_3$ reduction
C10	OUTFIL7	name of output file to contain the output of the pyrite oxidation submodel.
C10	OUTFIL8	name of output file to contain the output of the solute flux to the surface water.

Input file 10: The file containing the initial water contents and solute concentrations in the soil profile (INIFIL).

Type	Symbol	INIFIL Description		
Number of chemical components (we advise NRCOMP = 11)				
*	*	data header		
R		CO(i,j)	i=1,NRCOMP	
		if NRCOMP = 11 then:		
		CO(1,j)	pH in soil solution (-)	One
		CO(2,j)	Na^+ concentration in soil solution ($meq.l^{-1}$)	line
		CO(3,j)	K^+ concentration in soil solution ($meq.l^{-1}$)	for
		CO(4,j)	Ca^{2+} concentration in soil solution ($meq.l^{-1}$)	each
		CO(5,j)	Mg^{2+} concentration in soil solution ($meq.l^{-1}$)	compart-
		CO(6,j)	Fe^{2+} concentration in soil solution ($meq.l^{-1}$)	ment
		CO(7,j)	Al^{3+} concentration in soil solution ($meq.l^{-1}$)	(j=1,NL)
		CO(8,j)	HCO_3^- concentration in soil solution ($meq.l^{-1}$)	
		CO(9,j)	SO_4^{2-} concentration in soil solution ($meq.l^{-1}$)	
		CO(10,j)	Cl^- concentration in soil solution ($meq.l^{-1}$)	
		CO(11,j)	initial pE of soil solution	
		This group consists of NL lines		

Input file 11: The file containing chemical data required for chemical equilibria calculation (CHEMFIL).

Type	Symbol	C H E M F I L Description	
*	*	data header	
. . . . .			
*	*	data header	
. . . . .			
I	RHOD	dry soil bulk density ($gr.cm^{-3}$)	
R	CEC(i)	Cation Exchange Capacity ($meq.100\ gr^{-1}$)	For each compart-ment
R	CPRE(1,i)	initial content of first precipitate ($mol.kg^{-1}$)	
R	CPRE(2,i)	initial content of 2^{nd} precipitate ($mol.kg^{-1}$)	
R	CPRE(npre,i)	initial content of $(npre)^{th}$ precipitate	
		Number of precipitates is indicated as NPRE in COMTAB	
		This group consists of NL lines	

Input file 12: The file containing the oxygen regime parameters (OXFIL).

Type	Symbol	O X F I L Description
*	*	general header
*	*	data header
R	RCLOD(i)	average aggregate radius per compartment (m) (i=1,NCS)
*	*	data header
R	OMCONT(i)	organic matter content per compartment ($kg.m^{-3}$) (i=1,NCS)
*	*	data header
R	OMOXCO(i)	oxygen consumption by organic matter (kg O2.kg^{-1} o.m..d^{-1}) (i=1,NCS)
*	*	data header
R	TORT(i)	tortuosity factor in diffusion equation per compartment (i=1,NCS)
*	*	data header
R	TEMSO	average soil temperature (°C)
R	DFCFCLOD	oxygen diffusion coefficient in saturated soil aggregate ($m^2.d^{-1}$)
R	HENRY	Henrys constant
R	OXMAX	oxygen concentration in air at TEMSO at 100% oxygen ($kg.m^{-3}$)
R	DFCFOXATM	diffusion coefficent of oxygen in atmosphere ($m^2.d^{-1}$)
*	*	data header
R	PYRCONT	initial pyrite content per compartment ($kg.m^{-3}$ soil) (i=1,NCS)
*	*	data header
R	PYRDIA	initial average pyrite diameter per compartment (m) (i=1,NCS)

Input file 13: The file containing information about the irrigation practices (IRRFIL)
(only used if IRPAR = 1)

Type	Symbol	IRRFIL Description	
*	*	data header	
R	TIRR	Julian day number of irrigation gift	
R	IRR	size of application ($m.d^{-1}$)	
R	COIRR(i)	i=1,NRCOMP	
		if NRCOMP =11 then:	For
		COIRR(2) Na^+ concentration of irrigation	
		water ($meq.l^{-1}$)	each
		COIRR(3) K^+ concentration of irrigation	
		water ($meq.l^{-1}$)	day
	COIRR(4)	Ca^{2+} concentration of irrigation	
		water ($meq.l^{-1}$)	that
	COIRR(5)	Mg^{2+} concentration of irrigation	
		water ($meq.l^{-1}$)	irrigation
	COIRR(6)	Fe^{2+} concentration of irrigation	
		water ($meq.l^{-1}$)	occurs
	COIRR(7)	Al^{3+} concentration of irrigation	
		water ($meq.l^{-1}$)	
	COIRR(8)	HCO_3^- concentration of irrigation	
		water ($meq.l^{-1}$)	
	COIRR(9)	SO_4^{2-} concentration of irrigation	
		water ($meq.l^{-1}$)	
	COIRR(10)	Cl^- concentration of irrigation	
		water ($meq.l^{-1}$)	
	COIRR(11)	pE of irrigation water	

Input file 14: The file containing the quality of surface water for lateral infiltration. (INFILFIL)
(only used if INFILPAR = 1)

Type	Symbol	INFILFIL Description	
*	*	data header	
. . . . .			
*	*	data header	
. . . . .			
I	dummy	julian daynummer	
R	COINFIL(i)	chemical composition of the lateral infiltrating surface water	
		i = 1,NRCOMP	
		If NRCOMP = 11 then:	
		COPRECIP(1) pH	I
		COINFIL(2) concentration of Na^+ (mmol.l^{-1})	I
		COINFIL(3) concentration of K^+ (mmol.l^{-1})	I for
		COINFIL(4) concentration of Ca^{2+} (mmol.l^{-1})	I
		COINFIL(5) concentration of Mg^{2+} (mmol.l^{-1})	I each
		COINFIL(6) concentration of Fe^{2+} (mmol.l^{-1})	I
		COINFIL(7) concentration of Al^{3+} (mmol.l^{-1})	I day
		COINFIL(8) concentration of HCO_3^- (mmol.l^{-1})	I
		COINFIL(9) concentration of SO_4^{2-} (mmol.l^{-1})	I
		COINFIL(10) concentration of Cl^- (mmol.l^{-1})	I
		COINFIL(11) pE (= - log (59.2)*Eh (in mVolt))	I

Input file 15: The file containing the parameters used for the calculation of chemical equilibria in Subroutine EPIDIM (COMTAB), after Groenedijk (1993)

Type	Symbol	C O M T A B Description
C80	TEXT	general header
C25	*	description of parameter
I5	NCOM	number of components
C25	*	description of parameter
I5	NSPE	number of species in aqueous phase
C25	*	description of parameter
I5	NADS	number of adsorbed species
C25	*	description of parameter
I5	NPRE	number of species involved in precipitation/dissolutionreactions
C25	*	description of parameter
I5	KNDADS	type of exchange relation to be used in adsorption calculations
C25	*	description of parameter
I5	INUMPH	column number containing pH
C25	*	description of parameter
I5	INUMPE	column number containing pE
C25	*	description of parameter
I5	MITR	maximum number of iterations
C25	*	description of parameter
F10.5	CONVRG	convergence criterium in iteration procedure

1X,A5	COMPNT(1)	name of component 1	
1X,A5	COMPNT(2)	name of component 2	
.	.	.	
.	.	.	
1X,A5	COMPNT(NCOM)	name of component NCOM	
		For i=1,NSPE, (two lines for each species):	
1X,A10	SPECIE(i)	name of species i	
I5	RWNUS(i)	number of components in species i	
I5	VALSPE(i)	valence of the species (aqueous phase)	
G10.4	LOGK0(i)	logarithm of equilibrium constant	
G10.4	STENTS(i)	standard enthalpy	
G10.4	SIZE(i)	parameter in Debye Huckel equation (see below)	
G10.4	WRKDBE(i)	parameter in Debye Huckel equation (see below)	
G10.4	EXTEN(i)	parameter in Debye Huckel equation (see below)	
1X,I3	RWVLS(i,j)	array number of component j of species i	For j= 1, RWNUS(i)
F7.3	STOCH(j)	stoichiometric coefficient of component j	
		The last two groups are repeated NSPE times	
		For I= 1,NADS, (two lines for each adsorbed component):	
1X,A10	ADSORP(i)	name of adsorbate i	
I5	RWNUA(i)	number of components in adsorbate i	
I5	VALADS(i)	valence of the adsorbate	
G10.3	KSEL(i)	selectivity constant	
1X,I3	RWVLA(i,j)	array number of component j of adsorbate i	For j= 1, RWNUA(i)
F7.3	STOCH(j)	stoichiometric coefficient of component j	

		The last two groups are repeated NADS times	
		For I = 1,NPRE, (two lines for each precipitate):	
1X,A10	PRECIP(i)	name of precipitate i	
I5	RWNUP(i)	number of components in precipitate i	
G10.3	LOGKSO(i)	logarithm of solubility product of component i	
G10.3	STENTP(i)	standard enthalpy for component i	
G10.3	RATEPRE(i)	reaction rate constant for precipitation of component i	
G10.3	RATEDIS(i)	reaction rate constant for dissolution of component i	
1X,I3	RWVLP(i,j)	array number of component j of precipitate i	For j= 1, RWNUP(i)
F7.3	STOCH(j)	stoichiometric coefficient of component j	
		The last two groups are repeated NPRE times	

NOTE: In its present form SMASS expects $Fe(OH)_3$ to be PRECIP(1). This is neccessary for a correct computation of iron reduction and the saturation index for $Fe(OH)_3$. Furthermore, jurbanite is PRECIP(2), and jarosite is PRECIP(3), both for the correct computation of saturation indices. If jurbanite and jarosite are not PRECIP(2) and PRECIP(3), the model computations remain valid but the computed saturation indices are without meaning. If $Fe(OH)_3$ is not PRECIP(1), iron reduction is computed wrongly, and computations become invalid.

Input file 16: The file containing additional information on the configuration of the file COMPON.TAB (HELPTAB)

H E L P . T A B

Type	Symbol	Description
I	INUMFE2	rotation number of Fe^{2+} in the component table
I	INUMFE3	rotation number of Fe^{3+} in the component table (always equals INUMPE I)
I	INUMHCO$_3^-$	rotation number of HCO_3^- in the component table
I	INUMSO4	rotation number of SO_4^{2-} in the component table
I	NUMSPEH	number of aquous species containing H^+
I	SPENUMH(i)	rotation number of first aquous species containing H^+
I	SPEFACH(i)	factor of H^+ in first H^+ containing aquous species
	. . .	i= 1 to NUMSPEH
I	SPENUMH(NUMSPEH)	rotation number of NUMSPEH-th H^+ containing aquous species.
I	SPEFACH(NUMSPEH)	factor of H^+ in NUMSPEH-th H^+ containing aquous species
I	NUMSPEOH	number of aquous species containing OH^-
I	SPENUMOH(i)	rotation number of first aquous species containing OH^-
I	SPEFACOH(i)	factor of OH^- in first OH^- containing aquous species
	. . .	i= 1 to NUMSPEOH
I	SPENUMOH(NUMSPEOH)	rotation number of NUMSPEOH-th OH^- containing aquous species.

I	SPEFACOH(NUMSPEOH)	factor of OH^- in NUMSPEOH-th OH^- containing aquous species.
I	NUMSPEFE2	number of aquous species containing Fe^{2+}
I	SPENUMFE2(i)	rotation number of first aquous species containing Fe^{2+}
I	SPEFACFE2(i)	factor of Fe^{2+} in first Fe^{2+} containing aquous species
	. . .	i= 1 to NUMSPEFE2
I	SPENUMFE2(NUMSPEFE2)	rotation number of NUMSPEFE2-th Fe^{2+} containing aquous species.
I	SPEFACFE2(NUMSPEFE2)	factor of Fe^{2+} in NUMSPEFE2-th Fe^{2+} containing aquous species
I	NUMSPEFE3	number of aquous species containing Fe^{3+}
I	SPENUMFE3(i)	rotation number of first aquous species containing Fe^{3+}
I	SPEFACFE3(i)	factor of Fe^{3+} in first Fe^{3+} containing aquous species
	. . .	i= 1 to NUMSPEFE3
I	SPENUMFE3(NUMSPEFE3)	rotation number of NUMSPEFE3-th Fe^{3+} containing aquous species.
I	SPEFACFE3(NUMSPEFE3)	factor of Fe^{3+} in NUMSPEFE3-th Fe^{3+} containing aquous species

3.2 Output files from SMASS

The model SMASS creates default 10 output files. Optionally 10 extra files can be produced by activating the subroutines EPICHECK and CHEMCHECK. It is advised to do so only if specific information on the chemical calculations is required, or if the model is in a test phase.

Default output files:

1. File with chemical output data (pH, solute concentrations, pE) for selected output intervals (OUTFIL1).
2. File with chemical output data (contents of adsorbed components) for selected output intervals (OUTFIL2).
3. File with chemical output data (amounts of precipitates) for selected output intervals (OUTFIL3).
4. File with output of general SMASS-input (OUTFIL4).
5. File with calculated saturation indices (OUTFIL5).
6. File with produced amounts of H^+, OH^-, Fe^{3+}, Fe^{2+}, HCO_3^- and SO_4^{2-} (OUTFIL6).
7. File with output related to pyrite oxidation and oxygen transport (OUTFIL7).
8. Output file with solute fluxes to surface water (OUTFIL8)
9. Messages produced by SMASS (MESSAGE1.OUT).
10. Messages produced by subroutine TRANSOL (MESSAGE2.OUT).

Optional output files:

1. File with activities, input for EPIDIM (ACTIN.OUT)
2. File with activities, output of EPIDIM (ACTOUT.OUT)
3. File with concentrations of adsorbing components, input for EPIDIM (ADSIN.OUT).
4. File with concentrations of adsorbing components, output of EPIDIM (ADSOUT.OUT).
5. File with solute concentrations, input for EPIDIM (CONSIN.OUT).
6. File with solute concentrations, output of EPIDIM (CONSOUT.OUT).
7. File with amounts of precipitates, input for EPIDIM (PRECIN.OUT)
8. File with amounts of precipitates, output of EPIDIM (PRECOUT.OUT)
9. File with concentrations of components in surface water, precipitation water ans soil water after initialisation (CHEMCHECK1.OUT)
10. File with output of H^+ concentrations, OH^- concentrations, H^+ blance, Fe^{3+} concentrations, Fe^{2+} concentrations, Fe balance and e balance. (CHEMCHECK2.OUT).

In next part the contents of the default output files 1 to 8 are described in detail. In each output file, the daynumber and timestep number are given.

Output file 1: The file with chemical output data (pH, solute concentrations, pE) for selected output times (OUTFIL1).

For each day of output:

. . . . . .

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
PEHA(I)	: pH of compartment I
CEQ(J,I)	: concentration of chemical components in soil solution ($meq.l^{-1}$)
J=1,NRCOMP+1	if NRCOMP = 11 then: CEQ(1) = H^+ concentration CEQ(2) = Na^+ concentration CEQ(3) = K^+ concentration CEQ(4) = Ca^{2+} concentration CEQ(5) = Mg^{2+} concentration CEQ(6) = Fe^{2+} concentration CEQ(7) = Al^{3+} concentration CEQ(8) = HCO_3^- concentration CEQ(9) = SO_4^{2-} concentration CEQ(10) = Cl^- concentrtaion CEQ(11) = Fe^{3+} concentration
PEE(I)	: pE of compartment I

Output file 2: The file with chemical output data (contents of adsorbed components) for selected output times (OUTFIL2)

For each day of output:

. . . . . .

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
CADS(J,I)	: Adsorbed amount at exchange comples (meq. 100 gr^{-1} dry soil)
J=1,NADS	if NADS = 7 then: CADS(1) = H^+ adsorbed CADS(2) = Na^+ adsorbed CADS(3) = K^+ adsorbed CADS(4) = Ca^{2+} adsorbed CADS(5) = Mg^{2+} adsorbed CADS(6) = Fe^{2+} adsorbed CADS(7) = Al^{3+} adsorbed

Output file 3: The file with chemical output data (contents of precipitates) for selected output times (OUTFIL3)

For each day of output:

. . . . . .

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
CPRE(J,I) J=1,NPRE	: Amount of precipitates (mol.kg^{-1} dry soil) if NPRE = 3: CPRE(1) = Amount of $Fe(OH)_3$ CPRE(2) = Amount of jurbanite CPRE(3) = Amount of jarosite

NOTE: The kinetic species of the component table will be printed here. The names of the variables listed above are examples.

Output file 4: The file with output of general SMASS-input (OUTFIL4).

CO(J,I)	: initial solute concentrations for all compartments (meq.l^{-1}).
RHOD(I)	: dry bulkdensity in (gr.cm^{-3}) of all compartments.
CEC(I)	: Cation Exchange Capacity (meq.100 g^{-1}) of all compartments.
COPRECIP(J)	: Concentrations of considered components in precipitation (mmol.l^{-1}).
COAQUIF(J)	: Concentrations of considered components in aquifer (mmol.l^{-1}).
COINFIL(J)	: Concentrations of considered components in lateral infiltrating surface water (mmol.l^{-1}).

Output file 5: The file with calculated saturation indices (OUTFIL5).

For each day of output:

. . . . . .

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
SATIND1	: saturation index for $Fe(OH)_3$
SATIND2	: saturation index for jurbanite
SATIND3	: saturation index for jarosite

Output file 6. The file with produced amounts of H, Fe and SO_4 (OUTFIL6).

For each day of output:

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
HPROD(I)	: produced H^+ through oxidation of pyrite in last time-step for each compartment (mol.l^{-1} soil solution)
FEPROD(I)	: produced Fe^{3+} through oxidation of pyrite in last time-step for each compartment (mol.l^{-1} soil solution)
SO4PROD(I)	: produced SO_4^{2-} through oxidation of pyrite in last time-step for each compartment (mol.l^{-1} soil solution)
PYROX(I)	: amount of pyrite oxidized in last time-step (kg/m^3 soil)
OHPROD(I)	: produced OH^- through reduction of $Fe(OH)_3$ in last time-step for each compartment (mol.l^{-1} soil solution)
FE2PROD(I)	: produced OH^- through reduction of $Fe(OH)_3$ in last time-step for each compartment (mol.l^{-1} soil solution)
HCO3PROD(I)	: produced HCO_3^- through reduction of $Fe(OH)_3$ in last time-step for each compartment (mol.l^{-1} soil solution)
HPRODTOT	: Amount of H^+ produced through pyrite oxidation in last time-step for whole soil profile (mol/m^2)
SO4PRODTOT	: Amount of SO_4^{2-} produced through pyrite oxidation in last time-step for whole soil profile (mol.m^{-2})
FEPRODTOT	: Amount of Fe^{3+} produced through pyrite oxidation in last time-step for whole soil profile (mol.m^{-2})
PYROXTOT	: Amount of pyrite oxidized in last time-step for whole soil profile (kg.m^{-2})
HPRODCUM	: Amount of H^+ produced through pyrite oxidation since start of simulation for whole soil profile (mol.m^{-2})
SO4PRODCUM	: Amount of SO_4^{2-} produced through pyrite oxidation since start of simulation for whole soil profile (mol.m^{-2})

FEPRODCUM	: Amount of Fe^{3+} produced through pyrite oxidation since start of simulation for whole soil profile ($mol.m^{-2}$)
PYROXCUM	: Amount of pyrite oxidized since start of simulation for whole soil profile ($kg.m^{-2}$)

Output file 7: The file with output produced by the 'oxygen transport and pyrite oxidation sub-model' (OUTFIL7).

For each day of output:

ITO	: number of iterations required to reach convergence in last time step
SUSQDI	: sum of squares of difference for last two computed oxygen profiles in last time step
DTCHEM	: time step for chemical computations (d)
NUAE	: number of aerated layers
SUOXDDRAM	: total oxygen consumption by the soil profile (kg $O_2.m^{-2}.d^{-}$)
WALET	: groundwater level (m)

For each compartment:

I	: number of soil compartment with numbering starting from top to bottom
DP(I)	: position of the nodal point with respect to the soil surface (m)
SC(I)	: pressure head for layer i (cm)
MOFR(I)	: moisture fraction for layer i
100 * OXCO2(I)	: oxygen concentrations in macropore air (%)
100 * AEVO(I)	: aerobic volume (%)
PYRPERC(I)	: pyrite content (weight percentage)
PYRCONT(I)	: pyrite content ($kg.m^{-3}$ soil)
PYRDIA(I)	: average diameter pyrite crystals (m)
RDOXDDRAM(I)	: oxygen consumption (kg $O_2.m^{-3}$ soil.d^{-1})

Output file 8: The file with output of solute fluxes to surface water (OUTFIL8).

For each day of output:

TIWA	: day of output
YR	: year
SOLFLUX(J)	: load of solutes to surface water via drainage in last time step (mol/ha) if NRCOMP = 11 then: SOLFLUX(1) = H^+ load SOLFLUX(2) = Na^+ load SOLFLUX(3) = K^+ load SOLFLUX(4) = Ca^{2+} load SOLFLUX(5) = Mg^{2+} load SOLFLUX(6) = Fe^{2+} load SOLFLUX(7) = Al^{3+} load SOLFLUX(8) = HCO_3^- load SOLFLUX(9) = SO_4^{2-} load SOLFLUX(10) = Cl^- load SOLFLUX(11) = Fe^{3+} load
SOLFLUXTOT(J)	: same as above but then since start of simulations

4 Program evaluation

4.1 Validation and application

The SMASS model has been validated succesfully by comparing model computations with measurements from: i) two-year lysimeter experiments using actual and potential acid sulphate soils from Indonesia (AARD/LAWOO, 1993; Van Wijk et al., 1993), ii) two-year lysimeter experiments using potential acid sulphate soils from the Netherlands (Ritsena and Groeneneberg, 1993), iii) two year measurements from various field plots in Southern Kalimantan, Indonesia (AARD/LAWOO, 1993; Van Wijk et al., 1993; Bronswijk et al., 1994).

Examples of model application in the evaluation of various water management options for a coastal plain in South Kalimantan, Indonesia, are presented in AARD/LAWOO (1993) and Bronswijk et al. (1994).

4.2 Example of application

In this section an example of application of SMASS is presented. The complete set of input and output files is given in appendix 1. The example deals with the dranaige of a potential acid sulphate soil from Belawang, South Kalimantan, Indonesia. An initially submerged soil, with high pyrite contents, and reletively high pH is drained for a period of 442 days. Thereafter the soil was submerged for 1 month. Following submergence, the soil was leached under saturated conditions during a period of some 300 days. SMASS was used to compute the chemical changes that are caused by this drainage, submergence and leaching. The presented example corresponds with the laboratory experiments and model validation described in AARD/LAWOO (1993) (Chapters 3 and 7, column A).

In figure 3 the pyrite contents of the soil at various times are presented. In figure 4 the changes in chemical composition of the soil solution are given.

It is clear that lowering the groundwater level in a water logged potential acid sulphate soil below the pyritic layer, leads to rapid and severe acidification. Subsequent submergence increases the pH and the Fe concentration somewhat as a result of reduction processes. Only after leaching, however, there is a significant increase in pH and an improvement of soil conditions.

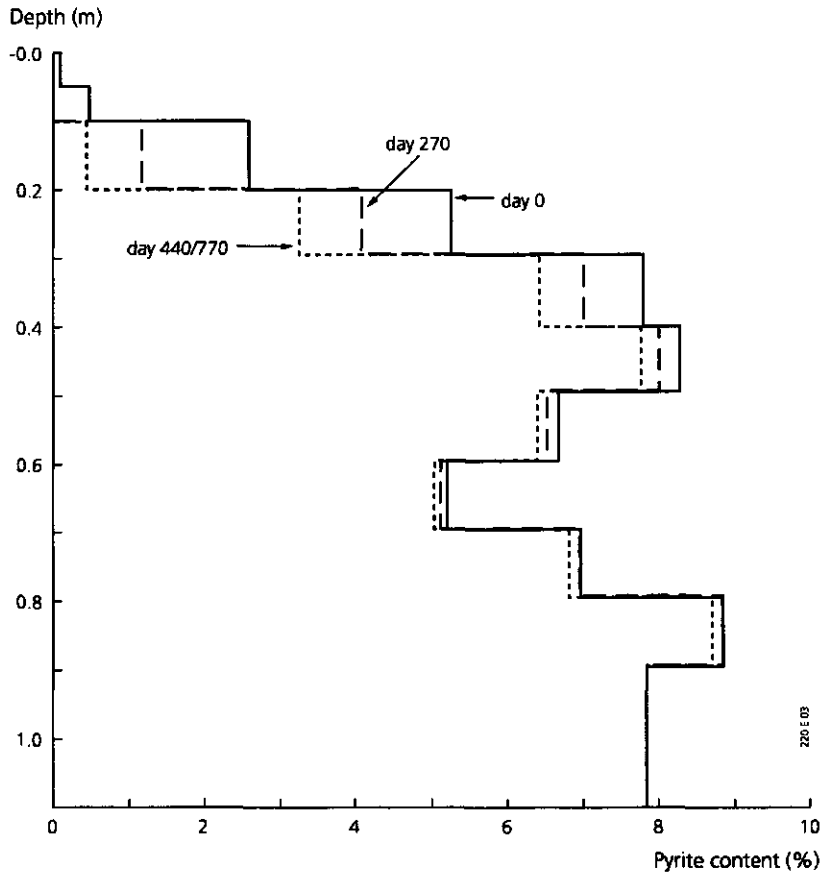

Fig. 3 The pyrite content of the soil at various times

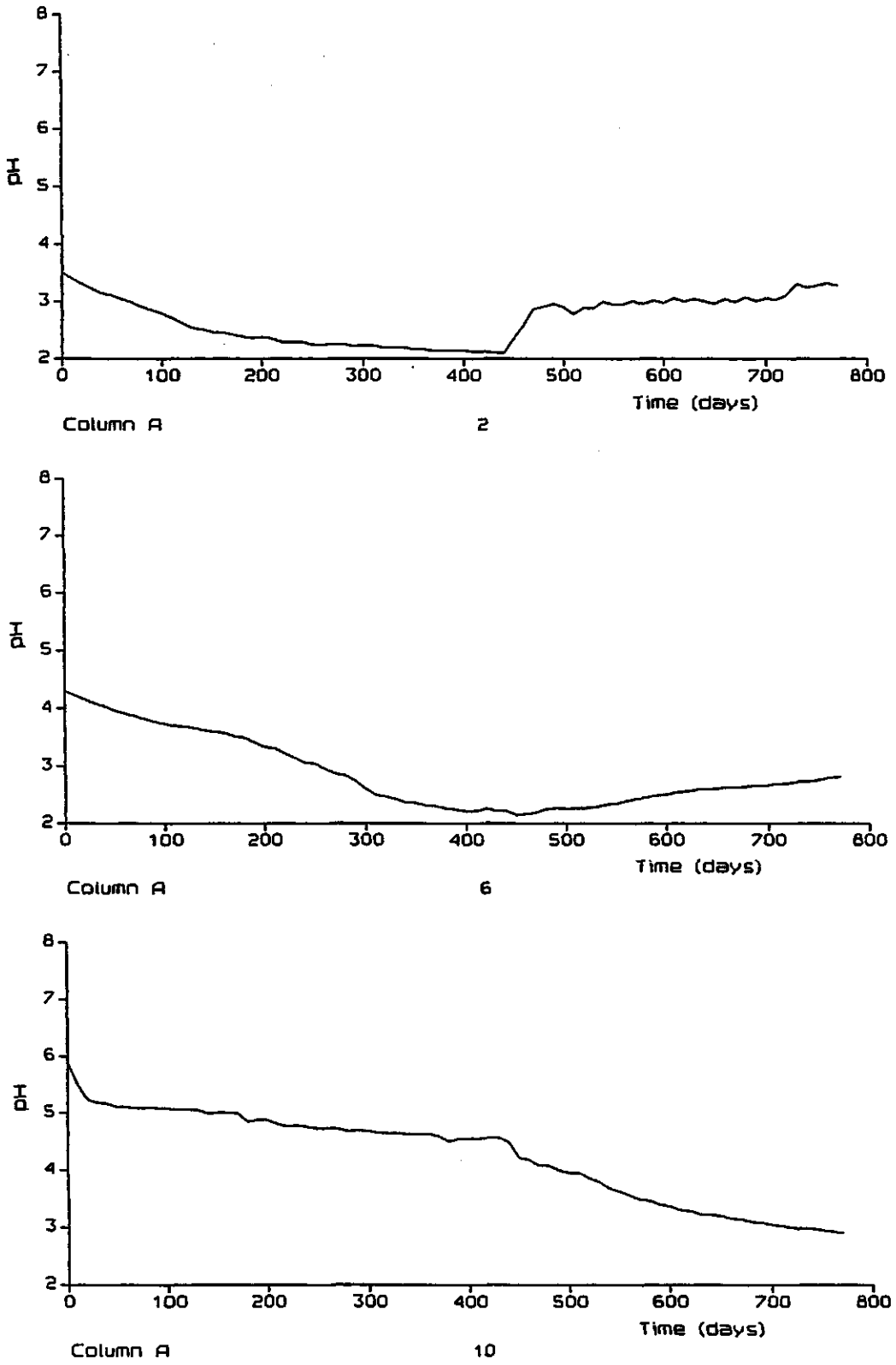

Fig. 4a The calculated course of the pH during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

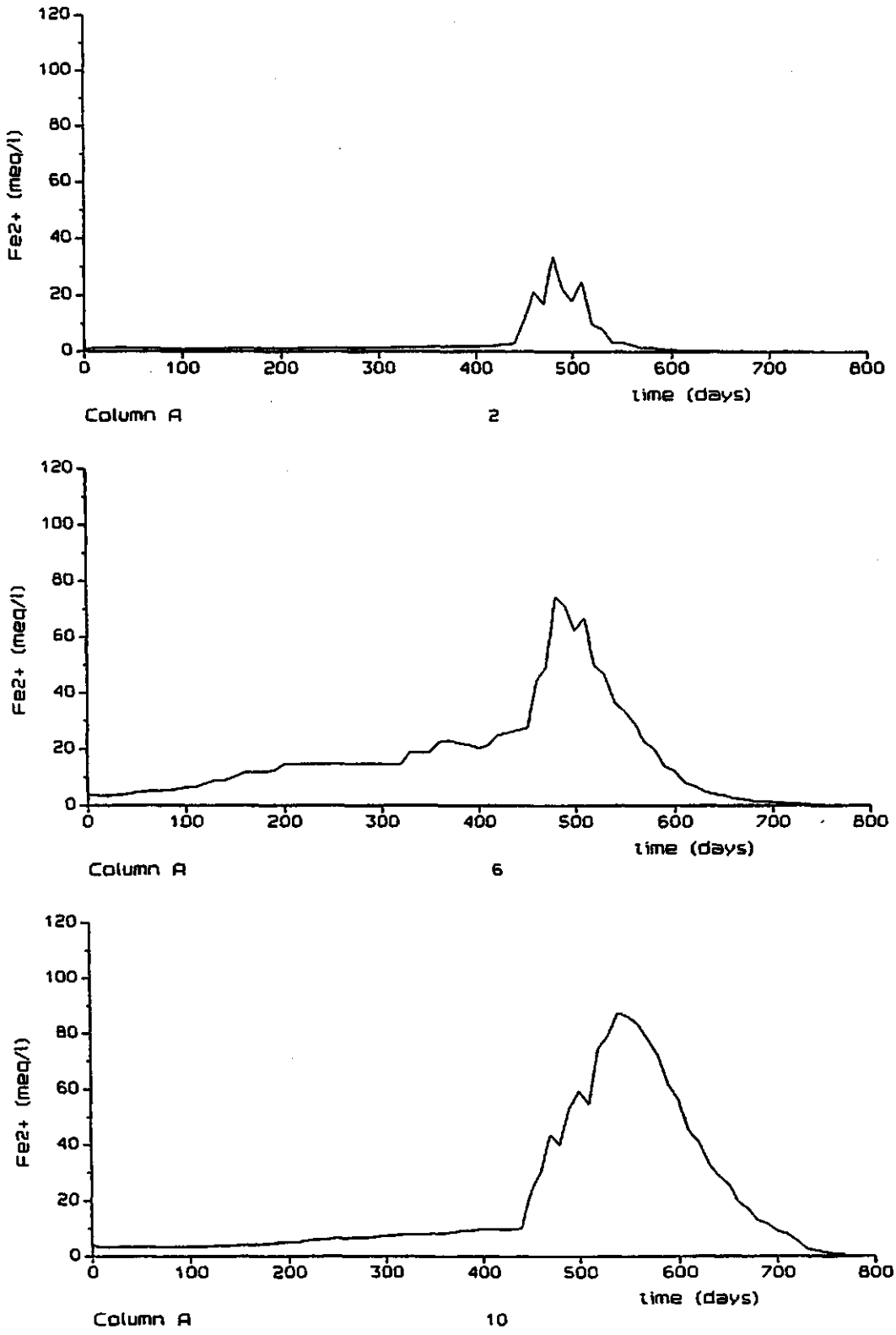

Fig. 4b The calculated course of the Fe^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

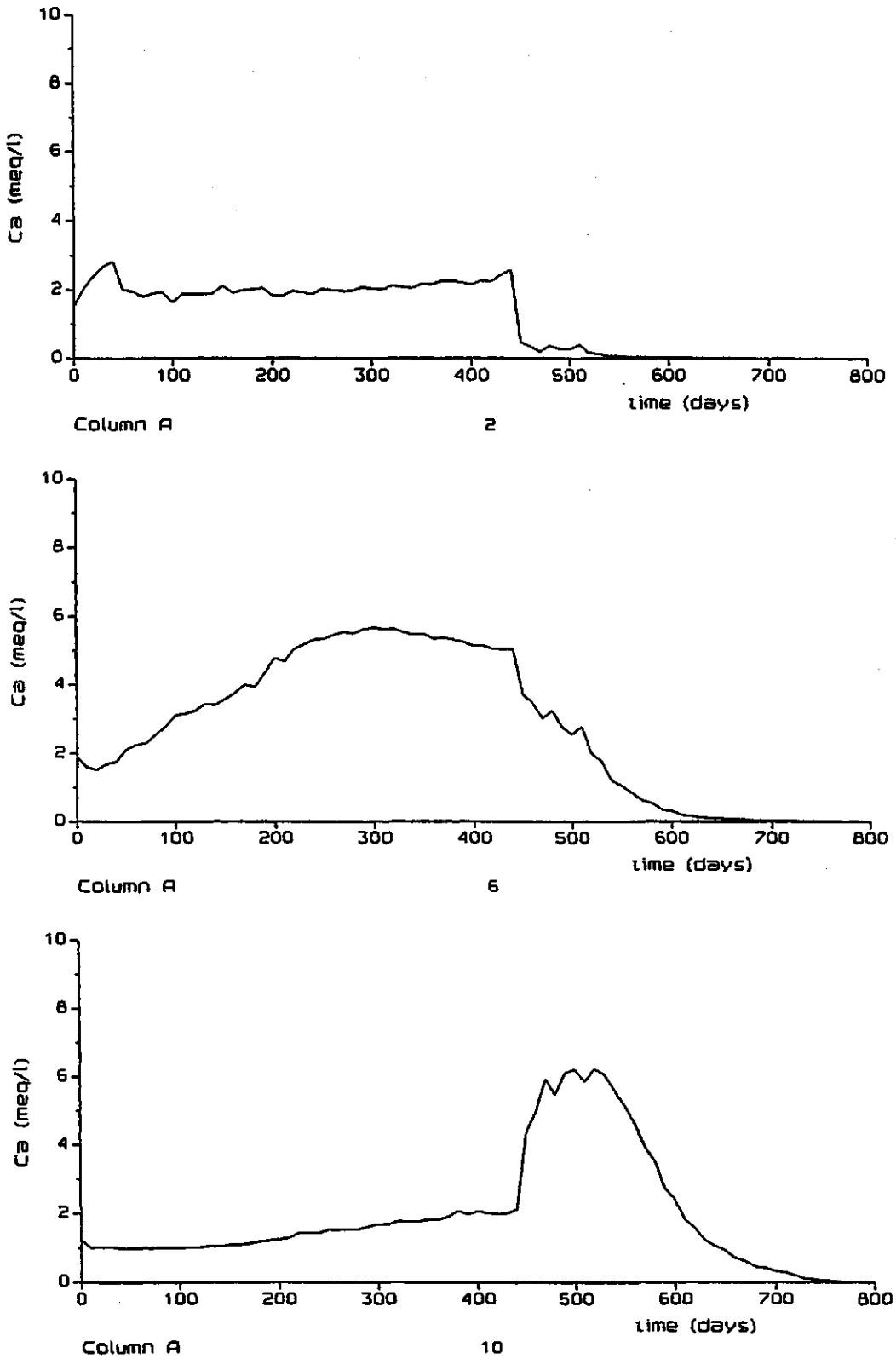

Fig. 4c The calculated course of the Ca^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

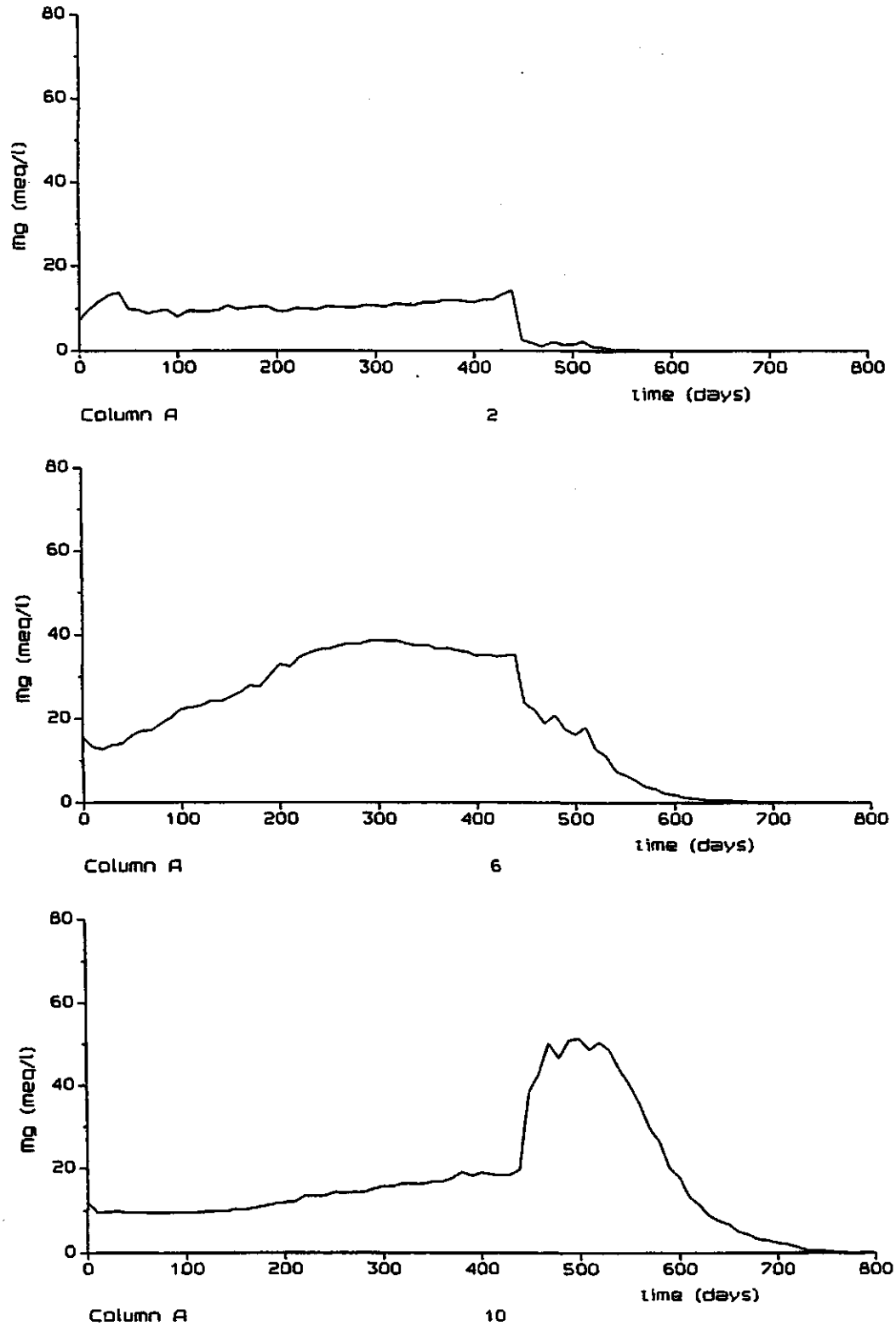

Fig. 4d The calculated course of the Mg^{2+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

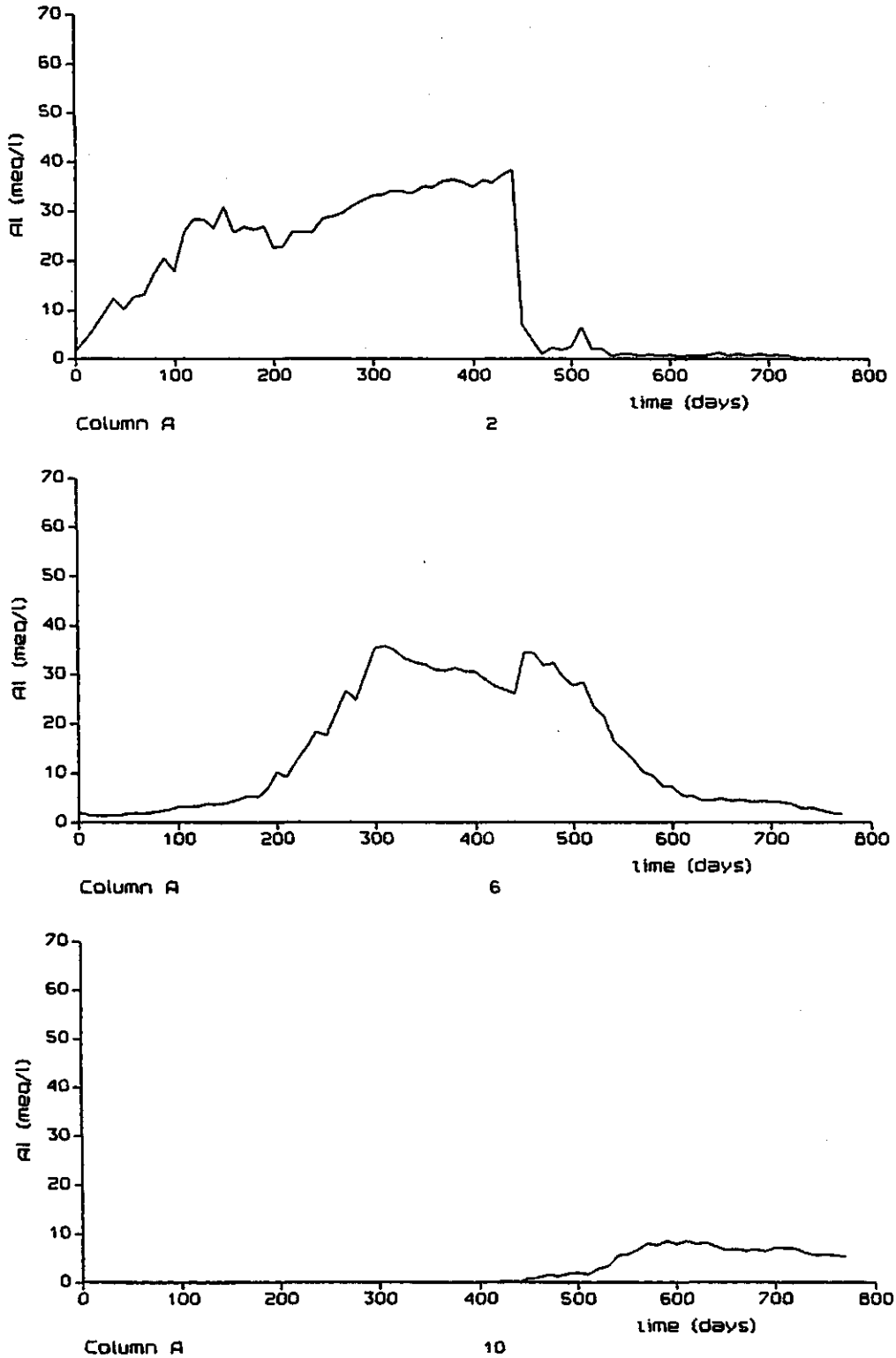

Fig. 4e The calculated course of the Al^{3+} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

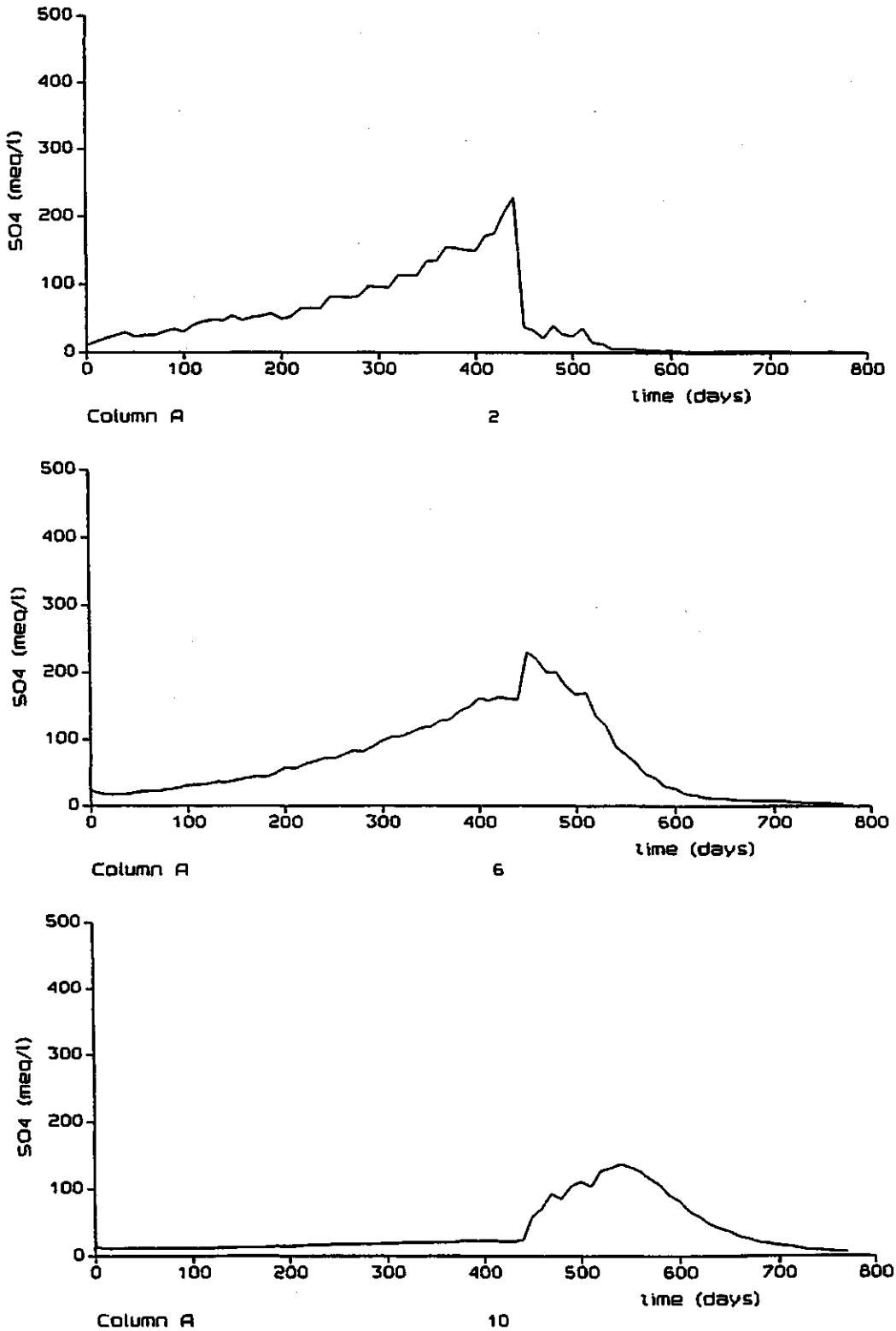

Fig. 4f The calculated course of the SO_4^{2-} concentration during a period of 770 days at depths of 7.5, 45, and 85 cm in a potential acid sulphate soils subjected to drainage (day 1 - day 442), submergence (day 443 - 473) and leaching (day 474 - day 770)

5 Installation

The SMASS model runs on a mainframe computer with the VMS operating system. SWACROP is available both for VMS and in a Personal Computer version under MS-DOS. Here we will outline the use of both models on a VAX-VMS computer.

1) Create the input files for SWACROP according to the instructions in section 3.1 and appendix 2, and the example in appendix 1.

2) The program SWACROP is written in Fortan 77. If an executable version of the model is not available, the source code should be compiled and linked with:

   $ FORTRAN SWACROP
   $ LINK SWACROP

   The executable can be executed with:
   $ RUN SWACROP

3) The unformated SWACROP outputfile OUTFILE should be renamed in SWATRE.UNF:
   $ RENAME OUTFILE SWATRE.UNF

4) The SMASS input files should be prepared according to the instructions of section 3.1 and the example in appendix 1.
   The Transol input file should be prepared according to appendix 3 and the example of appendix 1.

5) The programm of SMASS is written in VAX-VMS Fortran 77. The complete program consists of 4 files: SMASS1.FOR, SMASS2.FOR, SMASS3.FOR, and TRANSOL.FOR. The contents of these 4 files are:
   SMASS1.FOR : main program
   SMASS2.FOR : oxygen diffusion and pyrite oxidation subroutines
   SMASS3.FOR : chemical submodel, includes subroutines EPIDIM and IRON
   TRANSOL.FOR : solute transport submodel, includes subroutine TRANSOL

6) Model variables and parameters are defined and declared in 4 files: COMMON.FOR, VARSMASS.FOR, PARAM.FOR, and PARAM1.FOR. (These files are automatically incorporated in the program through INCLUDE statements.)

   If an executable version of the model is not available, the source code should be compiled and linked with:

```
$ FORTRAN/G_FLOATING SMASS1,SMASS2,SMASS3,TRANSOL
$ LINK SMASS1,SMASS2,SMASS3,TRANSOL
```

The executable can be executed with:

```
$ RUN SMASS1
```

6) The output can be analysed.

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Appendixes

Appendix Table of contents

1 Example of a complete set of input and output files for SWACROP and SMASS 67
2 Description of required format for input files for SWACROP 105
3 Description of required format for input file for TRANSOL 157

Appendix 1: Example of a complete set of input files and output files for SWACROP and SMASS

In the first part of Appendix 1 all 16 input files for running SWACROP and SMASS are given. The input files were used in the example of application, given in section 4.2. The numbering of the input files corresponds with the numbering in section 3.1.

In the second part of Appendix 1, the 10 SMASS output files, created from the input of the first part is given. Again the files correspond with the example of application of section 4.2. The numbering of the output files corresponds with the numbering given in section 3.2

INPUT FILES FOR SWACROP AND SMASS

File 1: **General input SWACROP**
Name: **SWADAT.INP**

```
>genhdr:
 'Column A, full period, groundwater level input'

>output:
 2  1  'Cola.bal'

>exfile:
 3
 'Cola.unf'
 'cola.out'
 1 1 1 1 1 1

>timeva:
 1987  1987  1 770  0.001  0.2   0  0
 0.25  5

>redeva:
 0  0.35

>irriva:
2
99
 29   3.98
 35    0.9
 42   3.98
 50   0.8
 56   1.59
 63   0.79
 70   1.59
 73    0.2
 78   0.66
 85   1.32
 91   0.88
 94   0.44
 98   1.59
110   0.5
112   1.59
127   1.59
140   1.5
152   0.8
154   1.6
166   0.7
180   1.59
187    0.6
193   0.8
196   1.59
210   1.59
224   1.59
238   1.76
252   1.59
266   1.59
280   1.59
295   1.59
308   1.59
322   1.59
336   1.59
351   1.59
371   1.59
385   1.76
399   1.76
413   1.76
442  13.17
449   6.68
459   4.29
```

```
469    6.59
484    6.55
498    4.10
511    5.06
518    5.06
525    5.06
532    5.06
539    5.06
546    5.06
553    5.06
560    1.61
563    1.61
565    3.21
569    3.21
574    5.06
581    5.06
588    5.06
595    5.06
602    5.06
607    1.61
610    4.29
617    5.06
623    5.06
630    5.06
637    5.06
644    5.06
651    5.06
658    5.06
663    0.44
665    5.06
672    5.06
679    5.06
686    5.06
695    5.06
700    4.40
707    5.50
712    2.20
714    4.40
717    4.40
721    6.60
724    5.50
728    5.50
730    2.20
738    4.40
740    4.40
742    4.40
744    2.20
747    4.40
750    4.40
752    4.40
754    2.20
756    4.40
758    4.40
761    2.20
763    4.40
765    4.40
767    4.40

>methdr:
 'meteo column A'

>topbnd:
 0 1

>metfil:
 1987 'Camet.inp'
```

```
>crphdr:
 'bare soil'

>sinkva:
 0 0 0

>rootac:
 0. 999. 999.

>crpfil:
 1987 'cacrop.inp'

>crppro:
 0

>profil:
 2  12  5  12
 5. 5. 10.0  10.0  10.0  10.0  10.0  10.0  10.0  10.0  10.0  10.0

>soilfl:
 'ca00.inp'
 'ca41.inp'

>pondmx:
 100.0

>incond:
 2
 -3.0

>bbdfil:
 'cagwl.inp'

>drains:
 0

>solute:
 0

>anafil:
 0
```

File 2: **Input top boundary SWACROP**
Name: **CAMET.INP**

```
>metd87:     day,   precip. (cm.d-1), pot. evap. (cm.d-1), pot. transP. (cm.d-1)
  1   0.00    0.095  0.0
  2   0.00    0.095  0.0
  3   0.00    0.095  0.0
  4   0.00    0.095  0.0
  5   0.00    0.095  0.0
  6   0.00    0.095  0.0
  7   0.00    0.095  0.0
  8   0.00    0.095  0.0
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
  .    .       .      .
744   0.00    0.172  0.0
745   0.00    0.172  0.0
746   0.00    0.172  0.0
747   0.00    0.172  0.0
748   0.00    0.172  0.0
749   0.00    0.172  0.0
750   0.00    0.172  0.0
751   0.00    0.172  0.0
752   0.00    0.172  0.0
753   0.00    0.172  0.0
754   0.00    0.172  0.0
755   0.00    0.172  0.0
756   0.00    0.172  0.0
757   0.00    0.172  0.0
758   0.00    0.172  0.0
759   0.00    0.172  0.0
760   0.00    0.172  0.0
761   0.00    0.172  0.0
762   0.00    0.172  0.0
763   0.00    0.172  0.0
764   0.00    0.172  0.0
765   0.00    0.172  0.0
766   0.00    0.172  0.0
767   0.00    0.172  0.0
768   0.00    0.172  0.0
769   0.00    0.172  0.0
770   0.00    0.172  0.0
```

File 3: **Input of crop data SWACROP**
Name: **CACROP.INP**

```
>sink87:
 0.   0.   0.   -1000. -2000. 100. -16000.

>root87:
 1
 1.   0.   365.   0./

>sink88:
 0.   0.   0.   -1000. -2000. 100. -16000.

>root88:
 1
 1.   0.   365.   0./
```

File 4A: Input of soil physical dat SWACROP, layer 1
Name: CA00.INP

```
>solhd1:
 'Column A, 0 - 40 cm depth'

>metho1:
 0

>soild1:     theta, pressure head (cm), k (cm.day-1)
0.78
0.01            -8562244.       1.6735144E-07
0.02            -7331203.       1.8859755E-07
0.03            -6277156.       2.1280997E-07
0.04            -5374654.       2.4043550E-07
0.05            -4601910.       2.7199073E-07
0.06            -3940268.       3.0807809E-07
0.07            -3373754.       3.4939475E-07
0.08            -2888690.       3.9675567E-07
0.09            -2473367.       4.5110616E-07
0.1000000       -2117758.       5.1355283E-07
0.1100000       -1813276.       5.8538393E-07
0.1200000       -1552571.       6.6810884E-07
0.1300000       -1329348.       7.6349016E-07
0.1400000       -1138220.       8.7359359E-07
0.1500000       -974572.9       1.0008403E-06
0.1600000       -834452.3       1.1480778E-06
0.1700000       -714478.4       1.3186415E-06
0.1800000       -611753.9       1.5164667E-06
0.1900000       -523798.7       1.7461772E-06
0.2000000       -448489.2       2.0132352E-06
0.2100000       -384007.4       2.3240718E-06
0.2200000       -328796.5       2.6863081E-06
0.2300000       -281523.6       3.1089298E-06
0.2400000       -241047.4       3.6026101E-06
0.2500000       -206390.7       4.1799631E-06
0.2600000       -176716.8       4.8559964E-06
0.2700000       -151309.2       5.6484996E-06
0.2800000       -129554.6       6.5786849E-06
0.2900000       -110927.9       7.6717406E-06
0.3000000       -94979.14       8.9577707E-06
0.3100000       -81323.46       1.0472619E-05
0.3200000       -69631.13       1.2259153E-05
0.3300000       -59619.88       1.4368647E-05
0.3400000       -51047.94       1.6862485E-05
0.3500000       -43708.55       1.9814201E-05
0.3600000       -37424.32       2.3312099E-05
0.3700000       -32043.59       2.7462300E-05
0.3800000       -27436.50       3.2392334E-05
0.3900000       -23491.83       3.8255766E-05
0.4000000       -20114.26       4.5237888E-05
0.4100000       -17222.32       5.3562031E-05
0.4200000       -14746.17       6.3498293E-05
0.4300000       -12626.03       7.5373260E-05
0.4400000       -10810.72       8.9582325E-05
0.4500000       -9256.399       1.0660491E-04
0.4600000       -7925.556       1.2702291E-04
0.4700000       -6786.051       1.5154347E-04
0.4800000       -5810.386       1.8102631E-04
0.4900000       -4974.995       2.1651921E-04
0.5000000       -4259.709       2.5929936E-04
0.5100000       -3647.267       3.1092542E-04
0.5200000       -3122.880       3.7330244E-04
0.5300000       -2673.887       4.4876110E-04
0.5400000       -2289.448       5.4015650E-04
0.5500000       -1960.279       6.5099105E-04
```

0.5600000	-1678.439	7.8556029E-04
0.5700000	-1437.121	9.4914768E-04
0.5800000	-1230.498	1.1482544E-03
0.5900000	-1053.583	1.3908896E-03
0.6000000	-902.1037	1.6869298E-03
0.6100000	-772.4024	2.0485742E-03
0.6200000	-661.3498	2.4908988E-03
0.6300000	-566.2639	3.0325681E-03
0.6400000	-484.8490	3.6967034E-03
0.6500000	-415.1396	4.5119976E-03
0.6600000	-355.4526	5.5140816E-03
0.6700000	-272.6132	7.7918898E-03
0.6799999	-221.6681	1.0229130E-02
0.6900000	-177.0300	1.3785436E-02
0.7000000	-119.7085	2.3315465E-02
0.7100000	-84.67094	3.7372310E-02
0.7200000	-47.82858	8.2507178E-02
0.7300000	-28.38736	0.1726433
0.7399999	-15.53840	0.4123802
0.7500000	-8.896491	0.9388809
0.7600000	-4.613840	20.525903
0.7700000	-1.762356	50.000000
0.7800000	0.0000000E+00	100.00000

File 4b: Input of soil physical dat SWACROP, layer 2
Name: CA41.INP

```
>solhd2:
 'Column A, 40-100 cm depth'

>metho2:
 0

>soild2:     theta, pressure head (cm), k (cm.day-1)
0.78
0.01            -8529311.       4.6634352E-10
0.02            -7274914.       6.4867473E-10
0.03            -6205000.       9.0018026E-10
0.04            -5292437.       1.2462765E-09
0.05            -4514084.       1.7214000E-09
0.06            -3850202.       2.3720925E-09
0.07            -3283957.       3.2610978E-09
0.08            -2800989.       4.4727702E-09
0.09            -2389051.       6.1203136E-09
0.1000000       -2037695.       8.3551113E-09
0.1100000       -1738014.       1.1379215E-08
0.1200000       -1482406.       1.5461628E-08
0.1300000       -1264390.       2.0959462E-08
0.1400000       -1078437.       2.8345719E-08
0.1500000       -919832.8       3.8245183E-08
0.1600000       -784553.9       5.1481177E-08
0.1700000       -669170.4       6.9135659E-08
0.1800000       -570756.3       9.2627133E-08
0.1900000       -486815.7       1.2381015E-07
0.2000000       -415220.2       1.6510367E-07
0.2100000       -354154.2       2.1965403E-07
0.2200000       -302069.1       2.9154427E-07
0.2300000       -257644.1       3.8605691E-07
0.2400000       -219752.7       5.1001223E-07
0.2500000       -187433.9       6.7219031E-07
0.2600000       -159868.2       8.8386486E-07
0.2700000       -136356.5       1.1594764E-06
0.2800000       -116302.7       1.5174677E-06
0.2900000       -99198.21       1.9813440E-06
0.3000000       -84609.23       2.5809686E-06
0.3100000       -72165.84       3.3541855E-06
0.3200000       -61552.49       4.3488444E-06
0.3300000       -52500.03       5.6252720E-06
0.3400000       -44778.90       7.2592989E-06
0.3500000       -38193.32       9.3460530E-06
0.3600000       -32576.27       1.2004492E-05
0.3700000       -27785.31       1.5383042E-05
0.3800000       -23698.95       1.9666255E-05
0.3900000       -20213.57       2.5083289E-05
0.4000000       -17240.78       3.1917531E-05
0.4100000       -14705.20       4.0518746E-05
0.4200000       -12542.52       5.1317405E-05
0.4300000       -10697.91       6.4841981E-05
0.4400000       -9124.571       8.1739090E-05
0.4500000       -7782.630       1.0279821E-04
0.4600000       -6638.051       1.2898019E-04
0.4700000       -5661.796       1.6145197E-04
0.4800000       -4829.122       2.0162559E-04
0.4900000       -4118.910       2.5120581E-04
0.5000000       -3513.145       3.1224577E-04
0.5100000       -2996.470       3.8720923E-04
0.5200000       -2555.784       4.7904497E-04
0.5300000       -2179.907       5.9127540E-04
0.5400000       -1859.311       7.2809029E-04
0.5500000       -1585.863       8.9446449E-04
0.5600000       -1352.632       1.0962842E-03
```

0.5700000	-1153.702	1.3404958E-03
0.5800000	-984.0284	1.6352698E-03
0.5900000	-839.3084	1.9901958E-03
0.6000000	-715.8722	2.4164882E-03
0.6100000	-610.5890	2.9272255E-03
0.6200000	-520.7903	3.5376055E-03
0.6300000	-444.1982	4.2652530E-03
0.6400000	-378.8709	5.1305234E-03
0.6500000	-323.1507	6.1568911E-03
0.6600000	-275.6253	7.3712892E-03
0.6700000	-242.1250	8.5208025E-03
0.6799999	-210.1250	9.9666938E-03
0.6900000	-178.7500	1.1891089E-02
0.7000000	-147.8750	1.4580846E-02
0.7100000	-119.7500	1.8222654E-02
0.7200000	-91.25000	2.4139430E-02
0.7300000	-63.12500	3.4957126E-02
0.7399999	-39.87500	5.4495100E-02
0.7500000	-19.25000	1.058393
0.7600000	-3.000000	20.467348
0.7700000	-1.0	50.0
0.7800000	0.0	200.0

File 5: Input bottom boundary data, SWACROP
Name: CAGWL.INP

```
>bothdr:
'Groundwater levels column A, at start of day'

>swbotb:
 0

>daygwl:
 770
  1    -60.0    /
  2    -65.0    /
  3    -70.0    /
  4    -75.0    /
  5    -65.0    /
  6    -64.0    /
  7    -63.0    /
  8    -62.0    /
  9    -63.5    /
 10    -65.0    /
 11    -68.0    /
 12    -71.0    /
 13    -74.0    /
 14    -77.0    /
 15    -83.0    /
 16    -89.0    /
 17    -89.5    /
 18    -90.0    /
 19    -90.5    /
 20    -91.0    /
  .       .
  .       .
  .       .
  .       .
  .       .
  .       .
  .       .
752    0.0 /
753    0.0 /
754    0.0 /
755    0.0 /
756    0.0 /
757    0.0 /
758    0.0 /
759    0.0 /
760    0.0 /
761    0.0 /
762    0.0 /
763    0.0 /
764    0.0 /
765    0.0 /
766    0.0 /
767    0.0 /
768    0.0 /
769    0.0 /
770    0.0 /
```

File 6: Input of bottom boundary data SWACROP
Name: -

This option was not used in the example calculations. File is not needed.

File 7: General input TRANSOL
Name: TRANSOL.INP

```
>hydmod: --------- kind of waterquantity model, 2 = SWACROP ------------
 2

! N.B. All values below are dummies. Chemical equilibria are computed with
  EPIDIM. TRANSOL is only used to compute conservative solute transport

>simper: ----------------- simulation period ---------------------------
 1
>sophys: ----------------- soil physical parameters --------------------
 10.0  25.0  0.01726   0.05184  3.457
 1310. 1650. 1700.
>sochem: ----------------- soil chemical parameters --------------------
 0.025  0.030  0.030
>rdepth: ----------------- depth-decomposition parameters --------------
 0.4  1.05   0.05
 0    1.0
>rvdose: ----------------- reservoir for additions to soil system ------
 0.025
>sorpti: ----------------- sorption-parameters -------------------------
 1
 0.200  0.001  0.9
>transf: ----------------- transformation rates or halflifetimes -------
 1
 1      0      0
 300.0  300.0  0.3
>metabo: ----------------- metabolite-param.; sorption- and decomp.-rate
 0
>uptake: ----------------- crop parameters -----------------------------
 0.0
>boucon: ----------------- boundary conditions -------------------------
 0.0
 0.0
 0.0
>inicon: ----------------- initial conditions --------------------------
 0.00335 0.00335 0.00335 0.02485 0.02485 0.06199 0.06199 0.06813 0.06813 0.03663
 0.03663 0.01396 0.01396 0.01396
>outopt: ----------------- output options ------------------------------
 1
 0  0  0  0  0
 0  0  0  0  0
 0  12  50.0
 0
```

File 8: Input of additions to the soil TRANSOL
Name: ADDIT.INP

! N.B. The values in this files are dummies. TRANSOL is only used for conservative tracer transport, and not for chemical reactions, etc.

```
>add001: ------------------- 1st addition ------------------------
 0.
 0.    0  0
 0.
```

File 9: **General input SMASS**
Name: **CAGEN.INP**

```
Column A, drainage and leaching potential acid sulphate soil
1        0
caini.inp
cacec.inp
compon.tab
caoxy.inp
cairr.inp
5.7  0.086  0.008  0.004  0.024  0.01  0.009  0.002  0.012  0.107  0.0
5.0  6.0    0.02   0.20   5.0    3.0   0.10   1.0    10.0   3.0    -2.0
3.5  0.4    0.07   0.20   0.50   0.15  0.30   0.00   3.00   0.20   0.0
1        10
0        0
casol.out
caads.out
caprec.out
cainp.out
caind.out
caprod.out
caoxy.out
caload.out
```

File 10: **Input of initial soil properties SMASS**
Name: **CAINI.INP**

```
11      !number of chemical components
Initial conc. in the soil solution (pH,Na,...,Cl,pE, conc. in meq/l)
3.50   1.0   0.2   1.5   7.3   0.9   1.8   1.00   10.7   1.42   5.75
3.50   1.0   0.2   1.5   7.3   0.9   1.8   1.00   10.7   1.42   5.75
4.00   1.0   0.2   1.5   7.3   0.9   1.8   1.00   10.7   1.42   5.75
4.00   1.5   0.2   1.6   9.8   4.2   1.4   1.00   13.5   0.01   5.75
4.20   1.5   0.2   1.6   9.8   4.2   1.4   1.00   13.5   0.01  -0.42
4.30   2.0   0.2   1.9  15.7   4.0   2.2   1.00   23.3   0.6   -0.42
5.00   2.0   0.1   1.4  12.8   4.0   1.5   2.00   18.8   0.6   -0.42
6.00   2.5   0.1   1.4  12.8   4.0   1.5   3.00   18.6   0.7   -0.42
6.00   2.5   0.1   1.4  12.8   4.0   1.5   3.00   18.6   0.7   -0.42
6.00   2.5   0.03  1.3  12.4   4.0   0.2   3.00   14.2   0.8   -0.85
6.00   2.5   0.03  1.3  12.4   2.4   0.2   3.00   14.2   0.8   -0.85
6.00   2.5   0.03  1.3  12.4   2.4   0.2   3.00   14.2   0.8   -0.85
```

File 11: Input of chemical soil data SMASS
Name: CACEC.INP

```
Dry bulk density,  CEC, Initial amount 1st, 2nd, and 3rd precipitate
(gr/cm3) (meq/100 g dry soil) (mol./kg dry soil)
  0.50   30.0    0.    0.1   0.
  0.49   30.0    0.    0.1   0.
  0.51   30.0    0.    0.1   0.
  0.52   30.0    0.    0.1   0.
  0.53   25.0    0.    0.1   0.
  0.56   25.0    0.    0.1   0.
  0.57   18.0    0.    0.1   0.
  0.58   18.2    0.    0.1   0.
  0.58   18.2    0.    0.1   0.
  0.57   18.0    0.    0.1   0.
  0.57   18.0    0.    0.1   0.
  0.57   18.0    0.    0.1   0.
```

File 12: Input of oxygen regime parameters SMASS
Name: CAOXY.INP

```
Column A, Drainage and leaching potential acid sulphate soil
Average aggregate radius per layer (m)
0.01 0.01 0.01  0.015 0.025 0.075 0.1 0.1 0.1 0.1 0.1 0.1
Organic matter content (kg/100 kg dry soil) per layer
18.7 20.9 16.4 14.25 12.50 11.28 9.68 7.33 8.36 9.21 9.07 9.07
Oxygen consumption rate organic matter (kg.kg org. matter .d-1) per layer
0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001 0.001
Tortuosity factor in macropore system
1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
Temp, Dfcfoxclod, Henry, Oxmax (100% O2) (kg.m-3 air), DfCfoxatm (m2.day-1)
30. 1.0E-5 52. 1.28 1.85
Initial pyrite content (kg pyrite/100kg dry soil)
0.13 0.48 2.62 5.30 7.86 8.28 6.69 5.23 6.97 8.86 7.84 7.84
initial diameter pyrite crystals (m)
50.E-06 50.E-06 50.E-06 50.E-06 50.E-06 50.E-06
50.E-06 50.E-06 50.E-06 50.E-06 50.E-06 50.E-06
```

File 13: **Input of irrigation data SMASS**
Name: **CAIRR.INP**

day	gift(m.d-1)	pH	Na+	K+	Ca2+	Mg2+	Fe2+	Al3+	HCO3-	SO42-	CL-	pE	(All conc. in meq/l)
29	0.03980	8.03	0.280	0.090	0.310	1.070	0.050	0.090	2.250	0.140	0.100	2.00	
35	0.00900	8.03	0.280	0.090	0.310	1.070	0.050	0.090	2.250	0.140	0.100	2.00	
42	0.03980	7.94	0.260	0.080	0.070	0.900	0.050	0.020	2.000	0.080	0.100	2.00	
50	0.00800	7.94	0.260	0.080	0.070	0.900	0.050	0.020	2.000	0.080	0.100	2.00	
56	0.01590	8.12	0.240	0.090	0.090	0.870	0.040	0.000	2.250	0.260	0.100	2.00	
63	0.00790	8.09	0.280	0.080	0.070	0.820	0.020	0.000	2.000	0.020	0.500	2.00	
70	0.01590	7.80	0.210	0.070	0.060	0.650	0.020	0.000	2.000	0.040	0.000	2.00	
73	0.00200	7.80	0.210	0.070	0.060	0.650	0.020	0.000	2.000	0.040	0.000	2.00	
78	0.00660	7.94	0.260	0.070	0.170	0.490	0.030	0.000	2.100	0.070	0.000	2.00	
85	0.01320	7.78	0.250	0.070	0.080	0.650	0.030	0.010	2.300	0.090	0.000	2.00	
91	0.00880	7.94	0.250	0.070	0.060	0.510	0.020	0.000	2.250	0.060	0.000	2.00	
94	0.00440	7.85	0.270	0.060	0.060	0.530	0.010	0.000	1.900	0.060	0.000	2.00	
98	0.01590	7.63	0.330	0.070	0.030	0.460	0.010	0.080	1.000	0.060	0.000	2.00	
110	0.00500	7.53	0.250	0.060	0.170	0.870	0.003	0.000	2.000	0.030	0.000	2.00	
112	0.01590	7.53	0.250	0.060	0.170	0.870	0.003	0.000	2.000	0.030	0.000	2.00	
127	0.01590	7.88	0.260	0.070	0.060	0.670	0.010	0.000	2.250	0.050	0.000	2.00	
140	0.01590	7.88	0.260	0.070	0.060	0.670	0.010	0.000	2.250	0.050	0.000	2.00	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	.	.	.	.	
728	0.05500	6.65	0.260	0.060	0.390	0.850	0.060	0.000	1.720	0.070	0.000	2.00	
730	0.02200	6.64	0.260	0.060	0.387	0.860	0.056	0.003	1.720	0.067	0.000	2.00	
738	0.04400	6.60	0.260	0.060	0.376	0.900	0.039	0.014	1.720	0.056	0.000	2.00	
740	0.04400	6.59	0.260	0.060	0.373	0.910	0.034	0.017	1.720	0.053	0.000	2.00	
742	0.04400	6.58	0.260	0.060	0.370	0.920	0.030	0.020	1.720	0.050	0.000	2.00	
744	0.02200	6.54	0.257	0.060	0.375	0.920	0.037	0.018	1.738	0.050	0.000	2.00	
747	0.04400	6.48	0.254	0.060	0.382	0.920	0.049	0.014	1.764	0.050	0.000	2.00	
750	0.04400	6.42	0.250	0.060	0.390	0.920	0.060	0.010	1.790	0.050	0.000	2.00	
752	0.04400	6.49	0.250	0.060	0.410	0.927	0.060	0.010	1.757	0.050	0.000	2.00	
754	0.02200	6.55	0.250	0.060	0.430	0.933	0.060	0.010	1.723	0.050	0.000	2.00	
756	0.04400	6.62	0.250	0.060	0.450	0.940	0.060	0.010	1.690	0.050	0.000	2.00	
758	0.04400	6.69	0.250	0.063	0.433	0.937	0.057	0.027	1.690	0.056	0.000	2.00	
761	0.02200	6.78	0.250	0.067	0.407	0.933	0.053	0.053	1.690	0.064	0.000	2.00	
763	0.04400	6.85	0.250	0.070	0.390	0.930	0.050	0.070	1.690	0.070	0.000	2.00	
765	0.04400	6.85	0.250	0.070	0.390	0.930	0.050	0.070	1.690	0.070	0.000	2.00	
767	0.04400	6.85	0.250	0.070	0.390	0.930	0.050	0.070	1.690	0.070	0.000	2.00	

File 14: Input of chemical composition of drainage water SMASS
Name: -

This option was not used in the example calculations. File is not needed.

File 15: Input for EPIDIM with chemical components SMASS
Name: COMPON.TAB

```
COMPON.TAB FILE  Column A computations, Fe(OH)3, jurbanite and jarosite
Number of components:     12
Number of Aq.species:     40
Number of Ads.species:    7
Number of Kin.species:    3
type of exchange rel.:    1
Column number pH:         1
Column number pe:         11
Maximum no. of iterat.:   1000
Convergence criterium:    0.01
 H+
 Na+
 K+
 Ca++
 Mg++
 Fe++
 AL+++
 HCO3-
 SO4--
 Cl-
 e-
 CEC
  H+          1    1       0.0        0.0        4.272      1.0      0.2463
   1   1.0
 OH-          1   -1     -14.0        0.0        3.181      1.0      0.2009
   1  -1.0
 HSO4-        2   -1       1.98       0.0        1.0        0.0     -0.25
   1   1.0    9   1.0
 Na+          1    1       0.0        0.0        4.152      1.0       0.07
   2   1.0
 NaCl         2    0       0.0        0.0        1.0        0.0     -0.125
   2   1.0   10   1.0
 NaHCO3       2    0      -0.25       0.0        1.0        0.0     -0.125
   2   1.0    8   1.0
 NaSO4-       2   -1       0.95       0.0        1.0        0.0     -0.25
   2   1.0    9   1.0
 K+           1    1       0.0        0.0        3.55       1.0       0.0161
   3   1.0
 KSO4-        2   -1       0.84       0.0        1.0        0.0     -0.25
   3   1.0    9   1.0
 Ca++         1    2       0.0        0.0        4.853      1.0       0.1781
   4   1.0
 CaCl+        2    1      -1.0        0.0        1.0        0.0     -0.25
   4   1.0   10   1.0
 CaCl2        2    0       0.0        0.0        1.0        0.0     -0.5
   4   1.0   10   2.0
 CaCO3        3    0      -8.13       0.0        1.0        0.0     -0.5
   1  -1.0    4   1.0    8   1.0
 CaHCO3+      2    1       1.26       0.0        1.0        0.0     -0.25
   4   1.0    8   1.0
 CaSO4        2    0       2.31       0.0        1.0        0.0     -0.5
   4   1.0    9   1.0
 Mg++         1    2       0.00       0.0        4.72       1.0       0.2414
   5   1.0
 MgCl2        2    0      -0.03       0.0        1.0        0.0     -0.5
   5   1.0   10   2.0
 MgCO3        3    0      -6.93       0.0        1.0        0.0     -0.5
   1  -1.0    5   1.0    8   1.0
```

```
MgHCO3+     2    1       1.16       0.0        1.0        0.0      -0.25
 5    1.0    8    1.0
MgSO4       2    0       2.25       0.0        1.0        0.0      -0.5
 5    1.0    9    1.0
Fe++        1    2       0.00       0.0        4.816      1.0       0.1859
 6    1.0
FeCl2       2    0      -0.07       0.0        1.0        0.0      -0.50
 6    1.0   10    2.0
FeSO4       2    0       2.30       0.0        1.0        0.0      -0.5
 6    1.0    9    1.0
Fe+++       2    3     -13.04       0.0        5.188      1.0       0.2177
 6    1.0   11   -1.0
FeCl++      3    2     -11.56       0.0        1.0        0.0      -0.25
 6    1.0   10    1.0   11   -1.0
FeCl2+      3    1     -10.91       0.0        1.0        0.0      -0.25
 6    1.0   10    2.0   11   -1.0
FeCl3       3    0     -12.27       0.0        1.0        0.0      -0.25
 6    1.0   10    3.0   11   -1.0
FeSO4+      3    1      -8.90       0.0        1.0        0.0      -0.6
 6    1.0    9    1.0   11   -1.0
Fe(SO4)2-   3   -1      -7.66       0.0        1.0        0.0      -0.5
 6    1.0    9    2.0   11   -1.0
FeOH++      3    2     -15.24       0.0        1.0        0.0      -0.5
 1   -1.0    6    1.0   11   -1.0
qFe2(OH)2   3    4     -29.00       0.0        1.0        0.0      -0.7
 1   -2.0    6    2.0   11   -2.0
Al+++       1    3       0.0        0.0        5.188      1.0       0.2177
 7    1.0
AlOH++      2    2      -5.02       0.0        1.0        0.0      -0.5
 1   -1.0    7    1.0
Al2(OH)2    2    4      -6.27       0.0        1.0        0.0      -0.7
 1   -2.0    7    2.0
AlSO4+      2    1       3.20       0.0        1.0        0.0      -0.6
 7    1.0    9    1.0
HCO3-       1   -1       0.0        0.0        5.34       1.0       0.0017
 8    1.0
CO3--       2   -2     -10.33       0.0        5.381      1.0       0.0039
 1   -1.0    8    1.0
H2CO3       2    0       6.35       0.0        1.0        0.0      -0.1
 1    1.0    8    1.0
SO4--       1   -2       0.0        0.0        2.989      1.0      -0.1013
 9    1.0
Cl-         1   -1       0.0        0.0        3.550      1.0       0.0161
10    1.0
CEC-H       2    1       225.
 1    1.0   12    1.0
CEC-Na      2    1       0.55
 2    1.0   12    1.0
CEC-K       2    1       9.2
 3    1.0   12    1.0
CEC-Ca      2    2       1.0
 4    1.0   12    2.0
CEC-Mg      2    2       1.0
 5    1.0   12    2.0
CEC-Fe      2    2       0.5
 6    1.0   12    2.0
CEC-Al      2    3       25.
 7    1.0   12    3.0
Fe(OH)3-T   3    15.74      0.0          1.0d-17    1.0d-17
 1   -3.0    6    1.0   11   -1.0
jurbanite   3    -3.23      0.0          1.0D-01    1.0D-01
 1   -1.0    7    1.0    9    1.0
jarosite    5    24.42      0.0          1.0d-28    1.0d-28
 1   -6.0    3    1.0    6    3.0    9    2.0   11   -3.0
```

File 16: Additional information about the configuration of COMTAB, SMASS
Name: HELP.TAB

```
6                   c- inumfe2; number of fe in component table
11                  c- inumfe3; number of fe3 (=inumpe !)
8                   c- inumhco3;
9                   c- inumso4;
3                   c- number aq. species, containing H+
1         1         c- rotation number of first aq. species + factor
3         1         c- idem second
38        1         c- idem third
8                   c- number aq. species, containing OH-
2         1         c- rotation number of first aq. species + factor
13        1         c- idem second
18        1         c- idem third
30        1         c- etc.
31        2
33        1
34        2
37        1
3                   c- number aq. species, containing Fe(ii)
21        1         c- rotation number of first aq. species + factor
22        1         c- idem second
23        1         c- idem third
8                   c- number aq. species, containing Fe(iii)
24        1         c- rotation number of first aq. species + factor
25        1         c- idem second
26        1         c- idem third
27        1         c- etc.
28        1
29        1
30        1
31        2
```

OUTPUT FILES FROM SMASS

File 1: File with chemical output data SMASS
Name: CASOL.OUT

Solute concentrations in soil solution (meq/l)

time : 1.00 days no. of t-steps = 1

i	depth m	pH	H+ meq/l	Na+ meq/l	K+ meq/l	Ca2+ meq/l	Mg2+ meq/l	Fe2+ meq/l	Al3+ meq/l	HCO3- meq/l	SO42- meq/l	Cl- meq/l	Fe3+ meq/l	pE
1	0.025	3.48	1.48	1.03	0.200	1.61	7.82	0.954	2.09	1.03	11.7	1.46	0.264E-03	7.88
2	0.075	3.49	1.44	1.01	0.198	1.56	7.60	0.927	1.99	1.00	11.3	1.42	0.257E-03	7.88
3	0.150	3.97	1.14	1.01	0.196	1.58	7.68	0.941	2.01	1.00	11.4	1.42	0.491E-04	6.92
4	0.250	3.98	1.14	1.51	0.196	1.66	10.2	4.33	1.52	1.00	14.2	0.100E-01	0.468E-04	6.24
5	0.350	4.18	1.08	1.51	0.196	1.63	9.95	4.25	1.44	1.00	13.8	0.100E-01	0.244E-04	5.84
6	0.450	4.29	1.07	1.99	0.195	1.86	15.3	3.93	2.06	0.999	22.7	0.597	0.149E-04	5.59
7	0.550	4.88	1.93	1.97	0.959E-01	1.30	11.9	3.78	1.18	1.99	17.3	0.600	0.191E-05	4.23
8	0.650	5.62	2.45	2.42	0.931E-01	1.21	11.0	3.55	0.502	2.98	15.9	0.699	0.528E-09	-0.01
9	0.750	5.62	2.46	2.42	0.931E-01	1.21	11.0	3.54	0.502	2.99	15.9	0.700	0.534E-09	-0.01
10	0.850	5.85	2.18	2.47	0.292E-01	1.22	11.7	3.80	0.136	3.00	13.4	0.799	0.219E-09	-0.68
11	0.950	5.85	2.18	2.46	0.291E-01	1.22	11.6	2.27	0.135	3.00	13.3	0.800	0.130E-09	-0.68
12	1.050	5.85	2.18	2.46	0.291E-01	1.21	11.6	2.26	0.134	3.00	13.3	0.800	0.129E-09	-0.68

time : 10.00 days no. of t-steps = 10

i	depth m	pH	H+ meq/l	Na+ meq/l	K+ meq/l	Ca2+ meq/l	Mg2+ meq/l	Fe2+ meq/l	Al3+ meq/l	HCO3- meq/l	SO42- meq/l	Cl- meq/l	Fe3+ meq/l	pE
1	0.025	3.35	1.94	1.31	0.168	2.51	12.2	1.39	5.50	1.27	20.4	1.80	0.959E-02	9.27
2	0.075	3.39	1.59	1.08	0.162	2.02	9.84	1.13	3.90	1.00	16.1	1.41	0.667E-02	9.21
3	0.150	3.77	1.24	1.13	0.130	2.16	10.6	1.39	4.13	1.00	17.1	1.29	0.655E-03	7.98
4	0.250	3.82	1.22	1.62	0.144	2.15	13.2	5.26	2.68	1.00	19.6	0.122E-01	0.504E-03	7.27
5	0.350	4.01	1.14	1.58	0.151	1.89	11.7	4.74	1.97	1.00	16.6	0.584E-01	0.160E-03	6.72
6	0.450	4.22	1.17	1.92	0.162	1.59	13.2	3.51	1.40	1.09	18.8	0.596	0.544E-04	6.25
7	0.550	4.58	2.07	1.89	0.848E-01	1.02	9.33	3.12	0.602	2.07	12.9	0.609	0.832E-05	5.19
8	0.650	5.10	2.84	2.23	0.786E-01	0.858	7.87	2.73	0.164	3.01	11.4	0.698	0.280E-05	4.29
9	0.750	5.15	2.80	2.22	0.773E-01	0.817	7.50	2.54	0.151	2.99	10.4	0.710	0.142E-07	1.97
10	0.850	5.49	2.58	2.35	0.269E-01	1.00	9.56	3.14	0.583E-01	3.00	10.8	0.793	0.411E-09	0.00
11	0.950	5.50	2.56	2.34	0.265E-01	0.984	9.42	1.90	0.575E-01	2.98	10.6	0.795	0.137E-09	-0.26
12	1.050	5.53	2.28	2.18	0.255E-01	0.899	8.61	1.71	0.525E-01	2.68	9.55	0.714	0.115E-09	-0.33

time : 20.00 days no. of t-steps = 20

i	depth m	pH	H+ meq/l	Na+ meq/l	K+ meq/l	Ca2+ meq/l	Mg2+ meq/l	Fe2+ meq/l	Al3+ meq/l	HCO3- meq/l	SO42- meq/l	Cl- meq/l	Fe3+ meq/l	pE
1	0.025	3.23	2.50	1.61	0.609E-01	3.47	16.9	1.84	10.9	1.56	31.5	2.20	0.262E-01	9.56
2	0.075	3.30	1.75	1.14	0.918E-01	2.39	11.7	1.32	6.33	1.00	20.8	1.37	0.109E-01	9.35
3	0.150	3.60	1.38	1.22	0.134E-01	2.62	13.0	1.84	6.75	1.00	22.5	1.17	0.203E-02	8.40

4	0.250	3.68	1.32	1.70	0.593E-01	2.60	15.9	6.01	4.21	1.00	24.7	0.165E-01	0.132E-02	7.67
5	0.350	3.86	1.21	1.65	0.911E-01	2.16	13.4	5.20	2.64	1.01	19.3	0.871E-01	0.387E-03	7.14
.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
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.	.	.	.	.	.	.	.	.	.	.	.	.	.	.
6	0.450	2.76	2.10	0.992E-01	0.348E-05	0.864E-02	0.382E-01	0.201	2.41	0.494E-01	3.87	0.127	0.155	11.66
7	0.550	2.72	2.35	0.103	0.355E-05	0.108E-01	0.501E-01	0.302	3.44	0.583E-01	4.74	0.129	0.187	11.55
8	0.650	2.68	2.64	0.107	0.368E-05	0.143E-01	0.703E-01	0.454	4.28	0.721E-01	5.70	0.132	0.227	11.44
9	0.750	2.69	2.61	0.112	0.230E-05	0.207E-01	0.112	0.678	4.59	0.910E-01	6.64	0.135	0.254	11.28
10	0.850	2.94	1.59	0.119	0.497E-05	0.427E-01	0.271	1.31	5.61	0.139	7.33	0.138	0.697E-01	10.38
11	0.950	3.46	0.630	0.134	0.240E-02	0.165	1.22	2.89	4.20	0.192	7.44	0.139	0.277E-02	8.47
12	1.050	4.54	0.276	0.150	0.142E-01	0.373	2.90	6.55	0.613E-01	0.243	8.37	0.136	0.220E-04	5.28

time : 760.00 days no. of t-steps = 760

i	depth m	pH	H+ meq/l	Na+ meq/l	K+ meq/l	Ca2+ meq/l	Mg2+ meq/l	Fe2+ meq/l	Al3+ meq/l	HCO3- meq/l	SO42- meq/l	Cl- meq/l	Fe3+ meq/l	pE
1	0.025	3.53	0.368	0.980E-01	0.115E-01	0.586E-02	0.241E-01	0.202	0.461E-01	0.517E-01	0.600	0.123	0.102E-02	9.24
2	0.075	3.32	0.564	0.943E-01	0.242E-02	0.551E-02	0.227E-01	0.153	0.130	0.502E-01	0.863	0.117	0.318E-02	9.99
3	0.150	3.09	0.946	0.917E-01	0.127E-03	0.529E-02	0.218E-01	0.132	0.364	0.506E-01	1.42	0.119	0.133E-01	10.78
4	0.250	2.95	1.30	0.917E-01	0.281E-04	0.549E-02	0.228E-01	0.123	0.701	0.487E-01	2.05	0.120	0.346E-01	11.24
5	0.350	2.87	1.58	0.932E-01	0.113E-04	0.606E-02	0.254E-01	0.134	1.24	0.476E-01	2.72	0.122	0.642E-01	11.47
6	0.450	2.80	1.91	0.948E-01	0.508E-05	0.687E-02	0.295E-01	0.153	1.89	0.473E-01	3.43	0.124	0.115	11.65
7	0.550	2.75	2.16	0.973E-01	0.648E-05	0.813E-02	0.360E-01	0.192	2.78	0.493E-01	4.17	0.126	0.132	11.60
8	0.650	2.69	2.49	0.101	0.721E-05	0.101E-01	0.469E-01	0.269	3.75	0.552E-01	4.98	0.128	0.165	11.54
9	0.750	2.69	2.57	0.105	0.516E-05	0.137E-01	0.688E-01	0.401	4.60	0.660E-01	5.80	0.130	0.194	11.42
10	0.850	2.92	1.59	0.111	0.604E-05	0.246E-01	0.145	0.797	5.42	0.994E-01	6.32	0.133	0.696E-01	10.62
11	0.950	3.39	0.628	0.121	0.109E-02	0.884E-01	0.634	1.66	5.02	0.130	6.10	0.135	0.193E-02	8.61
12	1.050	4.51	0.199	0.135	0.135E-01	0.342	2.66	5.53	0.713E-01	0.163	7.12	0.133	0.258E-04	5.43

time : 770.00 days no. of t-steps = 770

i	depth m	pH	H+ meq/l	Na+ meq/l	K+ meq/l	Ca2+ meq/l	Mg2+ meq/l	Fe2+ meq/l	Al3+ meq/l	HCO3- meq/l	SO42- meq/l	Cl- meq/l	Fe3+ meq/l	pE
1	0.025	3.55	0.378	0.102	0.129E-01	0.626E-02	0.258E-01	0.230	0.436E-01	0.764E-01	0.637	0.128	0.937E-03	9.12
2	0.075	3.28	0.606	0.993E-01	0.106E-02	0.713E-02	0.294E-01	0.166	0.190	0.368E-01	0.883	0.117	0.403E-02	10.09
3	0.150	3.09	0.943	0.939E-01	0.115E-03	0.569E-02	0.234E-01	0.145	0.401	0.430E-01	1.48	0.118	0.136E-01	10.74
4	0.250	2.96	1.29	0.936E-01	0.289E-04	0.562E-02	0.233E-01	0.139	0.736	0.471E-01	2.06	0.119	0.338E-01	11.17
5	0.350	2.89	1.51	0.921E-01	0.133E-04	0.557E-02	0.232E-01	0.134	1.14	0.487E-01	2.65	0.120	0.558E-01	11.40
6	0.450	2.82	1.79	0.924E-01	0.634E-05	0.594E-02	0.250E-01	0.146	1.66	0.498E-01	3.26	0.121	0.957E-01	11.59
7	0.550	2.78	2.02	0.936E-01	0.105E-04	0.663E-02	0.285E-01	0.155	2.39	0.490E-01	3.89	0.123	0.993E-01	11.57
8	0.650	2.72	2.33	0.959E-01	0.125E-04	0.779E-02	0.346E-01	0.188	3.24	0.503E-01	4.58	0.124	0.121	11.57
9	0.750	2.70	2.49	0.992E-01	0.110E-04	0.992E-02	0.469E-01	0.259	4.26	0.550E-01	5.28	0.126	0.143	11.49
10	0.850	2.90	1.59	0.104	0.723E-05	0.162E-01	0.895E-01	0.515	5.26	0.765E-01	5.67	0.129	0.689E-01	10.83
11	0.950	3.35	0.638	0.111	0.260E-03	0.535E-01	0.374	1.07	5.37	0.949E-01	5.27	0.131	0.374E-02	9.13
12	1.050	4.47	0.162	0.123	0.143E-01	0.329	2.56	4.83	0.925E-01	0.121	6.14	0.126	0.300E-04	5.59

File 2: File with chemical output data SMASS
Name: CAADS.OUT

Adsorbed amounts (meq/100g)

time : 1.00 days no. of t-steps = 1

i	depth m	H+ meq/100g	Na+ meq/100g	K+ meq/100g	Ca2+ meq/100g	Mg2+ meq/100g	Fe2+ meq/100g	Al3+ meq/100g
1	0.03	13.0	0.849E-01	0.275	0.372	1.86	0.111	14.3
2	0.08	13.0	0.842E-01	0.276	0.372	1.87	0.111	14.3
3	0.15	4.86	0.970E-01	0.314	0.495	2.48	0.148	21.6
4	0.25	5.24	0.157	0.339	0.587	3.71	0.769	19.2
5	0.35	2.87	0.135	0.293	0.521	3.29	0.685	17.2
6	0.45	2.19	0.170	0.279	0.487	4.18	0.519	17.2
7	0.55	0.483	0.146	0.119	0.378	3.58	0.553	12.7
8	0.65	0.122	0.250	0.161	0.680	6.45	1.01	9.53
9	0.75	0.122	0.251	0.161	0.680	6.45	1.01	9.53
10	0.85	0.861E-01	0.311	0.615E-01	1.07	10.5	1.68	4.26
11	0.95	0.883E-01	0.317	0.626E-01	1.11	10.9	1.04	4.48
12	1.05	0.883E-01	0.317	0.626E-01	1.11	10.9	1.04	4.48

time : 10.00 days no. of t-steps = 10

i	depth m	H+ meq/100g	Na+ meq/100g	K+ meq/100g	Ca2+ meq/100g	Mg2+ meq/100g	Fe2+ meq/100g	Al3+ meq/100g
1	0.03	14.0	0.822E-01	0.177	0.307	1.55	0.854E-01	13.8
2	0.08	13.8	0.746E-01	0.187	0.309	1.56	0.868E-01	14.0
3	0.15	6.47	0.877E-01	0.169	0.415	2.11	0.135	20.6
4	0.25	6.57	0.142	0.212	0.518	3.29	0.637	18.6
5	0.35	3.89	0.129	0.206	0.485	3.10	0.610	16.6
6	0.45	2.78	0.179	0.253	0.515	4.43	0.572	16.3
7	0.55	1.09	0.162	0.121	0.415	3.92	0.638	11.7
8	0.65	0.468	0.274	0.162	0.726	6.87	1.16	8.54
9	0.75	0.426	0.279	0.162	0.735	6.95	1.15	8.50
10	0.85	0.212	0.326	0.624E-01	1.10	10.8	1.74	3.74
11	0.95	0.216	0.332	0.629E-01	1.14	11.2	1.11	3.94
12	1.05	0.207	0.320	0.627E-01	1.14	11.2	1.09	4.00

time : 20.00 days no. of t-steps = 20

i	depth m	H+ meq/100g	Na+ meq/100g	K+ meq/100g	Ca2+ meq/100g	Mg2+ meq/100g	Fe2+ meq/100g	Al3+ meq/100g
1	0.03	15.4	0.829E-01	0.521E-01	0.260	1.32	0.696E-01	12.8
2	0.08	14.8	0.680E-01	0.914E-01	0.262	1.33	0.725E-01	13.4
3	0.15	8.30	0.812E-01	0.149E-01	0.352	1.82	0.124	19.3
4	0.25	8.09	0.130	0.758E-01	0.455	2.90	0.529	17.8
5	0.35	5.00	0.122	0.113	0.446	2.87	0.539	15.9
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.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.

time : 760.00 days no. of t-steps = 760

i	depth m	H+ meq/100g	Na+ meq/100g	K+ meq/100g	Ca2+ meq/100g	Mg2+ meq/100g	Fe2+ meq/100g	Al3+ meq/100g
1	0.03	21.8	0.168E-01	0.329E-01	0.848E-02	0.350E-01	0.146	8.02
2	0.08	23.6	0.109E-01	0.468E-02	0.353E-02	0.146E-01	0.492E-01	6.32
3	0.15	26.0	0.676E-02	0.157E-03	0.133E-02	0.554E-02	0.166E-01	4.00
4	0.25	27.1	0.509E-02	0.261E-04	0.755E-03	0.318E-02	0.846E-02	2.93
5	0.35	22.7	0.358E-02	0.726E-05	0.465E-03	0.198E-02	0.514E-02	2.25
6	0.45	23.1	0.308E-02	0.276E-05	0.367E-03	0.160E-02	0.410E-02	1.93
7	0.55	16.6	0.202E-02	0.225E-05	0.241E-03	0.109E-02	0.286E-02	1.36
8	0.65	17.0	0.187E-02	0.223E-05	0.231E-03	0.109E-02	0.307E-02	1.20
9	0.75	16.9	0.189E-02	0.155E-05	0.290E-03	0.148E-02	0.425E-02	1.28
10	0.85	13.9	0.279E-02	0.254E-05	0.101E-02	0.609E-02	0.164E-01	4.05
11	0.95	6.73	0.437E-02	0.661E-03	0.751E-02	0.549E-01	0.706E-01	11.1
12	1.05	2.05	0.195E-01	0.327E-01	0.440	3.51	3.58	8.37

time : 770.00 days no. of t-steps = 770

i	depth m	H+ meq/100g	Na+ meq/100g	K+ meq/100g	Ca2+ meq/100g	Mg2+ meq/100g	Fe2+ meq/100g	Al3+ meq/100g
1	0.03	21.5	0.180E-01	0.382E-01	0.966E-02	0.400E-01	0.178	8.26
2	0.08	23.4	0.102E-01	0.182E-02	0.363E-02	0.151E-01	0.424E-01	6.55
3	0.15	25.8	0.684E-02	0.140E-03	0.139E-02	0.579E-02	0.178E-01	4.19
4	0.25	26.9	0.521E-02	0.270E-04	0.778E-03	0.326E-02	0.965E-02	3.10
5	0.35	22.6	0.370E-02	0.892E-05	0.468E-03	0.198E-02	0.566E-02	2.39
6	0.45	22.9	0.318E-02	0.365E-05	0.358E-03	0.154E-02	0.441E-02	2.05
7	0.55	16.6	0.208E-02	0.390E-05	0.225E-03	0.986E-03	0.264E-02	1.44
8	0.65	16.9	0.189E-02	0.413E-05	0.202E-03	0.916E-03	0.245E-02	1.27
9	0.75	16.9	0.183E-02	0.340E-05	0.222E-03	0.107E-02	0.291E-02	1.32
10	0.85	14.1	0.256E-02	0.299E-05	0.653E-03	0.368E-02	0.104E-01	3.91
11	0.95	7.04	0.381E-02	0.149E-03	0.419E-02	0.298E-01	0.418E-01	10.9
12	1.05	2.14	0.167E-01	0.325E-01	0.382	3.05	2.82	9.57

File 3: File with chemical output data SMASS
Name: CAPREC.OUT

Amounts of precipitates in mol/kg soil

time : 1.00 days no. of t-steps = 1

	depth m	Fe(OH)3-T mol/kg	jurbanite mol/kg	jarosite mol/kg
1	0.03	0.000E+00	0.100	0.116E-03
2	0.08	0.000E+00	0.100	0.105E-03
3	0.15	0.000E+00	0.100	0.176E-03
4	0.25	0.000E+00	0.100	0.156E-03
5	0.35	0.000E+00	0.100	0.100E-03
6	0.45	0.000E+00	0.101	0.368E-04
7	0.55	0.619E-04	0.101	0.000E+00
8	0.65	0.000E+00	0.102	0.000E+00
9	0.75	0.000E+00	0.102	0.000E+00
10	0.85	0.000E+00	0.101	0.000E+00
11	0.95	0.000E+00	0.101	0.000E+00
12	1.05	0.000E+00	0.101	0.000E+00

time : 10.00 days no. of t-steps = 10

	depth m	Fe(OH)3-T mol/kg	jurbanite mol/kg	jarosite mol/kg
1	0.03	0.590E-05	0.101	0.123E-02
2	0.08	-.529E-22	0.100	0.108E-02
3	0.15	0.112E-04	0.103	0.172E-02
4	0.25	0.803E-05	0.102	0.150E-02
5	0.35	0.662E-05	0.102	0.103E-02
6	0.45	0.399E-05	0.104	0.333E-03
7	0.55	0.679E-03	0.105	0.000E+00
8	0.65	0.626E-05	0.105	0.181E-04
9	0.75	0.000E+00	0.105	0.000E+00
10	0.85	0.000E+00	0.102	0.000E+00
11	0.95	0.000E+00	0.102	0.000E+00
12	1.05	0.000E+00	0.102	0.000E+00

time : 20.00 days no. of t-steps = 20

	depth m	Fe(OH)3-T mol/kg	jurbanite mol/kg	jarosite mol/kg
1	0.03	0.000E+00	0.102	0.271E-02
2	0.08	0.000E+00	0.101	0.213E-02
3	0.15	0.217E-04	0.106	0.343E-02
4	0.25	0.575E-05	0.104	0.298E-02
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time : 760.00 days no. of t-steps = 760

	depth m	Fe(OH)3-T mol/kg	jurbanite mol/kg	jarosite mol/kg
1	0.03	0.618E-02	0.107	0.376E-02
2	0.08	0.210E-01	0.952E-01	0.378E-02
3	0.15	0.158E-01	0.118	0.396E-02
4	0.25	0.113E-01	0.123	0.406E-02
5	0.35	0.126E-01	0.129	0.360E-02
6	0.45	0.109E-01	0.148	0.331E-02

7	0.55	0.000E+00	0.138	0.180E-02
8	0.65	0.000E+00	0.132	0.204E-02
9	0.75	0.000E+00	0.146	0.190E-02
10	0.85	0.000E+00	0.144	0.989E-03
11	0.95	0.000E+00	0.132	0.519E-03
12	1.05	0.208E-05	0.112	0.443E-04

time : 770.00 days no. of t-steps = 770

	depth m	Fe(OH)3-T mol/kg	jurbanite mol/kg	jarosite mol/kg
1	0.03	0.586E-02	0.106	0.369E-02
2	0.08	0.208E-01	0.943E-01	0.385E-02
3	0.15	0.157E-01	0.117	0.397E-02
4	0.25	0.113E-01	0.122	0.407E-02
5	0.35	0.126E-01	0.128	0.360E-02
6	0.45	0.108E-01	0.147	0.331E-02
7	0.55	0.000E+00	0.138	0.180E-02
8	0.65	0.000E+00	0.132	0.204E-02
9	0.75	0.000E+00	0.145	0.190E-02
10	0.85	0.000E+00	0.144	0.988E-03
11	0.95	0.000E+00	0.133	0.529E-03
12	1.05	0.150E-04	0.112	0.359E-04

File 4: File with echo of general SMASS input
Name: CAINP.OUT

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Column A, drainage and leaching potential acid sulphate soil

This file contains only output from SMASS-input
Output of input for TRANSOL is given in GENERAL.OUT

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Number of chemical components is 11

Initial solute concentrations in meq/l

 pH      Na+     K+      Ca2+    Mg2+    Fe-tot  Al3+    HCO3-   SO42-   Cl-
  3.500  1.000   0.200   1.500   7.300   0.900   1.800   1.000  10.700   1.420   5.750
  3.500  1.000   0.200   1.500   7.300   0.900   1.800   1.000  10.700   1.420   5.750
  4.000  1.000   0.200   1.500   7.300   0.900   1.800   1.000  10.700   1.420   5.750
  4.000  1.500   0.200   1.600   9.800   4.200   1.400   1.000  13.500   0.010   5.750
  4.200  1.500   0.200   1.600   9.800   4.200   1.400   1.000  13.500   0.010  -0.420
  4.300  2.000   0.200   1.900  15.700   4.000   2.200   1.000  23.300   0.600  -0.420
  5.000  2.000   0.100   1.400  12.800   4.000   1.500   2.000  18.800   0.600  -0.420
  6.000  2.500   0.100   1.400  12.800   4.000   1.500   3.000  18.600   0.700  -0.420
  6.000  2.500   0.100   1.400  12.800   4.000   1.500   3.000  18.600   0.700  -0.420
  6.000  2.500   0.030   1.300  12.400   4.000   0.200   3.000  14.200   0.800  -0.850
  6.000  2.500   0.030   1.300  12.400   2.400   0.200   3.000  14.200   0.800  -0.850
  6.000  2.500   0.030   1.300  12.400   2.400   0.200   3.000  14.200   0.800  -0.850


 RHO (g/cm3)  CEC (meq/100g)
      0.50      30.00
      0.49      30.00
      0.51      30.00
      0.52      30.00
      0.53      25.00
      0.56      25.00
      0.57      18.00
      0.58      18.20
      0.58      18.20
      0.57      18.00
      0.57      18.00
      0.57      18.00


The chemical composition of precipitation
 pH      Na+     K+      Ca2+    Mg2+    Fe-tot  Al3+    HCO3-   SO42-   Cl-
  5.700  0.086   0.008   0.004   0.024   0.010   0.009   0.002   0.012   0.107   0.000


The chemical composition of the aquifer
 pH      Na+     K+      Ca2+    Mg2+    Fe-tot  Al3+    HCO3-   SO42-   Cl-
  5.000  6.000   0.020   0.200   5.000   3.000   0.100   1.000  10.000   3.000  -2.000


The chemical composition of surface water
 pH      Na+     K+      Ca2+    Mg2+    Fe-tot  Al3+    HCO3-   SO42-   Cl-
  3.500  0.400   0.070   0.200   0.500   0.150   0.300   0.000   3.000   0.200   0.000
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File 5: File with calculated saturation indices SMASS
Name: CAIND.OUT

Saturation indices
time : 1.00 days no. of t-steps = 1

i	depth	SI(FE(OH)3)	SI(Jurb)	SI(Jarosite)
1	0.03	-1.08	0.736E-01	0.116
2	0.08	-1.07	0.556E-01	0.103
3	0.15	-.565	0.546	0.162
4	0.25	-.591	0.426	0.144
5	0.35	-.399	0.599	0.105
6	0.45	-.420	0.900	0.371E-01
7	0.55	0.369E-03	1.20	-.918
8	0.65	-2.05	1.38	-9.32
9	0.75	-2.04	1.38	-9.30
10	0.85	-1.95	0.929	-10.4
11	0.95	-2.18	0.936	-11.1
12	1.05	-2.19	0.936	-11.1

time : 10.00 days no. of t-steps = 10

i	depth	SI(FE(OH)3)	SI(Jurb)	SI(Jarosite)
1	0.03	0.169E-04	0.379	3.96
2	0.08	-.467E-04	0.264	3.71
3	0.15	0.341E-04	0.674	2.50
4	0.25	0.449E-04	0.530	2.44
5	0.35	0.406E-04	0.576	1.80
6	0.45	0.345E-04	0.656	1.33
7	0.55	0.113E-01	0.616	-.197
8	0.65	0.636	0.522	0.211E-01
9	0.75	-1.56	0.517	-6.77
10	0.85	-2.39	0.348	-10.8
11	0.95	-2.86	0.352	-12.2
12	1.05	-2.88	0.319	-12.4

time : 20.00 days no. of t-steps = 20

i	depth	SI(FE(OH)3)	SI(Jurb)	SI(Jarosite)
1	0.03	-.204E-02	0.563	4.07
2	0.08	-.869E-01	0.395	3.59
3	0.15	-.865E-04	0.723	2.15
4	0.25	-.346E-05	0.589	2.60
5	0.35	0.405E-04	0.564	2.09
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time : 760.00 days no. of t-steps = 760

i	depth	SI(FE(OH)3)	SI(Jurb)	SI(Jarosite)
1	0.03	-.522E-02	-1.93	0.266E-01
2	0.08	0.150E-03	-1.59	0.255
3	0.15	-.431E-04	-1.28	0.100E-01
4	0.25	0.730E-05	-1.07	0.261E-03
5	0.35	-.300E-03	-.877	0.210E-02
6	0.45	0.654E-04	-.752	0.962E-03
7	0.55	-.113	-.622	0.652E-03
8	0.65	-.209	-.542	0.116E-02
9	0.75	-.195	-.450	0.174E-02
10	0.85	-.903E-02	-.136	0.396E-03
11	0.95	-.283	0.297	0.443E-03
12	1.05	0.398	-.407	-.695E-03

time : 770.00 days no. of t-steps = 770

i	depth	SI(FE(OH)3)	SI(Jurb)	SI(Jarosite)
1	0.03	-.118E-02	-1.92	0.757E-01
2	0.08	-.339E-03	-1.47	0.231E-01
3	0.15	-.171E-03	-1.23	-.920E-03
4	0.25	0.682E-05	-1.05	0.309E-03
5	0.35	-.399E-03	-.891	0.227E-02
6	0.45	-.635E-04	-.781	0.176E-02
7	0.55	-.148	-.659	0.437E-03
8	0.65	-.254	-.580	0.844E-03
9	0.75	-.277	-.483	0.151E-02
10	0.85	-.206E-01	-.182	0.410E-03
11	0.95	-.750E-01	0.250	0.575E-03
12	1.05	0.373	-.357	-.629E-02

File 6: File with produced amounts of H^+, OH^-, Fe^{2+}, Fe^{3+}, HCO_3^-, SO_4^{2-} SMASS
Name: CAPROD.OUT

Produced amounts H+, SO4-- and Fe3+ (mol/l)
time : 1.00 days no. of t-steps = 1

i	depth (m)	Production from pyrite oxidation: H-prod (mol/l soil sol./last t.st.)	SO4-prod	Fe3+-prod	pyr. ox. (kg/m3 soil/last t.st.)	Production from Fe(OH)3 reduction: OH-prod	Fe2+-prod	HCO3-prod
1	0.03	0.242E-03	0.484E-03	0.242E-03	0.207E-01	0.000E+00	0.000E+00	0.000E+00
2	0.08	0.212E-03	0.423E-03	0.212E-03	0.182E-01	0.000E+00	0.000E+00	0.000E+00
3	0.15	0.356E-03	0.713E-03	0.356E-03	0.308E-01	0.000E+00	0.000E+00	0.000E+00
4	0.25	0.309E-03	0.619E-03	0.309E-03	0.269E-01	0.000E+00	0.000E+00	0.000E+00
5	0.35	0.216E-03	0.432E-03	0.216E-03	0.190E-01	0.000E+00	0.000E+00	0.000E+00
6	0.45	0.701E-04	0.140E-03	0.701E-04	0.632E-02	0.000E+00	0.000E+00	0.000E+00
7	0.55	0.465E-04	0.930E-04	0.465E-04	0.422E-02	0.000E+00	0.000E+00	0.000E+00
8	0.65	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
9	0.75	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	0.85	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	0.95	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	1.05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Total production/consumption during last timestep:
H+ (mol.m-2): 0.889E-07
Fe3+ (mol.m-2): 0.178E-06
SO42- (mol.m-2): 0.889E-07
FeS2 (kg.m-2): 0.107E-04

Total production/consumption since start:
H+ (mol.m-2): 0.889E-07
Fe3+ (mol.m-2): 0.889E-07
SO42- (mol.m-2): 0.889E-07
FeS2 (kg.m-2): 0.107E-04

time : 10.00 days no. of t-steps = 10

i	depth (m)	Produktion from pyrite oxidation: H-prod (mol/l soil sol./last t.st.)	SO4-prod	Fe3+-prod	pyr. ox. (kg/m3 soil/last t.st.)	Production from Fe(OH)3 reduction: OH-prod	Fe2+-prod	HCO3-prod
1	0.03	0.272E-03	0.545E-03	0.272E-03	0.229E-01	0.000E+00	0.000E+00	0.000E+00
2	0.08	0.216E-03	0.431E-03	0.216E-03	0.183E-01	0.000E+00	0.000E+00	0.000E+00
3	0.15	0.370E-03	0.740E-03	0.370E-03	0.317E-01	0.000E+00	0.000E+00	0.000E+00
4	0.25	0.326E-03	0.651E-03	0.326E-03	0.281E-01	0.000E+00	0.000E+00	0.000E+00
5	0.35	0.227E-03	0.455E-03	0.227E-03	0.199E-01	0.000E+00	0.000E+00	0.000E+00

6	0.45	0.736E-04	0.147E-03	0.736E-04	0.661E-02	0.000E+00	0.000E+00	0.000E+00
7	0.55	0.485E-04	0.971E-04	0.485E-04	0.440E-02	0.000E+00	0.000E+00	0.000E+00
8	0.65	0.419E-04	0.838E-04	0.419E-04	0.387E-02	0.000E+00	0.000E+00	0.000E+00
9	0.75	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	0.85	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	0.95	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	1.05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

Total production/consumption during last timestep:
H+ (mol.m-2): 0.959E-07
Fe3+ (mol.m-2): 0.192E-06
SO42- (mol.m-2): 0.959E-07
FeS2 (kg.m-2): 0.115E-04

Total production/consumption since start:
H+ (mol.m-2): 0.924E-06
Fe3+ (mol.m-2): 0.924E-06
SO42- (mol.m-2): 0.924E-06
FeS2 (kg.m-2): 0.111E-03

time : 20.00 days no. of t-steps = 20

		Produktion from pyrite oxidation				Production from Fe(OH)3 reduction		
i	depth (m)	H-prod (mol/l soil sol./last t.st.)	SO4-prod	Fe3+-prod	pyr. ox. (kg/m3 soil/last t.st.)	OH-prod	Fe2+-prod	HCO3-prod
1	0.03	0.361E-03	0.722E-03	0.361E-03	0.297E-01	0.000E+00	0.000E+00	0.000E+00
2	0.08	0.219E-03	0.437E-03	0.219E-03	0.182E-01	0.000E+00	0.000E+00	0.000E+00
3	0.15	0.375E-03	0.750E-03	0.375E-03	0.314E-01	0.000E+00	0.000E+00	0.000E+00
4	0.25	0.327E-03	0.655E-03	0.327E-03	0.278E-01	0.000E+00	0.000E+00	0.000E+00
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time : 770.00 days no. of t-steps = 770

		Produktion from pyrite oxidation				Production from Fe(OH)3 reduction		
i	depth (m)	H-prod (mol/l soil sol./last t.st.)	SO4-prod	Fe3+-prod	pyr. ox. (kg/m3 soil/last t.st.)	OH-prod	Fe2+-prod	HCO3-prod
1	0.03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	0.08	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

3	0.15	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	0.25	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
5	0.35	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.240E-05	0.137E-05	0.343E-06
6	0.45	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.657E-05	0.376E-05	0.939E-06
7	0.55	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
8	0.65	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
9	0.75	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	0.85	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	0.95	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	1.05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.226E-04	0.129E-04	0.323E-05

Total production/consumption during last timestep:
H+ (mol.m-2): 0.000E+00
Fe3+ (mol.m-2): 0.000E+00
SO42- (mol.m-2): 0.000E+00
FeS2 (kg.m-2): 0.000E+00

Total production/consumption since start:
H+ (mol.m-2): 0.323E-04
Fe3+ (mol.m-2): 0.323E-04
SO42- (mol.m-2): 0.323E-04

File 7: File with output related to pyrite oxidation and oxygen transport, SMASS
Name: CAOXY.OUT

Column A, drainage and leaching potential acid sulphate soil

time : 1.00 days number of time step= 1

number of iterations = 3
susqdi = 0.265E-04
Dtchem (d) = 1
number aerated layers = 7
O2 consumption (kg O2.m-2.d-1)= 0.0289
Depth ground water level (m-soil surface) = 0.65

i	depth cm	prhead cm	theta	[O2]air %	aevo %	FeS2 %	FeS2 kg/m3	FeS2 dia m	Oxcons kg/m3.d
1	0.025	78.9	0.714	19.7	26.6	0.13	0.66	0.4949E-04	0.5170E-01
2	0.075	66.6	0.717	18.4	20.3	0.48	2.46	0.4988E-04	0.5393E-01
3	0.150	52.6	0.720	16.4	11.2	2.61	13.99	0.4996E-04	0.8367E-01
4	0.250	39.2	0.726	15.0	5.2	5.30	29.05	0.4998E-04	0.7273E-01
5	0.350	29.2	0.731	14.3	2.5	7.86	44.08	0.4999E-04	0.5136E-01
6	0.450	19.8	0.751	13.9	0.8	8.28	46.90	0.5000E-04	0.1726E-01
7	0.550	10.0	0.757	13.7	0.7	6.69	38.02	0.5000E-04	0.1158E-01
8	0.650	0.0	0.780	0.0	0.0	5.23	29.98	0.5000E-04	0.0000E+00
9	0.750	0.0	0.780	0.0	0.0	6.97	40.00	0.5000E-04	0.0000E+00
10	0.850	0.0	0.780	0.0	0.0	8.86	51.01	0.5000E-04	0.0000E+00
11	0.950	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00
12	1.050	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00

time : 10.00 days number of time step= 10
number of iterations = 2
susqdi = 0.112E-03
Dtchem (d) = 1
number aerated layers = 8
O2 consumption (kg O2.m-2.d-1)= 0.0307
Depth ground water level (m-soil surface) = 0.68

i	depth cm	prhead cm	theta	[O2]air %	aevo %	FeS2 %	FeS2 kg/m3	FeS2 dia m	Oxcons kg/m3.d
1	0.025	121.8	0.700	19.9	27.4	0.09	0.46	0.4398E-04	0.5365E-01
2	0.075	99.6	0.706	18.7	20.8	0.44	2.30	0.4874E-04	0.5410E-01
3	0.150	75.2	0.713	16.8	11.5	2.56	13.71	0.4962E-04	0.8512E-01
4	0.250	51.8	0.719	15.4	5.4	5.25	28.80	0.4984E-04	0.7474E-01
5	0.350	34.8	0.727	14.6	2.6	7.83	43.90	0.4993E-04	0.5295E-01

6	0.450	23.1	0.749	14.0	0.8	8.27	46.84	0.4998E-04	0.1779E-01
7	0.550	13.0	0.755	13.6	0.7	6.68	37.98	0.4998E-04	0.1190E-01
8	0.650	3.0	0.770	13.2	0.8	5.23	29.96	0.4999E-04	0.1050E-01
9	0.750	0.0	0.780	0.0	0.0	6.97	40.00	0.5000E-04	0.0000E+00
10	0.850	0.0	0.780	0.0	0.0	8.86	51.01	0.5000E-04	0.0000E+00
11	0.950	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00
12	1.050	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00

time : 20.00 days number of time step= 20
number of iterations = 1
susqdi = 0.101E-04
Dtchem (d) = 1
number aerated layers = 10
O2 consumption (kg O2.m-2.d-1)= 0.0329
Depth ground water level (m-soil surface) = 0.92

i	depth cm	prhead cm	theta	[O2]air %	aevo %	FeS2 %	FeS2 kg/m3	FeS2 dia m	Oxcons kg/m3.d
1	0.025	206.4	0.685	20.0	28.3	0.04	0.20	0.3349E-04	0.5990E-01
2	0.075	169.9	0.692	19.0	21.0	0.41	2.11	0.4742E-04	0.5371E-01
3	0.150	130.8	0.699	17.2	11.5	2.50	13.40	0.4925E-04	0.8459E-01
4	0.250	96.1	0.707	15.9	5.4	5.20	28.53	0.4968E-04	0.7413E-01
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.

time : 760.00 days number of time step= 760
number of iterations = 1
susqdi = 0.000E+00
Dtchem (d) = 1
number aerated layers = 0
O2 consumption (kg O2.m-2.d-1)= 0.0000
Depth ground water level (m-soil surface) = 0.00

i	depth cm	prhead cm	theta	[O2]air %	aevo %	FeS2 %	FeS2 kg/m3	FeS2 dia m	Oxcons kg/m3.d
1	0.025	0.0	0.780	0.0	0.0	0.00	0.00	0.0000E+00	0.0000E+00
2	0.075	0.0	0.780	0.0	0.0	0.00	0.00	0.0000E+00	0.0000E+00
3	0.150	0.0	0.780	0.0	0.0	0.50	2.63	0.2863E-04	0.0000E+00
4	0.250	0.0	0.780	0.0	0.0	3.28	17.81	0.4246E-04	0.0000E+00
5	0.350	0.0	0.780	0.0	0.0	6.45	35.96	0.4671E-04	0.0000E+00
6	0.450	0.0	0.780	0.0	0.0	7.83	44.28	0.4905E-04	0.0000E+00
7	0.550	0.0	0.780	0.0	0.0	6.43	36.50	0.4932E-04	0.0000E+00
8	0.650	0.0	0.780	0.0	0.0	5.06	28.99	0.4944E-04	0.0000E+00

9	0.750	0.0	0.780	0.0	0.0	6.84	39.26	0.4969E-04	0.0000E+00
10	0.850	0.0	0.780	0.0	0.0	8.77	50.46	0.4982E-04	0.0000E+00
11	0.950	0.0	0.780	0.0	0.0	7.84	44.96	0.5000E-04	0.0000E+00
12	1.050	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00

time : 770.00 days number of time step= 770
number of iterations = 1
susqdi = 0.000E+00
Dtchem (d) = 1
number aerated layers = 0
O2 consumption (kg O2.m-2.d-1)= 0.0000
Depth ground water level (m-soil surface) = 0.00

i	depth cm	prhead cm	theta	[O2]air %	aevo %	FeS2 %	FeS2 kg/m3	FeS2 dia m	Oxcons kg/m3.d
1	0.025	0.0	0.780	0.0	0.0	0.00	0.00	0.0000E+00	0.0000E+00
2	0.075	0.0	0.780	0.0	0.0	0.00	0.00	0.0000E+00	0.0000E+00
3	0.150	0.0	0.780	0.0	0.0	0.50	2.63	0.2863E-04	0.0000E+00
4	0.250	0.0	0.780	0.0	0.0	3.28	17.81	0.4246E-04	0.0000E+00
5	0.350	0.0	0.780	0.0	0.0	6.45	35.96	0.4671E-04	0.0000E+00
6	0.450	0.0	0.780	0.0	0.0	7.83	44.28	0.4905E-04	0.0000E+00
7	0.550	0.0	0.780	0.0	0.0	6.43	36.50	0.4932E-04	0.0000E+00
8	0.650	0.0	0.780	0.0	0.0	5.06	28.99	0.4944E-04	0.0000E+00
9	0.750	0.0	0.780	0.0	0.0	6.84	39.26	0.4969E-04	0.0000E+00
10	0.850	0.0	0.780	0.0	0.0	8.77	50.46	0.4982E-04	0.0000E+00
11	0.950	0.0	0.780	0.0	0.0	7.84	44.96	0.5000E-04	0.0000E+00
12	1.050	0.0	0.780	0.0	0.0	7.84	44.97	0.5000E-04	0.0000E+00

File 8: File with chemical output data SMASS
Name: -

This option was not used in the example calculations. File is not created.

File 9: Messages produced by SMASS
Name: MESSAGE1.OUT

```
Messages created by subroutines Chem and Epidim
 Day       1    Layer    1
 Day       1    Layer    2
 Day       1    Layer    3
 Day       1    Layer    4
 Day       1    Layer    5
 Day       1    Layer    6
 Day       1    Layer    7
 Day       1    Layer    8
 Day       1    Layer    9
 Day       1    Layer   10
 Day       1    Layer   11
 Day       1    Layer   12
 Day       2    Layer    1
 Day       2    Layer    2
 Day       2    Layer    3
 Day       2    Layer    4
 Day       2    Layer    5
  .        .        .
  .        .        .
  .        .        .
  .        .        .
  .        .        .
  .        .        .
  .        .        .
 Day     769    Layer    9
 Day     769    Layer   10
 Day     769    Layer   11
 Day     769    Layer   12
 Day     770    Layer    1
 Day     770    Layer    2
 Day     770    Layer    3
 Day     770    Layer    4
 Day     770    Layer    5
 Day     770    Layer    6
 Day     770    Layer    7
 Day     770    Layer    8
 Day     770    Layer    9
 Day     770    Layer   10
 Day     770    Layer   11
 Day     770    Layer   12

(NO ERROR MESSAGES)
```

File 10: Messages produced by subroutine TRANSOL
Name: MESSAGE2.OUT

```
Messages from subroutine Transol

 subr.FLWCHECK: watertransport is greater actual storage
   daynr =  29.00;  layernr =  1;  average waterflux = 0.377E-01  (m/d)
   average watertransport = 0.377E-01 (m)
   actual storage         = 0.355E-01 (m) ;  difference =    6.18 %

 subr.FLWCHECK: watertransport is greater actual storage
   daynr =  42.00;  layernr =  1;  average waterflux = 0.385E-01  (m/d)
   average watertransport = 0.385E-01 (m)
   actual storage         = 0.363E-01 (m) ;  difference =    6.19 %
      .
      .
      .
      .
      .
      .
      .
      .
      .
      .

 subr.FLWCHECK: watertransport is greater actual storage
   daynr = 728.00;  layernr =  1;  average waterflux = 0.429E-01  (m/d)
   average watertransport = 0.429E-01 (m)
   actual storage         = 0.390E-01 (m) ;  difference =    9.95 %

 subr.FLWCHECK: watertransport is greater actual storage
   daynr = 728.00;  layernr =  2;  average waterflux = 0.422E-01  (m/d)
   average watertransport = 0.422E-01 (m)
   actual storage         = 0.390E-01 (m) ;  difference =    8.14 %

 subr.FLWCHECK:    72 flowcheck-messages written to the file  MESSAGE2.OUT
```

Appendix 2: Description format for input files for SWACROP

December 1991

Staring Centre
Wageningen

SWATRE / SWACROP

INPUT INSTRUCTIONS MANUAL

Simulation model of the water balance of a cropped soil with different types of boundary conditions including the possibility of drainage and irrigation and the calculation of crop yield.

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Table of contents

Setup of input instructions manual 107

How tu create a data file 110

Section 1: The file containing the general input data (SWADAT.INP) 111

Section 2: The file containing the data for the upper boundary 123

Section 3: The file containing the crop data 127

Section 4: The file(s) containing the soil physical data 134

Section 5: The file containing the data for the lower boundary 136

Section 6: The file containing the data for drainage/subirrigation 139

References 143

Appendixes

2.1 Figures 144
2.2 Alphabetical list of labels and corresponding groups 146
2.3 List of variables 147

N.B. In its original form, SWACROP is designed to read input files for a one-year period. If more (succesive) years need to be calculated, seperate input files with for example crop data or meteorological data need to be prepared. However, for irrigation data, it was not yet possible to read different irrigation gifts over a period of more than one year. Therefore, the used SWACROP model is slightly adapted, with the result that all input files may now contain as much as 4000 data's. In this way, periods of up to 10 years can be simulated in one run. For example, in section 4.2 one meteo file with 770 values is used for a two years simulation period. The same aplies to the irrigation data, the groundwater levels etc.
Note: the manual in this appendix applies to the original SWACROP model.

SETUP OF *INPUT INSTRUCTIONS MANUAL*

The model SWATRE / SWACROP supports various hydrological options. Each option requires different input data with corresponding format. The input instructions given below describe how to make the required input files depending on your choice of options.

This *INPUT INSTRUCTIONS MANUAL* is made up of 6 separate SECTIONS each representing one datafile. Each of these SECTIONS is made up of GROUPS. The group nummering includes SECTION number and a letter of the alphabet, eg. GROUP 1.M (SECTION 1 with GROUP M). Some GROUPS are made up of a number of SUB-GROUPS which are separated by a grey line.

For **one** year of simulation, SWATRE / SWACROP uses 5 or 6 ASCII-files for data input :

- FILE 1 : contains input as described in SECTION 1 (general input data)	**default**
- FILE 2 : contains input as described in SECTION 2 (top boundary data)	"
- FILE 3 : contains input as described in SECTION 3 (crop data)	"
- FILE 4 : contains input as described in SECTION 4 (soil physical data)	"
- FILE 5 : contains input as described in SECTION 5 (bottom boundary data)	"
- FILE 6 : contains input as described in SECTION 6 (drainage data)	**optional**

Beginning of example GROUP 1.M as listed in this *INPUT INSTRUCTIONS MANUAL* ======

GROUP 1.M	**used only if SWTOPB = 2 or 4 (see GROUP 1.H)**
LABEL ">excons:"	**use 1 line**
	Constants used for calculating evapotranspiration.
	Use this line if SWTOPB = 2 :
R ALPHA	empirical constant in the Priestly and Taylor equation. We advise 1.35 ± 0.10
	Use this line if SWTOPB = 4 :
	Canopy resistances used in the Monteith-Rijtema equation.
R RSMIN	minimum canopy resistance ($s \cdot m^{-1}$)
R RSMAX	maximum canopy resistance ($s \cdot m^{-1}$)

End of example GROUP 1.M ==========

End of example GROUP 1.M ==========

Explanation of GROUP 1.M

GROUP 1.M on the previous page is made up of : i) **group heading**
ii) **group text**

The **group heading** (shaded) indicates:

- the group number	1.M
- when a group should be used	used only if ....
- the unique group label (max. 8 characters)	" >excons: "
- the amount of lines to use for input	use 1 line

The **group text** indicates :

- occasional explanatory text	Constants used for calculating evapotranspiration.
- variable name	ALPHA if SWTOPB = 2 and
	RSMIN and RSMAX if SWTOPB = 4
- type of variable	Real
- description of variables	empirical constant... or minimum canopy...

ADDITIONAL INFORMATION:

* Please note: FILE 1 containing the general input data as described in SECTION 1 of this *INPUT INSTRUCTIONS MANUAL*, **must at all times be named SWADAT.INP**
The other 5 data files have **user-definable names to be specified in FILE 1**

* Variable names correspond with those used in the source code. Variable names are either REAL (R), INTEGER (I) or STRING (S) as indicated before each variable name.
Please note: **STRING data should be quoted using single quotes (' ')**

* Special attention should be given to explanatory notes with a ☛ .

☛ For all equations, figures and page numbers you find in the **group text** please refer to the following publication, unless stated otherwise:

Feddes, R.A., Kowalik, P.J., and Zaradny, H., (1978): "Simulation of field water use and crop yield", Simulation Monographs, Pudoc, Wageningen.

* More background literature is listed in the **References**.

HOW TO CREATE A DATA FILE

For each GROUP in each data file, there are default and optional lines:

default lines are: - **a label line** containing the unique group label
- **data line(s)** containing the value(s) of the variables

optional lines are: - **comment lines**

Label line :
The first 8 characters of a label line should contain the label as given in the group heading. In the example this is: " >excons: " Any characters to the right of this label are not significant and may be used as comment. The label indicates that the next line **must be** a data line.

Data lines :
A data line **always** follows a label line. Data on one line must be separated by one or more blanks. The line should end with a <cr/lf> (carriage return/line feed).

Comment lines :
These may be used *before a label line* or *after a data line* (or group of data lines). They are not significant to the program. Their purpose is purely explanatory.

Example of GROUP 1.M as listed in the main input file *SWADAT.INP*

```
extra constants for calculating evapotranspiration          ← comment line
>excons:                                                      ← label line
1.35                                                          ← data line
alpha for Priestly and Taylor equation                        ← comment line
```

End of example GROUP 1.M ==========

SECTION 1. The file containing the general input data (SWADAT.INP)

GROUP 1.A **use 1 line**
LABEL ">genhdr:"

S HEADER — Desired heading to be printed. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters

☛ reminder: string data, e.g. HEADER, should be quoted using a single quote.

GROUP 1.B **use 1 line**
LABEL ">output:"

I SWSTAG
= 0 : the stage of computation is not shown during calculations
= 1 : the stage of computation is shown as: a bar on the screen showing % of computed days (advised for interactive systems)
= 2 : the stage of computation is shown as: 'year', 'daynumber' and '% mass balance error' (advised for batch processing)

I OUTIVL — interval between output written to all output files (d)

S OUTPUTFL — give name of output file, this output file contains: i) the echo of the input and ii) terms of the water balance. Use max. 40 characters

GROUP 1.C **if SWFILE1 = 0 use 1 line**
LABEL ">exfile:" **if SWFILE1 = 1 use 1 + 1 + 1 lines**
if SWFILE1 = 2 use 1 + 1 lines
if SWFILE1 = 3 use 1 + 1 + 1 lines

Whether extra output file containing supplementary data is needed.

I SWFILE1
= 0 : no extra file
= 1 : extra output file created containing soil-profile data
= 2 : extra **unformatted** output file created containing output data to be used as input for the water-quality model ANIMO
= 3 : Two extra files output created for water-quality model ANIMO:
  i) extra **unformatted** file created containing output data to be used as input by the water-quality model ANIMO
  ii) extra **formatted** (readable) file created containing the same data

If **SWFILE = 2** or **3**; then the following parameters are output to the ANIMO file(s):

	Initial values :	
**	YEAR	year when simulation starts (-)
**	YEAR	year when simulation ends (-)
	DAYSTA	day when simulation starts (d)
	DAYEND	day when simulation ends (d)
	OUTIVL	length of output interval (d)
**	NUMNOD	number of compartments (-)
	NUMLAY	number of different types of soil layers (-)
	NRLEVS	number of drainage levels (-)
**	BOTCOM()	bottom compartment of layer 1 to NUMLAY (-)
**	THETSN()	saturated moisture fr. layer 1 to NUMLAY ($m^3 \cdot m^{-3}$)
**	THETPFF()	moisture content at pF 2.0 layer 1 to NUMLAY (-)
**	THETPFW()	moisture content at pF 4.2 layer 1 to NUMLAY (-)
**	DZ()	height of compartment 1 to NUMNOD (m)
**	THETA()	moisture cont. of compartment 1 to NUMNOD ($m^3 \cdot m^{-3}$)
**	GWL(3)	groundwater table (m below soil surface, positive)
	POND	initial ponding level (m)
	At each interval :	
**	T	day number of output (d)
	IPREC	average precipitation during interval ($m \cdot d^{-1}$)
	IINTC	average interception during interval ($m \cdot d^{-1}$)
	IEVAP	average evaporation during interval ($m \cdot d^{-1}$)
	IEPND	average ponding evap. during interval ($m \cdot d^{-1}$)
	IPEVA	aver. pot. evaporation during interval ($m \cdot d^{-1}$)
	IPTRA	av. pot. transpiration during interval ($m \cdot d^{-1}$)
	IRUNO	average runoff during interval ($m \cdot d^{-1}$)
	GWL(3)	groundwater table at end of interval (m)
	POND	ponding level at end of interval (m)
**	H()	pressure head 1 to NUMNOD at end of interval (m), (negative when unsaturated)
**	THETA()	moisture content 1 to NUMNOD at end of interval(-)
**	INQROT()	average root extraction flux 1 to NUMNOD ($m \cdot d^{-1}$)
**	INQ()	average flux at the top of compartments 1 to NUMNOD+1 ($m \cdot d^{-1}$, positive = downwards). INQ(NUMNOD+1) represents seepage/drainage
**	INQDRA(1)	average flux of 1st drain level from compartment 1 to NUMNOD ($m \cdot d^{-1}$)
	▽repeat▽	
**	INQDRA(nrlevs)	average flux of level NRLEVS from compartment 1 to NUMNOD ($m \cdot d^{-1}$)
**	indicates a new record (unformatted output). Formatted output uses the same order of data but more records.	

Units and signs used for this output are **not** the same as units and signs used in SWATRE / SWACROP. Drainage fluxes are given for levels 1 to NRLEVS, if NRLEVS = 0 no fluxes are given. If there is no groundwater or perched water table a dummy value of -9.99 is given.

	Use this line if SWFILE1 = 1, 2 or 3:
S OUTFILE1	If SWFILE1 = 1; give name of extra output file containing soil profile data (see below for choice of soil profile data) If SWFILE1 = 2 or 3; give name of extra **unformatted** output file containing output data as input for ANIMO model, (see previous page for type of output data) Use max. 40 characters
	Use this line **only** if SWFILE1 = 3 :
S OUTFILE2	give name of extra **formatted** output file containing output data as input for ANIMO model, (see previous page for type of output data) Use max. 40 characters
	Use this line **only** if SWFILE1 = 1 :
	Make a choice of soil profile data to be written to the filename given in OUTFILE1 above. Output per nodal point with interval OUTIVL (see GROUP 1.B) of :
I SWOUTP(1)	= 0 : no output = 1 : output of the **volumetric moisture content** of the profile at the end of the interval
I SWOUTP(2)	as above, for the **pressure head** in the profile at the end of the interval
I SWOUTP(3)	as above, for the **hydraulic conductivity** of the profile at the end of the interval
I SWOUTP(4)	as above, for the **flux** through the compartments cumulated during the interval
I SWOUTP(5)	as above, for the **extracted volume** by the roots cumulated during the interval
I SWOUTP(6)	as above, for the **drainage fluxes** to each drainage medium cumulated during the interval
	Note: **ponding** thickness, **groundwater level** and **perched water level** are always given

GROUP 1.D **use 1 line**
LABEL ">timeva:"

Describes the calculation period and size of time step.

I YEARST	starting year of calculations (-)
I YEAREN	finishing year of calculations (-)
I DAYSTA	starting day of calculations (Julian day number, Janaury 1st = 1)
I DAYEND	finishing day of calculations (d)
R DTMAX	maximum value of time step allowed (d), this value may range from 0.01 to 0.5, We advise 0.2
R PRECIS	calculation precision criterium (-). This value may range from 1.0 (low accuracy, low computing time) to 10.0 (high accuracy, high computing time). We advise to use 5.0

GROUP 1.E **use 1 line**
LABEL ">redeva:"

Choice of reduction of potential soil evaporation.

I SWREDU	= 0 : no reduction = 1 : reduction is calculated using the Black (1969) model = 2 : reduction is calculated using the Boesten (1986) model = 3 : reduction is calculated using an adapted Boesten model taking into account the actual moisture condition of soil surface
R COFRED	coefficient α (Black, $cm \cdot d^{-½}$) or β ($cm^{½}$)

☛ for α we advise to use 0.35 ± 0.15
for β we advise to use 0.63 (range 0.54-0.95)
☛ if SWREDU = 0, a dummy value should be given for COFRED

GROUP 1.F **if SWIRRI = 0 use 1 line**
LABEL ">irriva:" **if SWIRRI = 1 use 1 + 1 lines**
if SWIRRI = 2 use 1 + 1 + COUNTI lines

I SWIRRI	= 0 : irrigation is not simulated = 1 : time of irrigation is simulated = 2 : time and amount of irrigation is given at prescribed days

---

Use this line if SWIRRI = 1 :

R IRRAMT	amount of each irrigation application (cm)
I TLAGIR	minimum time-lag between two successive applications (d)
R HCRIT	critical pressure head value below which irrigation is applied (cm), (the irrigation criterium)

I NCRIT	nodal point number where HCRIT applies (-), (see GROUP 1.P)
	Use these lines if SWIRRI = 2 :
I COUNTI	number of days that irrigation takes place
I DAYNR(I)	first daynumber at which irrigation takes place
R IRRAMT(DAYNR(1))	amount of irrigation applied on this first daynumber (cm)
	▽repeat▽ for each irrigation day (one data-pair per line)
I DAYNR(COUNTI)	last daynumber at which irrigation takes place
R IRRAMT(DAYNR(COUNTI))	amount of irrigation applied on this last daynumber (cm)

GROUP 1.G **use 1 line**
LABEL ">methdr:"

S HEADER Description of the meteorological conditions. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters

GROUP 1.H **use 1 line**
LABEL ">topbnd:"

Describes the upper boundary conditions.

I SWTOPB
- = 0 : pot. evapotranspiration ($cm \cdot d^{-1}$) is entered as pot. soil evaporation and pot. transpiration (see Group 2.B)
- = 1 : pot. evapotranspiration ($cm \cdot d^{-1}$) is entered as REFEVA (reference evapotranspiration) and then multiplied by a crop factor (see GROUP 3.H)
  (for choice of REFEVA as E_{OPEN} or E_{MAK}, see GROUP 2.B)
- = 2 : pot. evapotranspiration ($cm \cdot d^{-1}$) is calculated with the Priestly and Taylor equation (see GROUP 2.B)
- = 3 : pot. evapotranspiration ($cm \cdot d^{-1}$) is calculated with the Penman equation (eq'n. 3.26) as E_{OPEN} (see GROUP 2.B) and then multiplied by a crop factor (see GROUP 3.H)
- = 4 : pot. evapotranspiration ($cm \cdot d^{-1}$) is calculated with the Monteith-Rijtema equation (eq'n. 3.33) (see GROUP 2.B) Internal canopy resistance r_s is calculated from RSMIN, RSMAX and Ewet. (for RSMIN and RSMAX values see GROUP 1.M)
- = 5 : pot. evapotranspiration ($cm \cdot d^{-1}$) is calculated with the Makkink equation as E_{MAK} (see GROUP 2.B) and then multiplied by a crop factor (see GROUP 3.H)

If SWTOPB = 2, 3, 4 or 5: potential soil evaporation is calculated with eq'n. 35 [Belmans et al. (1983)] and the minimum allowed pressure head at the soil surface is calculated according to eq'n. 4.11

☛ **To calculate crop production, SWTOPB should be 2, 3, 4 or 5.**

I SWTBVA
= 0 : upper boundary condition is constant with time
= 1 : upper boundary condition is varying with time

GROUP 1.I **use YEARST - YEAREN + 1 lines**
LABEL ">metfil:"

SWATRE / SWACROP gives the option to calculate for several successive years.
Give name(s) of the input file(s) containing the meteorological data.
See SECTION 2 for the input description of these files.
For each simulation year, give yearnumber and matching filename.

I yearst
first year of calculation (see GROUP 1.D)
S METEOFL(yearst)
give name of the input file containing the parameters describing the boundary conditions at the top of the soil profile (meteo data) for year YEARST. Use max. 40 characters
▽repeat▽ for each year of calculation
I yearen
last year of calculation (see GROUP 1.D)
S METEOFL(yearen)
give name of the input file containing the parameters describing the boundary conditions at the top of the soil profile for year YEAREN

☛ If 'SWADAT.INP' is given as file name, then the corresponding meteo input data can be added to the file SWADAT.INP

GROUP 1.J **use 1 line**
LABEL ">crphdr:"

S HEADER
Description of the crop input data. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters

GROUP 1.K **if SWUPFU = 0 use 1 line**
LABEL ">sinkva:" **if SWUPFU = 1 use 1 + 1 lines**
if SWUPFU = 2 use 1 line

Description of sink term and root extraction pattern.
I SWSINK
= 0 : sink term according to Feddes
See fig. 1 (appendix 1) and Feddes et al. (1978)
= 1 : sink term according to Hoogland
See fig. 2 (appendix 1) and Feddes et al. (1988b)

I SWHYPR	= 0 : linear relationship between the points HLIM3 and HLIM4 of the sink term. See fig. 3 (appendix 1) = 1 : hyperbolic relationship between the points HLIM3 and HLIM4 of the sink term. See fig. 4 (appendix 1) For values of HLIM3 and HLIM4 see GROUP 3.A
I SWUPFU	= 0 : water uptake function according to Feddes See fig. 5 (appendix 1) and Feddes et al. (1988b) = 1 : water uptake function according to Hoogland See fig. 6 (appendix 1) = 2 : water uptake function according to Prasad (1988) See fig. 7 (appendix 1)

Use this line if SWUPFU = 1 :

R COFSZA	intercept 'a' of eq'n. $S_{max} = a - b \cdot \lvert z \rvert$ [Feddes et al. 1988a]
R COFSZB	slope 'b' of eq'n. $S_{max} = a - b \cdot \lvert z \rvert$ [Feddes et al. 1988a]

where: z = depth below soil surface (cm)

GROUP 1.L **use 1 line**
LABEL ">rootac:"

Nonactive layer of roots at the top of the profile.

R ZRONAM	maximum thickness (cm, absolute value) of the nonactive layer during the period t > TRONAE
R TRONAB	point of time (d) at which the nonactive layer starts, (drought damage or morphological reasons)
R TRONAE	point of time (d) at which the nonactive layer reaches its maximum thickness

$$\begin{aligned} t \le TRONAB &: ZRONA = 0 \\ TRONAB < t \ge TRONAE &: ZRONA = ZRONAM * \frac{t - TRONAB}{TRONAE - TRONAB} \\ t > TRONAE &: ZRONA = ZRONAM \end{aligned}$$

where: t = time (d)
ZRONA = actual thickness of the non-active layer (cm)

☞ to cancel this option: set ZRONAM = 0.0 and give dummy values for TRONAB and TRONAE

GROUP 1.M **used only if SWTOPB = 2 or 4** **(see GROUP 1.H)**
LABEL ">excons:" **use 1 line**

Constants used for calculating evapotranspiration.

Use this line if SWTOPB = 2 :

R ALPHA — empirical constant in the Priestly and Taylor equation,
We advise a value of 1.35 ± 0.10

Use this line if SWTOPB = 4 :

Canopy resistances used in the Monteith-Rijtema equation.

R RSMIN — minimum canopy resistance ($s \cdot m^{-1}$)
R RSMAX — maximum canopy resistance ($s \cdot m^{-1}$)

GROUP 1.N — use YEARST - YEAREN + 1 lines
LABEL ">crpfil:"

SWATRE / SWACROP gives the option to calculate for several successive years.
Give name(s) of the input file(s) containing the crop data.
See SECTION 3 for the input description of these file(s).
For each simulation year, give yearnumber and matching filename.

I yearst — first year of calculation (see GROUP 1.D)
S CROPINFL(yearst) — give name of the input file containing the crop data for year YEARST, Use max. 40 characters
▽repeat▽ for each year of calculation
I yearen — last year of calculation (see GROUP 1.D)
S CROPINFL(yearen) — give name of the input file containing the crop data for year YEAREN

☛ If 'SWADAT.INP' is given as file name, then the corresponding crop input data can be added to the file SWADAT.INP

GROUP 1.O — If SWPROD = 0 use 1 line
LABEL ">crppro:" — If SWPROD = 1 use 2 lines

I SWPROD — = 0 : crop production is not simulated
= 1 : crop production is simulated

☛ To calculate crop production SWTOPB should be 2, 3, 4 or 5 (see GROUP 1.H)

Use this line if SWPROD = 1 :

S CROOUTFL — give name of the output file containing crop production terms,
Use max. 40 characters

GROUP 1.P **use 1 line + max. 4 lines (assume 10 values/line)**
LABEL ">profil:"

Describes the geometry of the soil profile.

I NUMLAY	number of different types of soil layers (-) The maximum is 5
I NUMNOD	number of soil compartments (-) The maximum is 40
I BOTCOM(1)	compartment number at bottom of 1st soil layer (-) ▽repeat▽ for each compartment
I BOTCOM(NUMLAY-1)	compartment number at bottom of soil layer NUMLAY-1 (-)

☛ BOTCOM(NUMLAY) equals NUMNOD

Distribution of compartments over the soil profile.

R DZ(1)	thickness of 1st (top) compartment (cm) ▽repeat▽ for each compartment
R DZ(NUMNOD)	thickness of deepest compartment (NUMNOD) (cm)

☛ We advise to limit compartment thickness to a maximum of 25 cm (for unsaturated compartments)

GROUP 1.Q **use max. NUMLAY - lines**
LABEL ">soilfl:"

Input filename(s) containing the soil physical parameters.
See SECTION 4 for the input description of these files.

S SOILFL(1)	give name of the file containing the soil physical parameters of the 1st soil layer, Use max. 40 characters. ▽repeat▽ for each soil layer
S SOILFL(NUMLAY)	give name of the file containing the soil physical parameters of the deepest soil layer (NUMLAY)

☛ If 'SWADAT.INP' is given as file name, then the corresponding soil input data can be added to the file SWADAT.INP

GROUP 1.R **use 1 line**
LABEL ">pondmx:"

R PONDMX	maximum thickness of ponding water layer on the soil surface (cm)

GROUP 1.S	**if SWINCO = 0 use 1 + max. 4 lines (assume 10 values/line)**
LABEL ">incond:"	**if SWINCO = 1 use 1 + max. 4 lines (assume 10 values/line)**
	if SWINCO = 2 use 1 + 1 lines

Initial 'theta' or 'pressure head' condition for first day of calculation.

I SWINCO

= 0 : volum. moisture content ($cm^3 \cdot cm^{-3}$) at each nodal point is input
= 1 : pressure head (cm) at each nodal point is input, (**unsaturated** = negative value)
= 2 : pressure head at each nodal point is calculated as equilibrium with the initial groundwater table depth

---

Use these lines if SWINCO = 0 :

Input of initial volum. moisture-content profile (t = DAYSTA)

R THETA(1) initial volum. moisture content ($cm^3 \cdot cm^{-3}$) of 1st compartment (top compartment at the soil surface)

▽repeat▽ for each compartment

R THETA(NUMNOD) initial volum. moisture content of the NUMNODth compartment (deepest compartment at the bottom of the soil profile)

Use these lines if SWINCO = 1 :

Input of initial pressure-head profile (t = DAYSTA)

R H(1) initial pressure head (cm) of 1st compartment

▽repeat▽ for each compartment

R H(NUMNOD) initial pressure head of NUMNODth compartment

☛ pressure heads are negative in the unsaturated zone while in the saturated zone these values are positive and equal to the depth below groundwater level

---

Use this line if SWINCO = 2 :

Input of initial groundwater table depth. Absolute value may be given (soil surface is used as reference level)

R GWL initial groundwater table depth (cm)

☛ if SWBOTB = 0 (see GROUP 5.B) this line may be skipped

GROUP 1.T **use 1 line**
LABEL ">bbdfil:"

S BBOUNDFL — Give name of the input file containing the parameters describing the boundary conditions at the bottom of the soil profile.
See SECTION 5 for the input description of this file. Use max. 40 characters.

☛ If 'SWADAT.INP' is given as file name, then the corresponding bottom boundary input data can be added to the file SWADAT.INP

GROUP 1.U **if SWDRAI = 0 use 1 line**
LABEL ">drains:" **if SWDRAI = 1 use 2 lines**

I SWDRAI — = 0 : no drainage or subsurface irrigation simulated
= 1 : drainage and/or subsurface irrigation simulated

Use this line if SWDRAI = 1 :

S LBOUNDFL — Give name of the input file containing the parameters describing the boundary conditions at the lateral side of the soil profile: drainage.
See SECTION 6 for the input description of this file.
Use max. 40 characters.

☛ If 'SWADAT.INP' is given as file name, then the corresponding lateral boundary input data can be added to the file SWADAT.INP

GROUP 1.V **if SWSALT = 0 use 1 line**
LABEL ">solute:" **if SWSALT = 1 use 10 lines**

I SWSALT — = 0 : no solute transport simulated
= 1 : solute transport is simulated

Use these lines if SWSALT = 1:

S OUTFILE3 — give name of general output file for solute transport

---

R CIRR — solute concentration in irrigation water ($mg \cdot cm^{-3}$)
R CPRE — solute concentration in precipitation ($mg \cdot cm^{-3}$)
R CGRO — solute concentration in groundwater ($mg \cdot cm^{-3}$)

R SA(1)	initial solute concentration in 1st compartment ($mg \cdot cm^{-3}$)
	▽repeat▽ for each compartment
R SA(NUMNOD)	initial solute concentration in NUMNODth compartment ($mg \cdot cm^{-3}$)

$$h_{osm} = OSMOTA + OSMOTB * c$$

where: h_{osm} = osmotic potential (cm)
c = solute conc. of soil water ($mg \cdot cm^{-3}$)

R OSMOTA	regression coefficient (cm)
R OSMOTB	regression coefficient ($cm^4 \cdot mg^{-1}$)

I SALIVL	Interval between output of solute data (days)

GROUP 1.W **If SWFILE2 = 0 use 1 line**
LABEL ">anafil:" **If SWFILE2 = 1 use 2 lines**

Additional solute data output

I SWFILE2	= 0 : no extra output
	= 1 : extra output file created to facilitate the solute data

---

Use this line if SWFILE2 = 1:

S OUTFILE4	give name of extra output file containing values at each nodal point for:
	theta volumetric soil moisture content ($cm^3 \cdot cm^{-3}$)
	h pressure head (cm)
	cmsy conc. of mobile parts of the system ($mg \cdot cm^{-3}$)
	cisy conc. of immobile parts of the system ($mg \cdot cm^{-3}$)
	cml conc. of mobile parts of soil water ($mg \cdot cm^{-3}$)
	cil conc. of the immobile parts of soil water ($mg \cdot cm^{-3}$)
	cl average conc. of **cml** and **cil** weighted to **theta** ($mg \cdot cm^{-3}$)
	use max. 40 characters.

SECTION2. The file containing the data for the upper boundary.

The name of this file should be specified in GROUP 1.I of file SWADAT.INP

In the labels of this section the simulation year (minus 1900) should be given instead of the question marks, e.g. for 1991 the label of GROUP 2.A becomes " >radi91: "

GROUP 2.A — **used only if SWTOPB = 2, 3, 4 or 5 (see GROUP 1.H)**
LABEL ">radi??:" — **use 1 or 1 + 1 line(s)**

Determines available type of radiation and transformation factors, (if necessary)

I SWGRAD
= 0 : given type of radiation is global (see GROUP 2.B)
= 1 : given type of radiation is net

Use this line if SWGRAD = 0 :

Transformation factors to change global radiation to net.
These factors vary for each crop.

$$R_{NET} = (A * R_{GLOBAL}) + B \quad (global \triangleright net)$$

R COFNGA
coefficient A in above equation, $(1-\alpha)$
where: α = surface reflection coefficient (albedo) of short wave radiation (-)

R COFNGB
coefficient B in above equation, (R_l)
where: R_l = flux of net outgoing thermal or long wave radiation $(W \cdot m^{-2})$

☛ in case of **potatoes** we advise : COFNGA = 0.54
COFNGB = -4.0

☛ this line can be omitted if (SWTOPB = 3, Penman equation) is chosen (see GROUP 1.H)
Transformation will take place according to Penman (1948)

Use this line if:

SWGRAD = 1 (GROUP 2.A) and SWTOPB = 5 (GROUP 1.H) **or**
SWGRAD = 1 (GROUP 2.A) and SWPROD = 1 (GROUP 1.O)

Transformation factors to change net radiation to global.
These factors vary for each crop.

$$R_{GLOBAL} = \frac{R_{NET} - B}{A} \quad (net \triangleright global)$$

R COFNGA	coefficient A in above equation (-)
R COFNGB	coefficient B in above equation ($W \cdot m^{-2}$)

☛ in case of **potatoes** we advise : COFNGA = 0.54
COFNGB = -4.0

GROUP 2.B **use 1 or max. 366 lines**
LABEL ">metd??:"

Input of meteorological data to calculate potential evapotranspiration.

if SWTBVA = 0 (GROUP 1.H): 1 line required for **1st day of input**, the value of daynr is not significant
if SWTBVA = 1 (GROUP 1.H): 1 line required for **each day of input**, [DAYEND-DAYSTA + 1] lines

☛ first daynr ≤ DAYSTA and last daynr ≥ DAYEND
(see GROUP 1.D)

Use these lines if SWTOPB = 0 : (see GROUP 1.H)

Pot. evapotranspiration rate is entered as pot. soil evaporation and pot. transpiration.

I daynr	Julian day number (January 1st = 1)
R PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R PEVA(daynr)	potential soil evaporation rate ($cm \cdot d^{-1}$)
R PTRA(daynr)	potential transpiration rate ($cm \cdot d^{-1}$)

Use these lines if SWTOPB = 1 : (see GROUP 1.H)

Potential evapotranspiration rate ($cm \cdot d^{-1}$) entered as REFEVA (reference evapotranspiration) to be multiplied by crop factors. REFEVA may be entered as E_{OPEN} (Penman, open water evaporation) or as E_{MAK} (Makkink, reference crop evapotranspiration).
Depending on choice of REFEVA you must choose the right crop factors as asked for in GROUP 3.H

I daynr	Julian day number (January 1st = 1)
R PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R REFEVA(daynr)	reference evapotranspiration rate ($cm \cdot d^{-1}$)

Use these lines if SWTOPB = 2 : (see GROUP 1.H)

Potential evapotranspiration rate ($cm \cdot d^{-1}$) calculated with the Priestly and Taylor equation.

I daynr	Julian day number (January 1st = 1)
R PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R RADIA(daynr)	net radiation flux ($W \cdot m^{-2}$) (see GROUP 2.A)
R TEM(daynr)	mean daily air temperature (°C)
R RH(daynr)	mean daily air humidity (-)

Use these lines if SWTOPB = 3 : (see GROUP 1.H)

Potential evapotranspiration rate ($cm \cdot d^{-1}$) calculated with the Penman equation as E_{OPEN} (open water evaporation) and to be multiplied by the crop factors you will choose in GROUP 3.H

I daynr	Julian day number (January 1st = 1)
R PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R RADIA(daynr)	global radiation flux ($W \cdot m^{-2}$) (see GROUP 2.A)
R TEM(daynr)	mean daily air temperature (°C)
R RH(daynr)	mean daily air humidity (-)
R U(daynr)	mean daily wind velocity at 2 m height ($m \cdot s^{-1}$)
R DEGCLD(daynr)	degree of cloudiness (-)

☛ if net radiation is given instead of global radiation (default) degree of cloudiness can be omitted.

Use these lines if SWTOPB = 4 : (see GROUP 1.H)

Potential evapotranspiration rate ($cm \cdot d^{-1}$) calculated with the Monteith-Rijtema equation.

I daynr	Julian day number (January 1st = 1)
R PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R RADIA(daynr)	net radiation flux ($W \cdot m^{-2}$) (see GROUP 2.A)
R TEM(daynr)	mean daily air temperature (°C)
R RH(daynr)	mean daily air humidity (-)
R U(daynr)	mean daily wind velocity at 2 m height ($m \cdot s^{-1}$)

Use these lines if SWTOPB = 5 : (see GROUP 1.H)

Potential evapotranspiration rate ($cm \cdot d^{-1}$) calculated with the Makkink equation as E_{MAK} (reference-crop evapotranspiration) and to be multiplied by the crop factors you will choose in GROUP 3.H

I	daynr	Julian day number (January 1st = 1)
R	PREC(daynr)	precipitation ($cm \cdot d^{-1}$)
R	RADIA(daynr)	global radiation flux ($W \cdot m^{-2}$) (see GROUP 2.A)
R	TEM(daynr)	mean daily air temperature (°C)
R	RH(daynr)	mean daily air humidity (-)

SECTION 3. The file containing the crop data.

The name of this file should be specified in GROUP 1.N of file SWADAT.INP

In the labels of this section the simulation year (minus 1900) should be given instead of the question marks, e.g. for 1991 the label of GROUP 3.A becomes ">sink91:".

GROUP 3.A **use 1 line**
LABEL ">sink??:"

Limiting pressure head (matrix potential) values.

☛ if SWSINK = 0, (see GROUP 1.K and figure 1 (appendix)):
all values below must be given **except HLIM3** (give dummy)
☛ if SWSINK = 1, (see GROUP 1.K and figure 2 (appendix)):
all values below must be given **except HLIM3H and HLIM3L** (give dummy values)

R HLIM1 — pressure head value (cm) below which roots start to extract water from the soil (starting point)

R HLIM2U — pressure head value (cm) below which roots start to extract water **optimally** from the Upper soil layer

R HLIM2L — as above, but for all Lower soil layers

R HLIM3H — pressure head value (cm) below which roots cannot extract water optimally any more, for a High pot. transpiration rate equal to 0.5 $cm \cdot d^{-1}$ (limiting point)

R HLIM3L — as above, but for Low pot. transpiration rate equal to 0.1 $cm \cdot d^{-1}$

R HLIM3 — pressure head value (cm) below which the roots cannot extract water optimally any more (limiting point)

R HLIM4 — pressure head value (cm) below which no water uptake by roots is possible (wilting point)

☛ If FWSINK = 0, an **intermediate** value $HLIM3^{inter}$ is calculated between HLIM3H and HLIM3L under following 3 conditions:

- if $0.1 \leq PTRAN \leq 0.5$ then $HLIM3^{inter}$ is calculated from linear interpolation between HLIM3H and HLIM3L, according to :

$$HLIM3^{inter} = HLIM3H + \frac{(0.5 - PTRAN)}{(0.5 - 0.1)} (HLIM3L - HLIM3H)$$

- if $PTRAN < 0.1$ $cm \cdot d^{-1}$ then $HLIM3^{inter} = HLIM3L$
- if $PTRAN > 0.5$ $cm \cdot d^{-1}$ then $HLIM3^{inter} = HLIM3H$

where: PTRAN = potential transpiration rate ($cm \cdot d^{-1}$)

GROUP 3.B **use 1 + max. 37 lines (10 data-pairs/line)**
LABEL ">root??:"

Describes the rooting depth.

I NUMLIN	number of lines containing the data-pair values. (a data-pair consists of: daynr - rooting depth)

I firstd	first day of calculation (DAYSTA) (see GROUP 1.D)
R DROOTZ(firstd)	depth of root zone (cm) at firstd
	▽repeat▽
I lastd	last day of calculation (DAYEND) (see GROUP 1.D)
R DROOTZ(lastd)	depth of root zone (cm) at lastd

The data-pairs (daynr - rooting depth) may be given using intervals of one or more days.
If intervals of more than one day are used the values of DROOTZ for the intermediate days will be calculated by the program via linear interpolation.
If the value of DROOTZ is identical for two data-pairs, the rooting depth is constant for the intermediate days.
One line of data should contain at least 1 data-pair and a maximum of 10 data-pairs.

☛ **Every data-pair line must end with a slash (/)**

EXAMPLE:

```
1                                  ← no. of lines with data-pairs
120 10.  150 30.  250 30./           ← 3 data-pairs on one line
```

```
  ↑
data-pair
```

DROOTZ at daynr 120 is 10.0 cm	linear interpolation between day 120 and 150.
DROOTZ at daynr 150 is 30.0 cm	
DROOTZ at daynr 250 is 30.0 cm	linear interpolation between day 150 and 250 (in this case a constant DROOTZ of 30.0 cm)

☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

GROUP 3.C — **used only if SWTOPB = 4 (see GROUP 1.H)**
LABEL ">chwi??:" — **if SWCHFU = 0 use 1 line**
if SWCHFU = 1 use 1 + 1 lines

Describes the coefficients of the crop height-wind function FUNCCH; used to calculate the aerodynamic resistance of a crop.

$$FUNCCH = COFCHA * CH^{COFCHB} \quad \text{for } CH \geq COFCHX$$
$$FUNCCH = COFCHC * CH^{COFCHD} \quad \text{for } CH < COFCHX$$
$$FUNCCH_{MAX} = COFCHM$$

where: CH = crop height

I SWCHFU

= 0 : 6 coefficients of the FUNCCH-function don't need to be given. They are the same as in fig. 30 and given here:

COFCHA	= 0.37E-7	COFCHB	= 0.238
COFCHC	= 0.164E-7	COFCHD	= 0.59
COFCHM	= 1.3E-7	COFCHX	= 20.0

= 1 : 6 coefficients of the FUNCCH-function must be prescribed in this GROUP.

Use this line if SWCHFU = 1 :

R COFCHA
R COFCHB
R COFCHC
R COFCHD
R COFCHM
R COFCHX

coefficients of the FUNCCH-function used to estimate potential evapotranspiration flux (see eqn's. 8.3 to 8.5)

GROUP 3.D — **used only if SWTOPB = 1, 2, 3, 4 or 5 (see GROUP 1.H)**
LABEL ">lasc??:" — **use 1 line**

Describes the coefficients for the Leaf-Area-Index - Soil Cover function named: LAI(SC).

$$LAI = COFLSA * SC + COFLSB * SC^2 + COFLSC * SC^3$$

R COFLSA
R COFLSB
R COFLSC

coefficients of the leaf area index-soil cover function, for more detail see fig. 31 and equation 8.6

☛ this very important equation affects the partitioning of potential evapotranspiration into soil evaporation and plant transpiration. **The equation varies greatly for different crops.**

GROUP 3.E — **used only if SWTOPB = 1, 2, 3, 4 or 5 (see GROUP 1.H)**
LABEL ">prin??:" — **if SWPRFU = 0 use 1 line**
if SWPRFU = 1 use 1 + 1 lines

Describes coefficients for the precipitation - interception function INTC; where: SC = soil cover (-) and PREC = precip. ($cm \cdot d^{-1}$)

$$INTC = SC * COFIPA + PREC^{(COFIPB - COFIPC * (PREC - COFIPD))} \quad \text{for } \leq COFIPX$$
$$INTC = SC * COFIPE \quad \text{for } > COFIPX$$

I SWPRFU	= 0 : 6 coefficients of the INTCEP-function are the same as in fig. 32 but transformed to $cm \cdot d^{-1}$: COFIPA = 0.169; COFIPB = 0.516; COFIPC = 0.1787; COFIPD = 0.0593; COFIPE = 0.19; COFIPX = 2.0 = 1 : 6 coefficients of the INTCEP-function must be prescribed below.

Use this line if SWPRFU = 1 :

R COFIPA	coefficients of the INTCEP-function describing reduction in precipitation rate as caused by interception (see eqn's. 8.7 to 8.9)
R COFIPB	
R COFIPC	
R COFIPD	
R COFIPE	
R COFIPX	

GROUP 3.F — **used only if SWPROD = 0 (see GROUP 1.O) and**
LABEL ">soco??:" — **SWTOPB = 1, 2, 3, 4 or 5 (see GROUP 1.H)**
use 1 + max. 37 lines (10 data-pairs/line)

Describes the soil cover.

I NUMLIN	number of lines containing the data-pair values (a data-pair consists of: daynr - soil cover)

I firstd	first day of calculation (DAYSTA)
R SC(firstd)	soil cover at firstd (-)
	▽repeat▽
I lastd	last day of calculation (DAYEND)
R SC(lastd)	soil cover at lastd (-)

For explanation of the input format see GROUP 3.B
- ☛ Every data-pair line must end with a slash (/)
- ☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

GROUP 3.G **used only if SWTOPB = 4 (see GROUP 1.H)**
LABEL ">crhe??:" **use 1 + max. 37 lines (10 data-pairs/line)**

Describes the crop height.

I NUMLIN	number of lines containing the data-pair values, (a data-pair consists of: daynr - crop height)

I firstd	first day of calculation (DAYSTA)
R CROPHT(firstd)	crop height at firstd (cm)
	▽repeat▽
I lastd	last day of calculation (DAYEND)
R CROPHT(lastd)	crop height at lastd (cm)

For explanation of the input format see GROUP 3.B

- ☛ Every data-pair line must end with a slash (/)
- ☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

GROUP 3.H **used only if SWTOPB = 1, 3 or 5 (see GROUP 1.H)**
LABEL ">crfa??:" **use 1 + max. 37 lines (10 data-pairs/line)**

Describes the crop factors used.

I NUMLIN	number of lines containing the data-pair values, (a data-pair consists of: daynr - crop factor)

I firstd	first day of calculation (DAYSTA)
R CRPFAC(firstd)	crop factor (-) at firstd
	▽repeat▽
I lastd	last day of calculation (DAYEND)
R CRPFAC(lastd)	crop factor (-) at lastd

If SWTOPB = 1 (GROUP 1.H) and REFEVA = E_{OPEN} (GROUP 2.B)
use Penman crop factors.
If SWTOPB = 1 (GROUP 1.H) and REFEVA = E_{MAK} (GROUP 2.B)
use Makkink crop factors.
If SWTOPB = 3 (GROUP 1.H and 2.B): use Penman crop factors
If SWTOPB = 5 (GROUP 1.H and 2.B): use Makkink crop factors

For explanation of the input format see Group 3.B

- ☛ Every data-pair line must end with a slash (/)
- ☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see Group 1.D)

GROUP 3.I **used only if SWPROD = 1 (see GROUP 1.0)**
LABEL ">grow??:" **use 1 line**

R TCROPS	time (d) at which crop starts growing (emergence date or after)
R TCROPE	time (d) at which crop stops growing (harvest date)
R PINIT	dry matter weight of crop ($kg \cdot ha^{-1}$) at TCROPS

GROUP 3.J **used only if SWPROD = 1 (see GROUP 1.0)**
LABEL ">grfu??:" **use 1 + 1 + 1 + 1 lines**

Description of: i) SC - development stage function and ii) partitioning to tubers - development stage function. These two function are only valid for tubercrops (potatoes, beets). See [Feddes et al. (1988a)].

R FSX(1)	1st	values of DEVELOPMENT STAGE in SC(DVS) function
R FSX(2)	2nd	(values must range between 0.0 and 1.0 in
R FSX(3)	3rd	ascending order)
R FSX(4)	4th	first value must be 0.0, last value must be 1.0
R FSX(5)	5th	
R FSX(6)	6th	

R FSY(1)	1st	values of SOIL COVER in SC(DVS) function
R FSY(2)	2nd	corresponding to the FSX-values (see above)
R FSY(3)	3rd	Values must range between 0.0 and 1.0
R FSY(4)	4th	
R FSY(5)	5th	
R FSY(6)	6th	

R FTX(1)	1st	values of DEVELOPMENT STAGE in FTUBER(DVS)
R FTX(2)	2nd	function
R FTX(3)	3rd	Values must range between 0.0 and 1.0 in ascending order
R FTX(4)	4th	First value must be 0.0, last value must be 1.0
R FTX(5)	5th	
R FTX(6)	6th	

R FTY(1)	1st	values of FTUBER (fraction of production going to
R FTY(2)	2nd	tuber) in FTUBER(DVS) function corresponding to
R FTY(3)	3rd	the FTX-values (see above)
R FTY(4)	4th	Values must range between 0.0 and 1.0
R FTY(5)	5th	
R FTY(6)	6th	

☛ Intermediate SOIL COVER (FSY) and FTUBER (FTY) -values will be interpolated

GROUP 3.K **used only if SWPROD = 1 (see GROUP 1.0)**
LABEL ">grco??:" **use 1 line**

R	WUSEFF	maximum water use efficiency ($kg \cdot mbar \cdot ha^{-1} \cdot cm$)
R	CONFAC	conversion factor (sugars into starch) to account for growth respiration (-)
R	MATHFL	mathematical flexibility factor (eq'n. 5.18) We advise a value of 0.01

For more details see [Feddes et al. (1988a)]

SECTION 4. The file(s) containing the soil physical data.

The name(s) of the file(s) should be specified in GROUP 1.Q of file SWADAT.INP

In the labels of this section the number of the soil layer should be given instead of the question mark, e.g. for layer 1 the label becomes ">soihd1:".

GROUP 4.A	**use 1 line**
LABEL ">soihd?:"	
S HEADER	Description of soil type. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters.

GROUP 4.B	**use 1 line**
LABEL ">metho?:"	
	Selects which method is applied to describe the soil-physical relationships of the soil layer(s)
I SWPHYS	= 0 : the h(θ) and K(h) relation is described in **table format** = 1 : the h(θ) and K(h) relation is described as **Van Genuchten** parameters [see Van Genuchten, 1980]

GROUP 4.C	**if SWPHYS = 0 use 1 + max. 100 lines (see GROUP 4.B)**
LABEL ">soild?:"	**if SWPHYS = 1 use 1 + 1 lines**
	Use this line if SWPHYS = 0 :
R THETHI	saturated moisture content, θ_s ($cm^3 \cdot cm^{-3}$)
	Use these lines if SWPHYS = 0 :
R thet	volumetric moisture content value ($cm^3 \cdot cm^{-3}$)
R HTABLE(thet)	pressure head corresponding to moisture content thet (cm, **negative**)
R KTABLE(thet)	hydraulic conductivity corresp. to moisture content thet ($cm \cdot d^{-1}$)
	☛ **This line should be repeated starting from a low value of thet up to saturation (THETHI) with increments of 0.01.** The lowest starting value of **thet** allowed is 0.01 while the highest value of **thet** should equal THETHI. ☛ Value of pressure head (**corresponding to lowest thet**) must be between -1.0E8 and -1.0E6 for the top layer. Highest value of pressure head (**corresponding to THETHI**) = 0

Use this line if SWPHYS = 1 :

Input of soil moisture retention curve and the hydraulic conductivity as described by Van Genuchten.

R COFGEN(1)	residual moisture content, θ_r ($cm^3 \cdot cm^{-3}$)
R COFGEN(2)	saturated moisture content, θ_s ($cm^3 \cdot cm^{-3}$)
R COFGEN(3)	saturated hydraulic conductivity, K_s ($cm \cdot d^{-1}$)
R COFGEN(4)	fitting parameter α (cm^{-1})
R COFGEN(5)	fitting parameter L (-)
R COFGEN(6)	fitting parameter n (-)

SECTION 5. The file containing the data for the lower boundary.

The name of this file should be specified in GROUP 1.T of file SWADAT.INP

GROUP 5.A **use 1 line**
LABEL ">bothdr:"

S HEADER	Description of the bottom boundary conditions. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters.

GROUP 5.B **use 1 line**
LABEL ">swbotb:"

Choosing type of lower boundary conditions.

I SWBOTB	= 0 : daily groundwater tabel depth (cm) is input (see GROUP 5.C) = 1 : flux ($cm \cdot d^{-1}$) from saturated zone is input (see GROUP 5.D) = 2 : flux ($cm \cdot d^{-1}$) from deep aquifer is calculated (see GROUP 5.E) = 3 : flux ($cm \cdot d^{-1}$) from the saturated zone is calculated as a function of groundwater table depth (see GROUP 5.F) = 4 : press. head (cm) at bottom compart. is input (see GROUP 5.G) = 5 : zero flux at the bottom of the profile = 6 : free drainage at the bottom of the profile, flux ($cm \cdot d^{-1}$) equals hydraulic conductivity of bottom compartment

GROUP 5.C **used only if SWBOTB = 0 (see GROUP 5.B)**
LABEL ">daygwl:" **use 1 + max. 37 lines (10 data-pairs/line)**

Input of daily groundwater tabel depth.

I NUMLIN	number of lines containing the data-pair values, (a data-pair consists of: daynr - groundwater level)

I firstd	first day of calculation (DAYSTA)
R GW(firstd)	groundwater level (cm, negative, absolute value may be given) at the beginning of firstd
	▽repeat▽
I lastd	last day of calculation (DAYEND)
R GW(lastd)	groundwater level (cm, negative) at the beginning of lastd

For explanation of the input format see GROUP 3.B

☛ Every data-pair line must end with a slash (/)
☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

GROUP 5.D — **used only if SWBOTB = 1 (see GROUP 5.B)**
LABEL ">dayflx:" — **use 1 + max. 37 lines (10 data-pairs/line)**

Input of daily flux values from the saturated zone (positive = upwards, $cm \cdot d^{-1}$)

I NUMLIN — number of lines containing the data-pair values. (a data-pair consists of: daynr - flux)

I firstd — first day of calculation (DAYSTA)

R QBOTOM(firstd) — flux from the saturated zone (cm) at the beginning of firstd

▽repeat▽

I lastd — last day of calculation (DAYEND)

R QBOTOM(lastd) — flux from the saturated zone (cm) at the beginning of lastd

For explanation of the input format see GROUP 3.B

☛ Every data-pair line must end with a slash (/)
☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

GROUP 5.E — **used only if SWBOTB = 2 (see GROUP 5.B)**
LABEL ">semipl:" — **use 1 + 1 lines**

Describes infiltration to / seepage from the deep aquifer (the soil surface is **always** used as reference level for water table and pressure-head values).

R SHAPE — shape factor of groundwater table (reduction coefficient)
SHAPE: the shape of the groundwater table in between the drains.
Possible values are :
0.66 (parabolic) 0.64 (sinusoidal)
0.79 (elliptic) 1.00 (no drains present, see GROUP 1.U)

R RIMLAY — vertical resistance of semi-permeable layer (d)

R AQAVE — average distance between water level in piezometer (located in deep aquifer) and soil surface (negative when water level is below the soil surface) (cm)

R AQAMP — amplitude of sine function (cm)
(= maximum deviation from the average water level)

R AQTAMX — first time the water level reaches its highest position (d)

R AQPER — nr. of days between highest positions (period of sine-function) (d)

☛ If the water level of the deep aquifer remains constant at
AQAVE cm, the latter 3 variables of this line should be set to zero

GROUP 5.F **used only if SWBOTB = 3 (see GROUP 5.B)**
LABEL ">flgwfu:" **use 1 line**

Describes the flux - groundwater table relationship according to :

$$q = COFQHA * e^{(COFQHB * |\phi|)}$$

R COFQHA — value of COFQHA in above equation
R COFQHB — value of COFQHB in above equation
where:
q = basic discharge ($cm \cdot d^{-1}$)
$|\phi|$ = the groundwater level (cm, absolute value)
COFQHA and COFQHB are parameters to be determined from fig. 8 on appendix 1 or to be derived from measurements.

GROUP 5.G **used only if SWBOTB = 4 (see GROUP 5.B)**
LABEL ">dayprh:" **use 1 + max. 37 lines (10 data-pairs/line)**

Input of daily values of pressure head at bottom compartment.

I NUMLIN — number of lines containing the data-pair values,
(a data-pair consists of: daynr - pressure head)

I firstd — first day of calculation (DAYSTA)
R HGIVEN(firstd) — pressure head at bottom compartment (cm) at the beginning of firstd
▽repeat▽
I lastd — last day of calculation (DAYEND)
R HGIVEN(lastd) — pressure head at bottom compartment (cm) at the beginning of lastd

For explanation of the input format see GROUP 3.B

- Every data-pair line must end with a slash (/)
- firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)

SECTION 6. The file containing the data for drainage/subirrigation.

This section can be skipped if SWDRAI = 0 (see GROUP 1.U)
The name of this file should be specified in GROUP 1.U of file SWADAT.INP

WARNING: *Please note that although the model offers the option to choose more than one (1) drainage level, the manner in which drainage is currently described needs to be verified and further tested.*
We strongly advise you to use 1 drainage level only.

GROUP 6.A **use 1 line**
LABEL ">lathdr:"

S HEADER	Description of the lateral boundary conditions. Will be printed in the output file (see GROUP 1.B) Use max. 40 characters.

GROUP 6.B **use 1 + 1 + 1 lines**
LABEL ">dgener:"

I NRLEVS	number of drainage levels to be considered. ☛ the maximum of NRLEVS is 4; 1st order : channel 2nd order : ditch 3rd order : drain/trench 4th order : drain/trench
R BASEGW(1)	depth of semi-impermeable layer (m) (negative) ☛ This layer is located **below** the defined profile (base of the aquifer)

R COFANI(1)	an-isotropic factor for 1st soil layer; horizontal saturated conductivity divided by vertical saturated conductivity; k_h/k_v ▽repeat▽ for each soil layer
R COFANI(NUMLAY)	an-isotropic factor for the deepest soil layer (NUMLAY) (GROUP 1.P) Common values for this factor are between 3 and 10 If COFANI is unknown use a value of 1. (layer is isotropic)

GROUP 6.C **use NRLEVS lines**
LABEL ">drchar:"

Specifies parameters for the drainage calculation.

Repeat this GROUP for all drainage levels 1-NRLEVS.

I level — drainage level

R L(level) — spacing between drainage mediums (channel/ditch/trench) (m)

R ZBOTDR(level) — depth of bottom of drainage medium (cm) (negative)

R WETPER(level) — wet perimeter of the drainage medium (cm)
The wet perimeter u should be calculated according to:

$u = b + 2y\sqrt{s^2+1}$ *for ditch*
$u = b + 2R_o$ *for pipe drain*

where: b = bottom width of drainage medium or width of drain trench (cm)
y = average water depth in channel (cm)
s = side slope of channel; $\Delta h/\Delta v$ (-)
R_o = outer radius of the pipe drain (cm)

☛ If the water depth in the channel = 0 use u = b.

I SWDTYP(level)
= 0 : drainage medium is either channel/ditch/trench
= 1 : drainage medium is pipe drain only

I SWALLO(level)
= 0 : drainage and infiltration both allowed
= 1 : drainage not allowed
= 2 : infiltration not allowed

GROUP 6.D	**If SWWLEV(level) = 0 use 2 + max. 37 lines (assume 10 values/line)**
LABEL ">level?:"	**If SWWLEV(level) = 1 use 1 line**
	Open water level in the drainage mediums (channel/ditch/trench); open water level is taken at ZBOTDR(level)
	☛ **Repeat this GROUP for all drainage levels 1-NRLEVS except if SWDTYP(level) = 1 (GROUP 6.C); then skip this GROUP**
I SWWLEV(level)	= 0 : open water level in channel/ditch/trench is input = 1 : open water level in channel/ditch/trench calculated as sinusoidal function
	Use this line if SWWLEV(level) = 0 :
I NUMLIN	number of lines containing the data-pair values, (a data-pair consists of: daynr - open water level)
	Use these lines if SWWLEV(level) = 0 :
I firstd	first day of calculation (DAYSTA)
R DRAIN(firstd,level)	open water level on 1st day of input (cm) (below the top of the soil profile)
	▽repeat▽
I lastd	last day of calculation (DAYEND)
R DRAIN(lastd,level)	open water level on last day of input (cm)
	For explanation of the input format see GROUP 3.B
	☛ Every data-pair line must end with a slash (/) ☛ water levels may be given as absolute value ☛ firstd ≤ DAYSTA and lastd ≥ DAYEND (see GROUP 1.D)
	Use this line if SWWLEV(level) = 1 :
R AVELEV(level)	average water level in the channel/ditch/trench (cm) (negative)
R DRNAMP(level)	amplitude of sine function (cm) (= maximum deviation from the average level)
R TAMMAX(level)	1st time water level in drainage medium reaches highest position (d)
R PERIOD(level)	nr. of days between highest positions (period of sine-function) (d)

References

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Van Genuchten, M.Th. and D.R. Nielsen, 1985. *On describing and predicting the hydraulic properties of unsaturated soils.* Annales Geophysicae 3(5): 615-628.

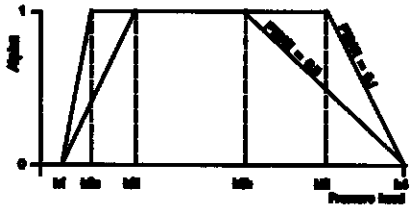

Figure 1. SWSINK=0

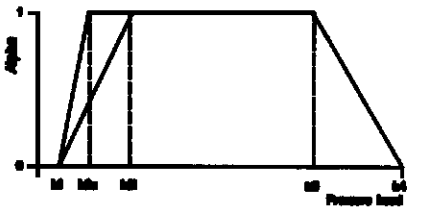

Figure 2. SWSINK=1

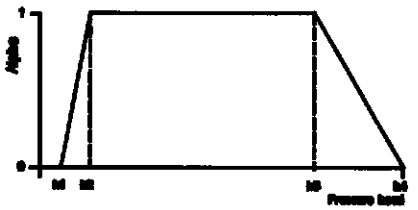

Figure 3. SWHYPR=0

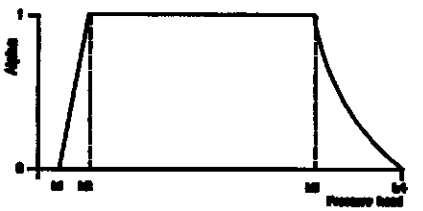

Figure 4. SWHYPR=1

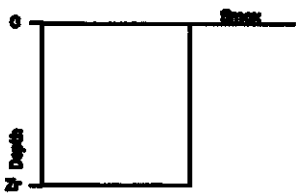

Figure 5. SWUPFU=0

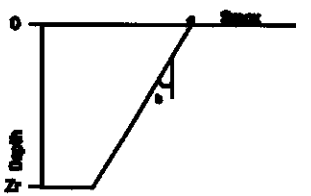

Figure 6. SWUPFU=1

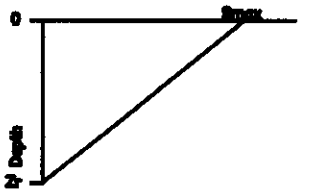

Figure 7. SWUPFU=2

Figure 1, 2, 3, 4, 5, 6 and 7

Appendix 2.2. Alphabetical list of labels and corresponding groups.

label	group	label	group
>bbdfil:	1.T	>radi??:	2.A
>bothdr:	5.A	>redeva:	1.E
>chwi??:	3.C	>rootac:	1.L
>crhe??:	3.G	>root??:	3.B
>crfa??:	3.H	>semipl:	5.E
>crpfil:	1.N	>sink??:	3.A
>crphdr:	1.J	>sinkva:	1.K
>crppro:	1.O	>soco??:	3.F
>dayflx:	5.D	>soild?:	4.C
>daygwl:	5.C	>soilfl:	1.Q
>dayprh:	5.G	>solhd?:	4.A
>dgener:	6.B	>solute:	1.V
>drains:	1.U	>swbotb:	5.B
>drchar:	6.C	>timeva:	1.D
>excons:	1.M	>topbnd:	1.H
>exfile:	1.C		
>flgwfu:	5.F		
>genhdr:	1.A		
>grco??:	3.K		
>grow??:	3.I		
>grfu??:	3.J		
>incond:	1.S		
>irriva:	1.F		
>lasc??:	3.D		
>lathdr:	6.A		
>level?:	6.D		
>metd??:	2.B		
>metfil:	1.I		
>methdr:	1.G		
>metho?:	4.B		
>output:	1.B		
>pondmx:	1.R		
>prin??:	3.E		
>profil:	1.P		

Appendix 2.3. List of variables

variable	description	type	units
A			
ALPHA	empirical constant of Priestly-Taylor equation	R	-
AQAMP	amplitude of piezometric level in deep aquifer	R	cm
AQAVE	average piezometric level in deep aquifer	R	-
AQOMEG	periodic frequency of level in deep aquifer	R	$rad \cdot d^{-1}$
AQPER	period of sinusoidal piezometric level in aquifer	R	d
AQTAMX	first day piezometric level in aquifer at a maximum	R	d
ATMPOT	potential evapotranspiration (atmospheric demand)	R	$cm \cdot d^{-1}$
AVELEV[5]	average water level of each drainage system	R	cm
B			
BASEGW[2]	depth of base of (perched) water table	R	cm
BELL	ASCII character 7	S	-
BOTCOM[5]	bottom compartment of each layer	I	-
C			
CEPND	cumulative evaporation of ponding layer	R	cm
CEVAP	cumulative actual soil evaporation	R	cm
CINTC	cumulative actual interception by leaves	R	cm
COBPPL	compartment at bottom of poorly permeable layer	I	-
COFANI[5]	an-isotropic factor for each soil layer	R	-
COFCHA	coeff. a of crop-height function 'FUNCCH'	R	-
COFCHB	coeff. b of crop-height function 'FUNCCH'	R	-
COFCHC	coeff. c of crop-height function 'FUNCCH'	R	-
COFCHD	coeff. d of crop-height function 'FUNCCH'	R	-
COFCHM	maximum value of 'FUNCCH'	R	-
COFCHX	breakpoint of 'FUNCCH'	R	-
COFGEN[7,5]	i^{th} coeff. (i=1-7) of Van Genuchten for layer j (j=1-5)	R	-
COFIPA	coeff. a of INTCEP('PREC') function	R	-
COFIPB	coeff. b of INTCEP('PREC') function	R	-
COFIPC	coeff. c of INTCEP('PREC') function	R	-
COFIPD	coeff. d of INTCEP('PREC') function	R	-
COFIPE	coeff. e of INTCEP('PREC') function	R	-
COFIPX	breakpoint of INTCEP('PREC') function	R	-
COFLSA	coeff. a of 'LAI'('SC') function	R	-

COFLSB	coeff. b of 'LAI'('SC') function	R	-
COFLSC	coeff. c of 'LAI'('SC') function	R	-
COFNGA	coeff. a for transformation of radiation	R	-
COFNGB	coeff. b for transformation of radiation	R	-
COFPCA	coeff. a of gross photosyn. function on a clear day	R	-
COFPCB	coeff. b of gross photosyn. function on a clear day	R	-
COFPCC	coeff. c of gross photosyn. function on a clear day	R	-
COFPOA	coeff. a of gross photosyn. function on overcast day	R	-
COFPOB	coeff. b of gross photosyn. function on overcast day	R	-
COFPOC	coeff. c of gross photosyn. function on overcast day	R	-
COFQHA	coeff. a of q(h)-relation	R	$cm \cdot d^{-1}$
COFQHB	coeff. b of q(h)-relation	R	-
COFRCA	coeff. a of solar radiation flux for photosynthesis	R	-
COFRCB	coeff. b of solar radiation flux for photosynthesis	R	-
COFRCC	coeff. c of solar radiation flux for photosynthesis	R	-
COFRED	coeff. α or β in reduction of soil evaporation	R	$cm \cdot d^{-1}$
COFSZA	coeff. a of S(z)-relation (Hoogland)	R	$cm \cdot d^{-1}$
COFSZB	coeff. b of S(z)-relation (Hoogland)	R	d-1
CONFAC	conversion factor (sugars into starch)	R	-
COTPPL	compartment at top of poorly permeable layer	I	-
CPEVA	cumulative potential soil evaporation	R	cm
CPREC	cumulative precipitation	R	cm
CPTRA	cumulative potential transpiration	R	cm
CQBOT	cumulative flux through bottom of profile	R	cm
CQDRA	cumulative total drainage flux	R	cm
CQROT	cumulative root water uptake	R	cm
CQTOP	cumulative flux through top of profile	R	cm
CROPHT[366]	crop height for each day	R	cm
CRPFAC[366]	crop factor for each day	R	-
CRUNO	cumulative surface runoff	R	cm
D			
DAYIRL	day at which last irrigation took place	R	d
DAYNR	day on which calculations are performed	R	d
DAYSTA	first day of calculation	I	d
DAYEND	last day of calculation	I	d
DEEPGW	calculated water level in deep aquifer	R	cm
DEGCLD	degree of cloudiness (Penman)	R	-
DMCC[5,99]	C-values of C(h) table (max. 5 layers)	R	cm^{-1}

DMCH[5,99]	'H '-values of C(h) table (max. 5 layers)	R	cm
DIMOCA[40]	differential moisture capacity at node	R	cm^{-1}
DISNOD[41]	distance between two nodes	R	cm
DOMEGA[5]	radial frequency of each drainage level	R	$rad \cdot d^{-1}$
DPTRA	incrementing daily potential transpiration	R	cm
DQROT	incrementing daily root extraction	R	cm
DRAIN[366,5]	daily water level in each drainage system	R	cm
DRNAMP[5]	amplitude of each drainage level	R	cm
DROOTZ[366]	depth of root zone for each day	R	cm
DRZ	depth of root zone	R	cm
DSOILP	depth of soil profile	R	cm
DT	time step	R	d
DTM1	previous time step	R	d
DTMAX	maximum allowed time step	R	d
DVS	development stage	R	-
DZ[40]	compartment size	R	cm
E			
EWET	maximum possible evaporation of a cropped surface (Monteith-Rijtema)	R	$cm \cdot d^{-1}$
EWETHI	'EWET' at upper limit of 'RS'	R	$cm \cdot d^{-1}$
EWETLO	'EWET' at lower limit of 'RS'	R	$cm \cdot d^{-1}$
F			
FACLAI	reduction coefficient for 'LAI'	R	-
FLENDD	indicates if time is at end-of-day	L	-
FLEQUA	indicates if input data on first and last day of calculation are of equal value	L	-
FLGENU[5]	indicates if soil characteristics are according to van Genuchten or via table input	L	-
FLGIFT[366]	indicates whether irrigation gift is applied	L	-
FLGROW	indicates if crop growth should be simulated	L	-
FLIOUT	indicates if intermediate output should be given	L	-
FLLAST	indicates last time step of day	L	-
FLOUTP[10]	indicates type of output	L	-
FLPPLA	indicates presence of poorly permeable layer	L	-
FLREAD	indicates if meteo. data are to be read	L	-
FLREDY	indicates if end of calculations is reached	L	-
FSX[6]	development stage in SC(DVS) relationship	R	-
FSY[6]	soil cover in SC(DVS) relationship	R	-

FTX[6]	development stage in FTUBER(DVS) relationship	R	-
FTY[6]	tuber partitioning in FTUBER(DVS) relationship	R	-
FUNCCH	function of crop-height	R	-
G			
GAMMA	time fraction that sky is overcast	R	-
GW[366]	given groundwater tabel depth for each day	R	cm
GWL[2]	water level (groundwater and perched water)	R	cm
H			
H[40]	pressure head at nodal point	R	cm
HATM	min. allowed 'H ' at soil surface for present time step	R	cm
HATMD	min. allowed 'H ' at soil surface obtained or calculated from meteorological data	R	cm
HCRIT	critical 'H ' below which irrigation is required	R	cm
HGIVEN[366]	given 'H ' at bottom node for each day	R	cm
HLIM1	'H' below which roots start to extract water (O_2 deficie.)	R	cm
HLIM2U	'H' below which root extraction is optimal for upper soil layer	R	cm
HLIM2L	'H ' below which root extraction is optimal for lower layers	R	cm
HLIM3	'H ' below which water can not be optimally extracted (reduction point)	R	cm
HLIM3H	'H ' below which water can not be optimally extracted at a high evaporative demand	R	cm
HLIM3L	'H ' below which water can not be optimally extracted at a low evaporative demand	R	cm
HLIM4	'H ' below which roots can not extract water (wilting point)	R	cm
HM1[40]	'H ' at previous time step	R	cm
HM2[40]	'H ' at second last time step	R	cm
HTABLE[5,99]	table containing 'H ' - values	R	cm
I			
IEPND	intermediate cumulative ponding evaporation	R	cm
IEVAP	intermediate cumulative soil evaporation	R	cm
IINTC	intermediate cumulative interception	R	cm
INQ[41]	intermediate cumulative flux between compartments	R	cm
INQDRA[4,40]	intermediate cumulative drainage per level per node	R	cm
INQROT[40]	intermediate cumulative root extr. volume per node	R	cm
INTC	interception flux	R	$cm \cdot d^{-1}$
IPEVA	intermediate cumulative potential evaporation	R	cm

IPREC	intermediate cumulative precipitation	R	cm
IPTRA	intermediate cumulative potential transpiration	R	cm
IQDRA	intermediate cumulative drainage flux	R	cm
IQROT	intermediate cumulative root extraction	R	cm
IRRAMT	depth of each irrigation application	R	cm
IRUNO	intermediate cumulative runoff	R	cm
K			
K[41]	hydraulic conductivity at nodal point	R	$cm \cdot d^{-1}$
KGEOM[41]	hydraulic conduc. between two nodes (geometric mean)	R	$cm \cdot d^{-1}$
KSURF	'K ' between top node and soil surface	R	$cm \cdot d^{-1}$
KTABLE[5,99]	table containing 'K '- values	R	$cm \cdot d^{-1}$
L			
L	distance between two channels	R	m
LAI	leaf area index	R	$m^2 \cdot m^{-2}$
LASTD	last day of calculations	I	d
LAYER[40]	soil layer in which node is situated	I	-
LDWET	last day it rained and/or irrigation took place	I	d
LUNBAL	logical unit number for water balance output	I	-
LUNCON	logical unit number for screen output	I	-
LUNCRP	logical unit number for crop production output	I	-
LUNERR	logical unit number for error messages	I	-
LUNEXA	logical unit number for supplementary output	I	-
LUNEXB	logical unit number for supplementary output	I	-
LUNIN	logical unit number for input	I	-
M			
MAINTA	maintenance respiration for actual production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
MAINTP	maintenance respiration for potential production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
MATHFL	mathematical flexibility factor	R	-
MAXITR	maximum allowed number of iterations	I	-
MAXTIT	maximum allowed number of decrements of 'DT' in iteration procedure	I	-
N			
NCRIT	critical node where 'HCRIT' is checked	I	-
NDYEAR	number of days in year	I	d
NODDRZ	bottom node of root zone	I	-
NRLEVS	number of drainage levels	I	-
NUMLAY	number of soil layers	I	-
NUMNOD	number of nodes	I	-

O			
OUTIVL	interval between intermediate outputs	I	d
P			
PARAM	decision parameter for subroutine INTERPOL	I	-
PASYMA	actual asymptotic daily production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PASYMP	potential asymptotic daily production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PC	gross photosyn. rate of standard canopy on clear day	R	$kg \cdot ha^{-1} \cdot d-1$
PDA	daily actual production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PDAPRT	daily actual production of productive parts	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PDP	daily potential production	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PDPPRT	daily potential production of productive parts	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PEVA	potential evaporation flux	R	$cm \cdot d^{-1}$
PI	pi	R	-
PINIT	initial dry matter weight of crop	R	$kg \cdot ha^{-1}$
PO	gross photosyn. rate of standard canopy on overcast day	R	$kg \cdot ha^{-1} \cdot d^{-1}$
POND	thickness of ponding water layer	R	cm
PONDMX	maximum allowed 'POND'	R	cm
PREC	precipitation	R	cm
PRECIS	calculation precision factor	R	-
PST	gross photosynthesis of standard canopy	R	$kg \cdot ha^{-1} \cdot d^{-1}$
PTA	total actual production	R	$kg \cdot ha^{-1}$
PTAPRT	total actual production of productive parts	R	$kg \cdot ha^{-1}$
PTP	total potential production	R	$kg \cdot ha^{-1}$
PTPPRT	total potential production of productive parts	R	$kg \cdot ha^{-1}$
PTRA	potential daily transpiration	R	$cm \cdot d^{-1}$
Q			
QBOT	flux through bottom of soil profile	R	$cm \cdot d^{-1}$
QBOTOM[366]	given flux through bottom of profile	R	$cm \cdot d^{-1}$
QDRA[4,40]	flux per node to/from each drainage system	R	$cm \cdot d^{-1}$
QROT[40]	root extraction flux per node	R	$cm \cdot d^{-1}$
QTOP	flux through top of soil profile (demand)	R	$cm \cdot d^{-1}$
R			
RA	aerodynamic diffusion resistance	R	$s \cdot m^{-1}$
RC	part of solar radiation flux involved in photosynthesis	R	$W \cdot m^{-2}$
REVA	reduced potential soil evaporation	R	$cm \cdot d^{-1}$
RGLOB	global radiation	R	$W \cdot m^{-2}$
RH	mean daily relative humidity	R	-
RIMLAY	vertical resistance of poorly permeable layer	R	d

RNET	net radiation	R	$W \cdot m^{-2}$
ROOTMAX	maximum rooting depth	R	cm
RS	internal canopy resistance	R	$s \cdot m^{-1}$
RSMAX	maximum internal canopy resistance	R	$s \cdot m^{-1}$
RSMIN	minimum internal canopy resistance	R	$s \cdot m^{-1}$
S			
SATVAP	saturation vapour pressure	R	mbar
SHAPE	shape factor of the groundwater table	R	-
SC[366]	soil cover for each day	R	-
SINFAC	proportionality factor for sink term	R	-
SLOPE	slope of 'SATVAP' - curve	R	$mbar \cdot K^{-1}$
SWALLO[4]	switch for allowance of drainage/infiltration	I	-
SWBOTB	switch for bottom boundary conditions	I	-
SWCHFU	switch selecting 'FUNCCH'-variables	I	-
SWDCAS[4]	switch indicating which drainage formula to use	I	-
SWDRAI	switch indicating drainage should be simulated	I	-
SWDTYP[4]	switch for type of drainage medium	I	-
SWEROR	switch to direct error messages	I	-
SWFILE1	switch for extra output file with supplementary data	I	-
SWFILE2	switch for extra output file with solute data	I	-
SWGRAD	switch for type of given radiation	I	-
SWHYPR	switch for linear/hyperbolic shape of sink term between 'HLIM3' and 'HLIM4'	I	-
SWINCO	switch indicating type of initial conditions	I	-
SWIRRI	switch for irrigation option	I	-
SWOUTP[6]	switch selecting of data written to extra file	I	-
SWPHYS	switch describing soil-physical relation	I	-
SWPRFU	switch for reading of INTCEP - variables	I	-
SWPROD	switch for production option	I	-
SWREDU	switch for reduction of soil evaporation	I	-
SWSALT	switch for solute transport		
SWSINK	switch of sink term (Feddes, Hoogland or Prasad)	I	-
SWSTAG	switch for showing the computing stage	I	-
SWTBVA	switch for varying bottom boundary conditions	I	-
SWTOPB	switch for the top boundary conditions	I	-
SWUPFU	switch for root water uptake function	I	-
SWWLEV[5]	switch specifying 'DRAIN'	I	-

T			
T	time of calculation	R	d
TAMMAX[4]	day of highest water level in drain	R	-
TCROP	time at which crop starts growing (emergence date)	R	d
TEM	mean daily air temperature	R	°C
THETA[40]	volumetric soil moisture content of each compartment	R	$cm^3 \cdot cm^{-3}$
THETHI[5]	position highest 'THETA' in array for each layer	I	-
THETLO[5]	position lowest 'THETA' in array for each layer	I	-
THETM1[40]	'THETA' of previous time-step	R	$cm^3 \cdot cm^{-3}$
THETSL[5]	saturated 'THETA' of each soil layer	R	$cm^3 \cdot cm^{-3}$
THETSN[40]	saturated 'THETA' of each compartment	R	$cm^3 \cdot cm^{-3}$
TLAGIR	minimum time-lag between 2 irrigation gifts	R	d
TM1	previous time of calculation	R	d
TRONAB	time at which roots become inactive at depth 'ZRONA'	R	d
TRONAE	time at which maximum depth of inactivity is reached	R	d
TVPD	ratio between TRAN and 'SATDEF'	R	-
U			
U	mean daily wind speed at 2 m height	R	$m \cdot s^{-1}$
V			
VOLACT	total volume of water in the profile	R	cm
VOLBD	volume of water at beginning of day	R	cm
VOLINI	initial volume of water in the profile	R	cm
VOLM1	volume of water at previous time step	R	cm
VPD	vapour pressure deficit	R	
W			
WUSEFF	water use efficiency	R	$kg \cdot mbar \cdot ha^{-1} \cdot cm$
Y			
YEARST	first year of calculation	I	-
YEAREN	last year of calculation	I	-
Z			
Z[40]	position of nodal point	R	cm
ZBOTDR[4]	depth of bottom of drainage medium	R	cm
ZRONA	depth above which roots are non-active	R	cm
ZRONAM	maximum allowed value of 'ZRONA'	R	cm

Appendix 3 Description of required format for input file for TRANSOL

(From Kroes, 1991)

F I L E - D E S C R I P T I O N

Filename: GENERAL.INP

Contents: input-data for TRANSOL with parameters concerning general simulation- and output-options

number of pages: 2 page-nr: 1

Mnemonic	Description	Unit	F
>hydmod:	..... kind of waterquality model		
IWA	kind of waterquantity model has been used (1 = WATBAL, 2 = SWATRE)		I
>simper:	..... simulation period		
NUYR	number of calendar-years to simulate	-	I
>sophys:	..... soil physical parameters		
APTE	amplitude of yearly sinus temperature wave	°C	R
AVTE	average yearly temperature at soil surface	°C	R
FQTE	frequency of yearly temperature wave	rad.d-1	R
TESMCF	thermal diffusivity	m2.d-1	R
PHSH	phase shift	rad	R
* RHBS(1-NUHO)	dry bulk density for each horizon (RHBS should have dummy values if sorption is not simulated)	kg.m-3	R
>sochem:	..... soil chemical parameters		
ORFR(1-NUHO)	organic matter fraction for each horizon (ORFR should have dummy values if sorption is not simulated)	kg.kg-1	R
>rdepth:	..... decomposition-reduction (depth, saturation)		
RDFADPH1	1st bend point for depth-related reduction	m-ss	R
RDFADPH2	2nd bend point for depth-related reduction	m-ss	R
RDFADPMI	minimum for depth-related reduction	m-ss	R
OPTRDSA	option for input of reduct. in sat. layers	-	I
RDFASA	reduction factor for decomposition in saturated layers (operational if OPTRDSA=1)		R
>rvdose:	..... reservoir for additions		
HE(0)	reservoir content for additions	m	R
>sorpti:	..... sorption-parameters		
OPTCX	option for linear/nonlinear sorption 1=no sorption, 2=linear sorption, 3=Freundlich sorption	-	I
SORAME(1)	average sorption rate	m3.kg-1	R
COSORA	concentr. at which SORA has been measured	kg.m-3	R
FHEXPME(1)	Freundlich exponent	-	R

Filename: GENERAL.INP

Nr of pages: 2 page-nr: 2

Mnemonic	Description	Unit	F
>transf:	..... solute-parameters; sorption and decomp.-rate		
OPTRECF	option for input of decomposition-rate	-	I
	1=no decomposition, 2=input as rate, 3=input as halflifetime		
OPTREKI(1-3)	options for input of kind of decomposition	-	I
	1 = on, OPTREKI(1) and OPTREKI(3) can not both be on		
* REKISOAVME(1)	aver. decomp.rate for amount in solution	d or d-1	R
REKICXAVME(1)	aver. decomp. rate for amount at complex	d or d-1	R
MOFRREKI	moisture fraction corresponding to REKISOAV	m3.m-3	R
(dummy values must be given if no decomposition is to be simulated)			
>metabo:	..... metabolite-parameters; sorption,decomposit.		
NME	number of simulated metabolites	-	I
For each metabolite I the following 4 values must be given:			
* SORAME(I)	average sorption rate	m3.kg-1	R
FHEXPME(I)	Freundlich exponent	-	R
REKISOAVME(I)	average decomp. rate for amount in sol.	d or d-1	R
REKICXAVME(I)	average decomp. rate for amount at compl.	d or d-1	R
>uptake:	..... crop uptake		
RDFAUPNH	reduction factor for uptake by plants	-	R
>boucon:	..... boundary conditions		
COPRNHIN	solute concentration in precipitation	kg.m-3	R
* COIDNH	solute conc. in infiltr.drainwater	kg.m-3	R
* COAQNH	solute conc. below vert.profile	kg.m-3	R
>inicon:	..... initial conditions		
CONH(1-NL)	solute concentration in layers 1-NL	kg.m-3	R
>outopt:	..... output options		
OUTSC	output of simulation-stage to screen (1=output)	-	I
* OUTSE(1-5)	selection of timestep-output (1 = output)	filename	I
	OUTSE(1) = solute conc. per layer,tstep	SOL-CONC.OUT	
	OUTSE(2) = solute amount per layer,tstep	SOL-AMOU.OUT	
	OUTSE(3) = adsorbed amount per layer,tstep	ADSORB.OUT	
	OUTSE(4) = conc. and tot.amount of metab.1	META-1.OUT	
	OUTSE(5) = conc. and tot.amount of metab.2	META-2.OUT	
* OUTBA(1-5)	output of balance-type (1 = output)	filename	I
	OUTBA(1) = water balance per tstep	BAWAST.OUT	
	OUTBA(2) = solute balance per tstep	BASOST.OUT	
	OUTBA(3) = water balance per year	BAWAYR.OUT	
	OUTBA(4) = solute balance per year	BASOYR.OUT	
	OUTBA(5) = water and solute balance per year	YRBAL.OUT	
the following 3 variabels arrange output to the files created with OUTBA(1-5)			
* BALNMI	first layer of massbalance (0=reservoir)	-	I
BALNMA	last layer of massbalance (0=reservoir)	-	I
TIBA	timestep for updating of year-balances	d	R
* OUTCDS	output to SCDATA.OUT file (1 = output)	-	I

I = data type INTEGER

* = new record

R = data type REAL

date: 9-10-1991

F I L E - D E S C R I P T I O N

Filename: ADDIT.INP

Contents: input-data for TRANSOL with parameters concerning additions to the soil

number of pages: 1 page-nr: 1

Mnemonic	Description	Unit	
>add001:	..... 1st addition		
TINEAD	time of first addition	d	R
*QUMT	amount of material added	kg.ha-1	R
WYAD	way of addition (=nr of layers over which additions are distributed) if WYAD=0 the addition goes into the surface reservoir	-	I
PL	number of layers to be ploughed (must be 0, ploughing is not yet possible !!)	-	I
*TINEAD	time of next addition	d	R
>add002:	..... 2nd addition		
*QUMT	amount of material added	kg.ha-1	R
WYAD	way of addition (=nr of layers over which additions are distributed) if WYAD=0 the addition goes into the surface reservoir	-	I
PL	number of layers to be ploughed (must be 0, ploughing is not yet possible !!)	-	I
*TINEAD	time of next addition	d	R
>addxxx:	..... xxx addition		
QUMT,WYAD,PL,TINEAD	next addition, etc.		

* = new record

I = data type INTEGER
R = data type REAL

date: 9-10-1991