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Illustration of the present Capabilities of the ECCES Program System

Brian Christensen, Peer Bo Mortensen and Torben Petersen

Risø National Laboratory, DK-4000 Roskilde, Denmark
April 1985

Risø-M-2501

ILLUSTRATION OF THE PRESENT CAPABILITIES OF THE ECCES PROGRAM SYSTEM

Brian Christensen, Peer Bo Mortensen and Torben Petersen

Abstract. This report describes the status of the development of the ECCES program system. The capabilities of the model are described together with the results of a scenario calculation. Furthermore a series of calculations are shown in order to demonstrate some phenomena concerning the soil chemistry and plant models.

EDB descriptors: ACID RAIN; AGRICULTURE; CADMIUM; COMPUTERIZED SIMULATION; CROPS: DISPERSIONS; E CODES; ENERGY SYSTEMS; ENVIRONMENTAL IMPACTS; ION EXCHANGE; PH VALUE; POINT POLLUTANT SOURCES; POWER PLANTS; SOIL CHEMISTRY; SOILS; SULFATES; SULFUR DIOXIDE; UPTAKE.

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April 1985
Risø National Laboratory, DK-4000 Roskilde, Denmark

The project is carried out at Risø National Laboratory, Department of Energy Technology.

The work is followed by a group of experts from government institutions and electric utilities:

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Danish summary. Denne rapport beskriver status for udvikling af programsystemet ECCES. Mulighederne i programmet er beskrevet sammen med et eksempel på en stor scenarieberegning. Beregninger, der illustrerer jordkemimodellens og plantemodellens mekanismer, er ligeledes udført.

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1. INTRODUCTION

This report shows some examples of calculations with the ECCES program system. The report should be considered an extension to the status report (Petersen 1984) which summarized the state of development of the ECCES system. The ECCES system is designed to predict environmental impacts from a given energy production scenario in a given geographical area for a period of time.

Presently the ECCES system contains submodels for atmospheric dispersion and deposition of pollutants, soil chemistry and uptake in selected crops. These are linked together in a main program which contains a description of the geographical area in question and positions of sources and which can handle data transfer between the submodels.

The report falls in two main sections. In the first section the result of a scenario calculation is shown. In this calculation all the submodels are brought into play.

In the second section a series of calculations is shown in order to demonstrate some phenomena concerning the soil chemistry model and the interaction with the plant model.

The intention of the calculations shown in the second section is to demonstrate some phenomena the soil chemistry and plant models may be used to study. It is also the intention to show the sensitivity of the results to some of the key parameters of the models. It is of course vital to the quality of the results that the parameters for the models can be determined with sufficient accuracy. At this stage it is not yet possible to get an assessment of the accuracy of the models, however, the study of sensitivity may be considered a first step.

The dispersion and deposition model is based on a traditional plume model and is therefore considered "proven technology".

Because of this, sensitivity studies at this stage are concentrated on the soil chemistry and plant models. Testing of the dispersion and deposition model has taken place against other well established programs also based on the plume model. Parameters (deposition velocity etc.) will, of course, influence results of scenario calculations, and calculations to demonstrate this may be performed later in the project.

The main body of the data for all the calculations is chosen as realistic as possible. But since the calculations are meant to show results of variation in parameters, the results are not intended to represent situations which can be encountered in nature.

2. DESCRIPTION OF THE CAPABILITIES OF THE ENVIRONMENTAL MODEL

The model for calculation of environmental consequeces of energy production has been implemented in a FORTRAN-77 program on the B7800 computer at Risø National Laboratory. The program consists of about 12800 lines of code, where a little more than half are real FORTRAN-statements, and the rest are comments. The program is run as a batch program with input from an input file. There is a number of input checks incorporated in the program and it has been attempted to give useful error reactions.

Output from the program are partly printer output, partly some data-files from which it is possible to transfer the results to an independent plot program. This plot program is run interactively on a graphic screen, but it will not be further described here.

The FORTRAN-77 program is stored on a file with the generic name ECCES (Environmental Calculation of Consequences from Energy Systems) followed by a version number. At present the latest version is ECCES version 2.2.

ECCES is divided into two parts: the dispersion part and the soil chemistry part - with or without crops - which are nearly independent. The two parts can be used in common or separately.

2.1. The dispersion model

The dispersion model is able to calculate dispersion of pollutants from a number of sources to a number of recipients. The sources are the point sources: power plants and the area sources: cities and counties (Danish: amt). The actual sources can be selected in a library of plants, cities and areas. The sources are characterised by their coordinates in a cartesian coordinate system and by the source strength (kg/sec) for each pollutant at maximum energy production for each source. For power plants moreover the chimney height is given.

Pollutants which are studied in a scenario, are also chosen by the input. The data for the pollutants: mole weight, valency, decay constants, deposition velocity, etc., are fetched from a pollutant library.

The dynamics in the model are introduced by a loadfactor (0 - 1) for each source. The load factors are given as input, but at present the time step length in the dispersion model is half a year, so only seasonal variation and long term changes in the power production scheme can be modelled.

The recipients of the pollution are the areas, the data of which are also selected from a library of areas. Deposition of pollutants of an area is calculated as if deposition takes place at the position of the "center of mass" for the area. Later in this report a scenario with 7 power plants at Zealand as sources and Roskilde Amt as recipient is set up.

"Above" the source- and recipient-defining data is a datafile describing the weather through out the scenario. This datafile contains data describing wind, etc. For further details see the report by Højerup (1984).

Output from the dispersion model is airconcentration (µg/m^3) and deposition (g/m^2/year) of the pollutants. If the pollutants undergo a chemical transformation in the air under the transport, the concentration and deposition are calculated for both the parent and the daughter product. An example of output from the dispersion model is shown in App. A, Fig. 1a.

2.2. The soil chemistry model

The soil chemistry model starts where the dispersion model ends, namely with the deposition as input to the model. The soil chemistry model can be used in conjunction with the dispersion model or alone. If it is used alone it is possible to select one or more soil types from a soil type library. The soil type library contains data such as the number of layers, the water capacity for each layer, the ion exchange capacity for each layer, etc. Today 7 different typical Danish soil types have been defined.

The soil chemistry model alone calculates chemical equilibrium in each soil layer as described by Brodersen (1984). Pollutants are added to the upper layer either by dry deposition or contained in rain. The water containing the different ions percolates through the soil layers (Maximum 5), and through this the gradual change of chemical equilibrium is modelled.

If the soil chemistry is used together with the dispersion model it is not possible to specify the soil types. Instead the actual geographical recipient areas in the scenario are simulated and typically these have areas with all soil types. The area library contains information about the area of each soil type (km^2) for the geographical areas. The model calculates the chemical equilibrium for all soil types in the recipient area with supply to the upper layer of rain plus the calculated deposition from the dispersion calculation.

2.3. The crop model

The crop model is the third and last module in the simulation complex and this module demand at least that the soil chemistry model also is used. It is possible to simulate uptake of ions in different crops and again the actual crop data are selected through the input from a crop library. This library contains information about crops, such as biomass, water uptake, etc. for each month in the year.

The crop model is closely connected to the soil chemistry model - the ion uptake is proportional to the equilibrium concentrations of the ions in the soil water as described by Mortensen (1984). Fertilizers are supplied to the upper soil layer once a year. A lime supply has not yet been incorporated.

When more soil types are simulated all combinations of crops and soil types are calculated, and with many areas and crops it results in a huge amount of calculations. There is no rotation of crops incorporated in the model.

The output from the crop model is concentrations (μg/kg) of ions (pollutants) in the harvested crop each year in a given area. These resulting concentrations are summed over the soil types weighted with the soil type areas. Additional output is the pH in the upper soil layer of all the soil types "beneath" the crops. An example of output from the crop model is given in Fig. 2a. The actual quantities are not adjusted to any experiments, so the figures are only for illustration purposes.

2.4. General remarks

The system which is incorporated in the program ECCES version 2.2 is a flexible simulation system and relatively easy to use The incorporated models can be used independently or in common.

Input to the program can be divided into three parts:

1. Scenario-defining information: areas, power plants, cities, crops, soil types and pollutants. Start time, simulation time and time step.

2. Model-defining information: which models are to be used. Output options for print and plot.

3. Dynamic information: load factors for each time step with the dispersion model.

There is a large number of output possibilities so nearly all combinations can be made. This is especially useful for testing purposes.

2.5. A scenario example

As an example of the capacity of the model a scenario with Roskilde Amt and seven power plants (Asnæsværk, Amagerværk, Kyndbyværk, Masnedøværk, Stigsnæsværk, Svanemølleværk and H.C. Ørsted værk) has been set up. Two different crops: winter cereals and grass is simulated in Roskilde Amt. This scenario is simulated first for 20 years with the power plants at full power and then further for 10 years with all power plants at zero power.

The result of the dispersion calculation for sulphur (SO_2 and SO_4^{--}) is shown in Fig. 1a. All curves shown in this report are based on 12 calculations per year. Calculations for nitrogen oxides and cadmium have also been made but are not shown here.

Soil chemistry and crop uptake calculations have also been made for 30 years. The results are partly in the output example in Fig. 2a, partly in the curves in Figs. 3a - 5a. Fig. 3a shows the resulting content of sulphate in the harvest of the two crops and there is a characteristic drop in the uptake, when the power plants are shut down.

Fig. 4a shows the corresponding curves for cadmium. The cadmium concentration is steadily increasing due to input from fertilizers since it is not washed out. When the power plants are shut down the curves shift due to an increase in pH in the soil (see Fig. 5a). The curves are less steep after the plant shut down and this is due to the missing supply of cadmium from the dispersion calculations. Finally Fig. 5a shows the pH-variation in the upper soil layer in the soil (sandy clay) when winter cereals are growing upon it. There is a rather large year variation, mainly due to the supply of fertilizers but also due to the growing crops. When the power plants shut down pH raises about 0.06.

3. SOIL CALCULATIONS

3.1. Introduction

This part of the report shortly describes some calculations from the ECCES program. These calculations shall predict the impact of different rainfall chemistries and other inputs to the soil chemistry system during a period of 20 years.

We have used a theoretical four layer test soil to show the changes of pH and concentrations of ions in the soil. For simplification all the soil layers are given the same soil parameters and start concentrations which makes it easier to compare the time dependent development of pH and ion concentrations down through the soil layers. Most test calculations are run without crops but one calculation with winter cereals growing upon the soil is shown. All results shall be regarded as preliminary because most parameters are theoretical or estimated.

3.2. Basis test

Constants used for this calculation are shown in Table 1b. A permanent ion-exchange capacity (CECP) of 10 meq/100 g and a variable ion exchange capacity (CECV) of 1 meq/100 g are used to describe a sandy-clay soil.

A low anion-exchange capacity for sulphate with maximum capacity of $5.4 \cdot 10^{-5}$ mol/l(s) is assumed (s stands for system or total soil volume).

Table 1. Constants used for basis test calculations.

Layer no.		I	II	III	IV
Soil depth	(mm)	200	300	500	1000
Solid content	(mm)	120	180	300	600
Max. water	(mm)	60	90	150	300
Min. water	(mm)	20	30	50	100
Density	(kg/l)	2.65	2.65	2.65	2.65
Max.Cap.SO_4	(mol/l(s))	5.4E-5	5.4E-5	5.4E-5	5.4E-5
Halfsat.SO_4	(mol/l)	1.8E-5	1.8E-5	1.8E-5	1.8E-5
CECV	(meq/100g)	1	1	1	1
CECP	(meq/100g)	10	10	10	10
CO_2 Partial	(atm)	0.003	0.003	0.003	0.003
Start water	(mm)	60	90	150	300
Start pH		7.0	7.0	7.0	7.0

Adsorption of ions to clay particles relative to calcium are shown in Table 2. Ca^{++} is bound somewhat stronger to clay particles than Mg^{++}, while K^{+} and Na^{+} is bound stronger than NH_4^{+}.

Table 2. Adsorption constants.

$K_{Ca/Mg}$	3.0
$K_{K/Ca}$	0.22
$K_{Na/Ca}$	0.22
$K_{NH4/Ca}$	0.17
$K_{Cd/Ca}$	0.44

The rain input (mm) from January to December in this simulation is shown in Table 3. Evaporation is assumed zero. These values are the same during all years.

Table 3. Rainfall (mm) from January to December. (Lund and Dorph-Petersen 1978).

J	F	M	A	M	J	J	A	S	O	N	D
54	40	34	40	45	49	76	89	68	70	70	62

Rainfall chemistry used in the simulation is shown in Table 4. A proton concentration as shown makes the pH in rain 4.9.

Table 4. Rainfall chemistry (mol/l). *This value makes a cadmium deposition of 0.2 mg · m^{-2} · $year^{-1}$.

Ions	No.	Concentration (mol/l)	References
H^+	1	1,3 · 10^{-5}	Brodersen (1984)
$SO4^{--}$	2	8,29 · 10^{-5}	Bentholm et al. (1983)
Ca^{++}	3	7,05 · 10^{-5}	Brodersen (1984)
Cl^-	4	2,04 · 10^{-4}	estimated
K^+	5	1,5 · 10^{-5}	Brodersen (1984)
Mg^{++}	6	2,55 · 10^{-5}	-
Na^+	7	1,47 · 10^{-4}	-
$NH4^+$	8	7,1 · 10^{-5}	-
$NO3^-$	9	5,6 · 10^{-5}	-
$HCO3^-$	10	1,26 · 10^{-5}	estimated
*Cd^{++}	14	1,3 · 10^{-9}	Miljøministeriet (1980)

Start concentrations for all adsorbed ions involved are calculated in the beginning of the program when dissolved concentrations are known. All start values are shown in App. B, Table 1b. Units for dissolved ions are mol/l (water) while permanent and variable adsorbed ions are mol/l(system).

Permanent adsorbed SO_4^{--} is sulphate adsorbed to the defined anion exchanger of the soil.

3.2.1. pH

App. B, Fig. 1b, shows the development of pH in the above defined basis test soil during 20 years. pH in the upper soil layer decreases most rapidly because of the acid rainfall to the soil surface. There is a delay down through the soil layers. pH of the soil goes towards 4.9, which is pH of rain.

3.2.2. Cadmium concentrations

Fig. 2b, App. B, shows a drastic decrease in cadmium concentration in the beginning of the simulation period. The explanation is that the start concentration in the soil water ($2.8 \cdot 10^{-9}$ mol/l) is higher compared to the rainwater concentration ($1.3 \cdot 10^{-9}$ mol/l) and that the permanent cation exchanger in the upper soil layer adsorbs most of the supplied cadmium (Fig. 3b, App. B). This high affinity for adsorption causes the concentration of dissolved cadmium to drop in soil layers 2-4 because percolation of cadmium from the upper soil layer becomes small. The amount of variable adsorbed cadmium decreases in soil layers 2-4 (Fig. 4b, App. B), because a decrease in pH are followed by a decrease in the variable cation exchange capacity (CECV).

3.3. Calculation with acid rain

This calculation was made to show the soil pH development and cadmium content as a function of time when the ECCES computer model was run with a very acid rain input of pH = 2.0. Sulphate concentration was changed to $5.0764 \cdot 10^{-3}$ mol/l to establish ion neutrality in the rain. All other ion concentrations in the rain, start values and parameters are as shown in the basis test (Section 3.2).

Plots for pH and cadmium concentrations are shown in App. C.

3.3.1. pH

Fig. 1c shows increasing acidification of all soil layers most pronounced in the upper soil layer (No. 1) with a clear timelack down through the soil. Most interesting are the two upper soil layers where all the buffer capacity are used during the simulation. After a very steep drop a plateau is reached in soil layer 1 for pH = 4.5 - 3.8. This buffer effect is a function of the permanent ion exchange capacity. The same effect is seen for soil layer 2.

3.3.2. Cadmium concentrations

Fig. 2c shows Cd^{++} concentrations in the four soil layers. In the beginning increase of cadmium concentration in the soil water is seen. Then a gradual decrease ending with a sudden drop in soil layers 1 and 2 down to the rain water concentration ($1.3 \cdot 10^{-9}$ mol/l) is seen. The increase is caused by release of Cd^{++} from the permanent and variable ion exchanger (see Fig. 4c).

The gradual decrease is mostly a consequence of cadmium release from the permanent cation exchanger just like the steep drop in 1989 and 1997 for soil layers 1 and 2 respectively. As seen in Fig. 3c, this steep drop coincide with the near disappearance of permanent adsorbed cadmium in these layers.

A greater wash out of cadmium from the upper soil layer to the underlying layers causes the variation in concentration levels down through the soil.

3.4. CECP and CECV sensitivity test

In this section the intention is to show how the permanent (CECP) and variable (CECV) cation exchanger influence pH-development and cadmium concentration in the soil system. Values used in the calculations are shown in Table 5. All other start values and parameters are defined in the basis test.

Table 5. Values of permanent and variable cation exchange capacities (meq/100 g). Figs. 2d and 6d are identical.

CECP	CECV	Plotparameters	Figures
10	0.1	pH	fig. 1d
10	1	pH	fig. 2d
10	5	pH	fig. 3d
10	10	pH	fig. 4d
1	1	pH, Cd	fig. 5d, 9d
10	1	pH	fig. 6d
20	1	pH	fig. 7d
30	1	pH, Cd	fig. 8d, 10d

As seen in Table 5 four runs have been made when either CECP or CECV is fixed while the other is changed within expected realistic values. CECP = 1 corresponds to a very sandy soil while a CECP = 30 corresponds to is a clayey soil. Low CECV is expected in a non humic soil while a high value corresponds to a very humic soil. From Table 5 is seen that only two plots of cadmium are shown. A value of 1 for CECV is assumed realistic for agricultural soils, while a wider range of CECP is expected.

3.4.1. pH

Figs.1d-4d, App. D, show pH development in four soil layers when CECP = 10 and CECV range from 0.1 to 10. From the figures it is clear that CECV very much influence the buffer capacity of the soil. A low value CECV (0.1) brings pH down to about 5.6 in the upper soil layer, while a high value (10) create a strong buffer effect where pH only drops to 6.5 in the upper soil layer after 20 years. The same acidification pattern down through the soil layers is seen in the basis calculations (Fig. 1b).

Figs. 5d-8d show pH development in the soil when CECP changes from 1 to 30 and CECV is fixed. CECP does not affect the buffer capacity as strongly as CECV. Soils with low CECP = 1 meq/100 g (very sandy soil) result in a pH of about 5.7 after 20 years, while a very clayey soil (CECP = 30 meq/100 g) results in a pH of 5.8 after 20 years of simulation.

This shows that pH in this model is very sensitive to changes in the variable cation exchange capacity and determination of this parameter is important.

3.4.2. Cadmium concentrations

Two figures (9d and 10d) of cadmium concentration development in the soil are shown with fixed CECV = 1 and CECP = 1 and 30 meq/100 g. The difference in permanent adsorbed cadmium is clear. A high CECP = 30 meq/100 g create more permanently adsorbed cadmium 10^{-7} mol/l (system) compared to 10^{-8} mol/l(system). Besides there is a clear difference between the levels of dissolved cadmium. Fig. 9d with a small CECP shows a much higher concentration of dissolved cadmium than soils with a high CECP (Fig. 10d). After 20 years the concentrations are $1 \cdot 10^{-9}$ and $2 \cdot 10^{-10}$ mol/l respectively or about 5 times higher in a soil with low CECP.

Because of higher permanent adsorption capacity in Fig. 10d compared to Fig. 9d, most of the supplied cadmium is adsorbed on the permanent cation exchanger and therefore creates a lower content of dissolved and variable adsorbed cadmium.

3.5. K_{Cd}-sensitivity test

Figs. 1e-3e show the effect on dissolved cadmium with changes in the adsorption constant (K_{Cd}). K_{Cd} describes the amount of cadmium adsorption to the permanent and variable ion exchanger.

The calculations were made with K_{Cd} values of 0.1, 1.0 and 10. The figures for soluble cadmium are shown in App. E.

3.5.1. Cadmium concentrations

The three figures (App. E) do not differ much except for the concentration of cadmium in the upper soil layer. Fig. 1e (K_{Cd} = 0.1) shows an increase of dissolved cadmium in this upper layer compared to Figs. 2e and 3e. This reaction was expected because K_{Cd} = 0.1 describes a weak cadmium adsorptive soil. The steep drop in the beginning of simulation has been discussed earlier in Section 3.2.2.

For every 10 times increase in K_{Cd}, 10 times increase in the adsorbed amount of cadmium is seen. Plots showing this effect are not included.

3.6. Sulphate adsorption

The effect of anion adsorption on the pH-development in the soil system was tested. Two calculations were made, one soil with a strong and one with a weak sulphate adsorption capacity.

No clear effects on either pH or sulphate concentration in the soil water were seen. Plots from these tests are not shown.

3.7. Basis test with crops

Calculations were made for the soil described in Section 3.2 with a crop (winter cereal) grown on the soil. The same rain-water input was used and every year fertilizer was supplied in May. The amount is shown in Table 6 together with crop uptake coefficients. The uptake coefficients are estimated values creating concentrations in the crop within expected magnitudes. Figures for pH-development and cadmium concentrations in the soil are shown in App. F.

Table 6. Fertilizer applied to the soil surface in May (mol/m^2), and uptake coefficient for winter cereals. Amount of fertilizer are estimated from Norsk Hydro (1984), *Hansen and Tjell (1981) and ** estimated to maintain ion neutrality.

Ions	Fertilizer (mol/m^2)	Uptake coefficient
SO_4^{--}	0.0224	1
Ca^{++}	0	3
Cl^-	** 0.1438048	0
K^+	0.11	10
Mg^{++}	0.0193	5
Na^+	0	0
NH_4^+	0.506	3
NO_3^-	0.466	1
Cd^{++}	* 0.0000024	1

3.7.1. PH

Fig. 1f shows the calculated pH in the basis soil grown with winter cereals as a function of time. The figure shows a yearly variation as a consequence of root uptake of ions. The small peak on the top of every curve are related to the input of fertilizer which influence the ion strength of the soil water creating a small increase in pH. The steep drop especially in the two uppermost soil layers is a consequence of protons released from the crop roots as a response to uptake of more cations than anions. This creates an acidifying reaction in the soil. During wintertime pH increases until fertilizer is supplied again and crops are grown next spring. Soil layer 4 is unaffected by the roots because these mostly grow in the upper soil layers.

Compared to pH-development in testsoil without crops (Fig. 1b) a much more acid soil is seen after 20 years. All the upper soil layers develop a pH about 5 during the winter and it drops to about 4.6 in the summer. In the test soil without crops pH is greater than 5.7 for all soil layers after 20 years (Fig. 1b).

3.7.2. Cadmium concentrations

Fig. 2f shows the concentration of dissolved cadmium and the concentration of protons in the soilwater. Dissolved cadmium increases during the simulated period and the yearly variation is closely related to the hydrogen concentration in the soilwater. Increase of hydrogen is followed by an increase of dissolved cadmium. This is a consequence of cadmium released from the variable cation exchanger (Fig. 3f). Variable and permanent adsorbed cadmium also increase in the simulated period as a consequence of input via rainfall and the yearly input of fertilizer.

4. CONCLUSION

Three different models, an atmospheric dispersion model, a soil chemistry model and a model for ion uptake in crops have been developed. These three models are assembled in a single program, ECCES, where it is possible to run the three models independently or in common. The program is very flexible and many input and output options are available. Besides some databases for areas, cities, plants, crops, soil types, pollutants and meteorology have been created.

The program has now reached the stage of development which was planned for the present phase of the project, as illustrated by the scenario calculations in the report. Even so, the models are still to be improved and extended in many areas.

The soil and plant models have been run independently to illustrate their function. The report presents a number of calculations which show how results depend on a number of parameters used in some of the submodels. The submodel for atmospheric dispersion has not been tested in this manner. This submodel is considered "proven technology" in the sense it is based on the well known plume model concept. Thus its accuracy and the permissible domain for use is well understood. This does not mean that the model may not be improved or replaced by other models at a later stage. One of the obvious improvements would be to use deposition velocities dependent on the surface on which deposition takes place.

Calculations of pH and cadmium concentrations in a theoretical test soil showed as expected a pH decrease with time in all soil layers when pH in rainfall was 4.9 and the start pH in soil was 7.0. The decrease was most pronounced in the upper soil layer.

Sensitivity tests were run to show the sensitivity of different parameters. Changes in CECV (variable cation exchange capacity) within the expected range showed a high buffer effect, while CECP (permanent cation exchange capacity) did not influence pH development very much. For this model, determination of CECV appears therefore very important for realistic calculations of soil acidification. CECP on the other hand influences concentration levels of permanent adsorbed ions in the soil. These levels influence the soluble amount of ions and create lower concentrations of dissolved cadmium in the soil water with a high CECP value and higher cadmium concentrations with low CECP.

Changes in sulphate adsorption capacity within the expected range did not show remarkable changes in either pH or sulphate concentration.

Variation of K_{Cd} (adsorption constant for cadmium) affects the concentration of cadmium in the upper soil layer, creating increase of soluble cadmium for small K_{Cd}.

The same testsoil with crops growing on it develops stronger acidification than the same soil without crops. A yearly variation of soil pH is seen as a consequence of released hydrogen ions from the root system. This calculation also showed an increase of soluble cadmium and permanent and variable adsorbed cadmium after 20 years due to cadmium input via rainfall and fertilizer.

It should be stressed again that the results in this report are meant to illustrate how the models work within their theoretical framework. Thus one should be careful in drawing conclusions from the calculations presented. To some extent the models may be used to reveal trends in the development of pollution effects in the environment. However, before more quantitative conclusions can be drawn from the model calculations, more data collection and verification of the models are needed. This will take a considerable part of the future work within this project.

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APPENDIX A

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        YEAR = 1984  'SUBPERIOD' =    1
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RESULT OF DISPERSION CALCULATION FOR POLLUTANT NO.  2  SULPHATE

POLLOTION TO AREA NO. 11113000  ROSKILDE      AMT

FROM :                                                PARENT PRODUCT                 DAUGHTER PRODUCT
                                  SOURCE STRENGTH    IN AIR    DEPOSITION           IN AIR    DEPOSITION
                                      KG/SEC        MICROG/M3   G/M2/YEAR          MICROG/M3   G/M2/YEAR

     PLANT NO. 11114011 ASVTOT (180 M) 1.40E+00     1.19E+00    3.25E-01           1.46E-01    1.17E-02
     PLANT NO. 11111011 AMVTOT (150 M) 2.70E-01     2.34E-01    6.34E-02           2.90E-02    2.30E-03
     PLANT NO. 11112011 KYVTOT (100 M) 8.60E-01     1.12E+00    3.03E-01           1.30E-01    1.02E-02
     PLANT NO. 11115011 MAVTOT ( 60 M) 1.40E-01     8.99E-02    2.41E-02           1.28E-02    9.76E-04
     PLANT NO. 11114021 STVTOT (130 M) 4.30E-01     3.80E-01    1.02E-01           5.04E-02    3.85E-03
     PLANT NO. 11111012 SMVTOT (100 M) 1.80E-01     1.81E-01    4.85E-02           2.59E-02    1.95E-03
     PLANT NO. 11111013 HCVTOT ( 88 M) 3.10E-01     3.54E-01    9.50E-02           4.92E-02    3.73E-03
  PLANTS                                            3.54E+00    9.61E-01           4.43E-01    3.47E-02

  CITIES                                            0.00E+00    0.00E+00           0.00E+00    0.00E+00

     AREA NO.  11113000 RSKLD. ( 10 M) 8.80E-02     0.00E+00    0.00E+00           0.00E+00    0.00E+00
  AREAS                                             0.00E+00    0.00E+00           0.00E+00    0.00E+00

TOTAL TO THIS AREA                                  3.54E+00    9.61E-01           4.43E-01    3.47E-02
```

Fig. 1a. Example of print from the dispersion model.

```
UPTAKE IN CROPS IN YEAR : 1995  FOR AREA :  11113000  ROSKILDE       AMT


                           CONCENTRATIONS IN MICROGR./KG
POLLUTANT    NAME
   NO.                          W.CER.    GRASS

     2     SULPHATE           1.70E+06  1.38E+06
     9     NITRATE            4.37E+06  2.68E+06
    14     CADMIUM            5.02E+01  3.23E+01
     3     CALCIUM            4.40E+06  2.51E+06
     5     POTASSIUM          2.16E+06  1.41E+06
     6     MAGNESIUM          3.08E+05  1.93E+05
     7     SODIUM             1.17E+06  8.66E+05
     8     AMMONIUM           3.62E+06  2.33E+06

HARVEST IN KG/M2              1.33E+00  2.70E+00
CROP AREA IN KM2              1.23E+02  3.84E+01


                           QUANTITIES IN CROPS IN T/YEAR
POLLUTANT    NAME
   NO.                          W.CER.    GRASS

     2     SULPHATE           2.78E+02  1.43E+02
     9     NITRATE            7.15E+02  2.79E+02
    14     CADMIUM            8.21E-03  3.35E-03
     3     CALCIUM            7.20E+02  2.60E+02
     5     POTASSIUM          3.54E+02  1.46E+02
     6     MAGNESIUM          5.04E+01  2.00E+01
     7     SODIUM             1.91E+02  8.98E+01
     8     AMMONIUM           5.92E+02  2.42E+02

HARVEST IN T                  1.64E+05  1.04E+05


ACIDITY  AT TIME :  JANUARY    1996
                   PH IN THE UPPER SOIL LAYER
  SOIL       NAME
  NO.                         W.CER.     GRASS

  100     COARSE-FINE          5.21       5.14
  200     CLAYEY SAND          5.29       5.16
  300     SANDY CLAY           5.35       5.45
  400     CLAY                 5.45       5.72
  500     HEAVY CLAY           5.61       5.81
  600     ORGANIC SOIL         5.63       5.82
```

Fig. 2a. Example of print from the crop uptake model.

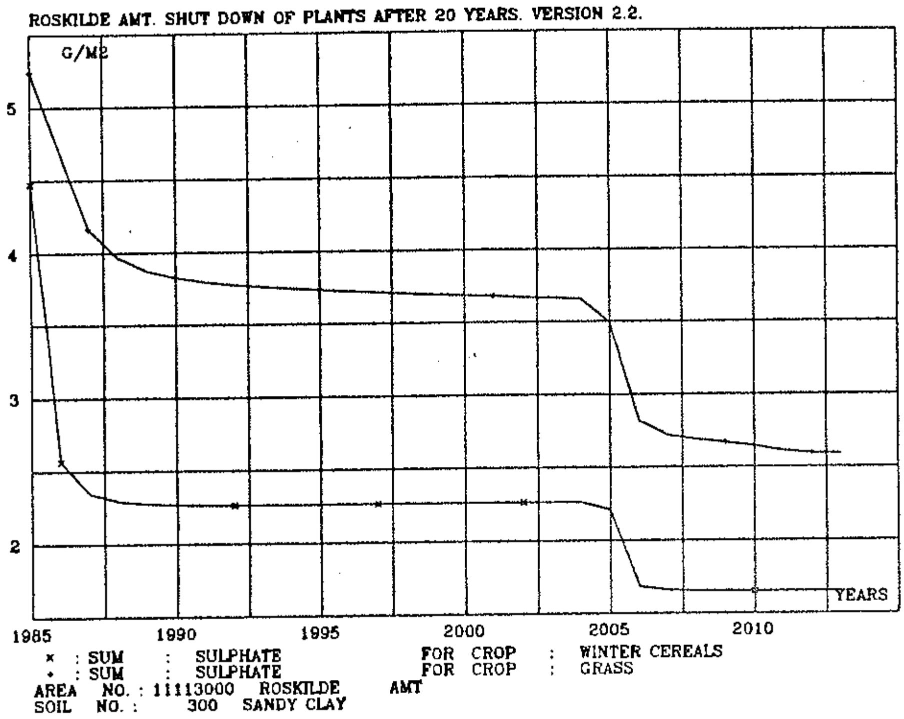


Fig. 3a. Uptake of sulphate in the harvest of winter cereals and grass in Roskilde during a 30 year period. The marks on the curves are for identification only.

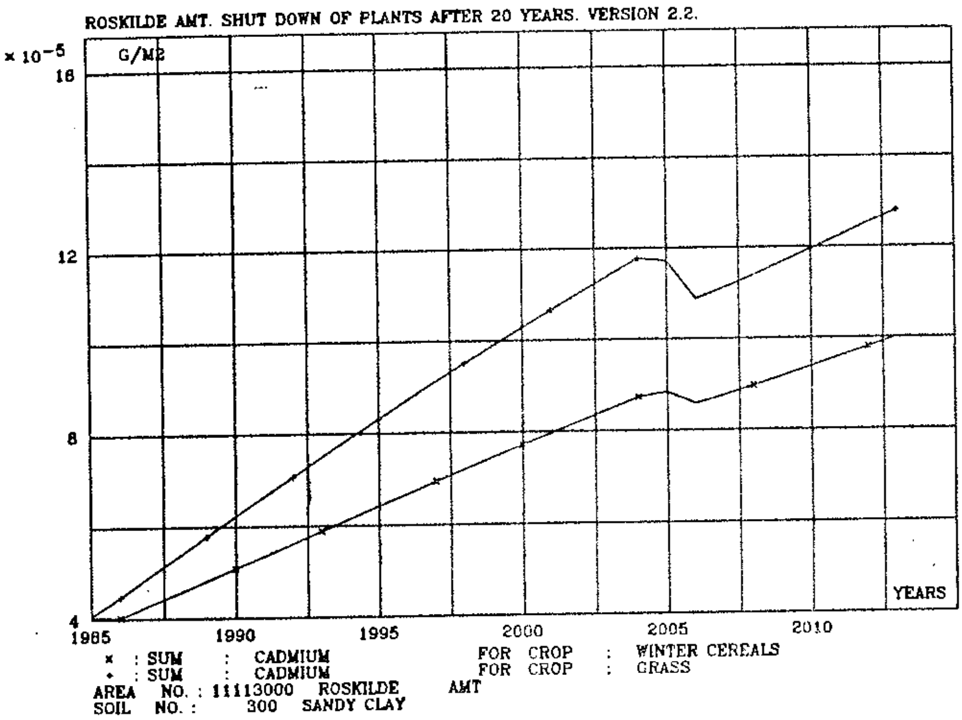


Fig. 4a. Uptake of cadmium in the harvest of winter cereals and grass in Roskilde during a 30 year period.

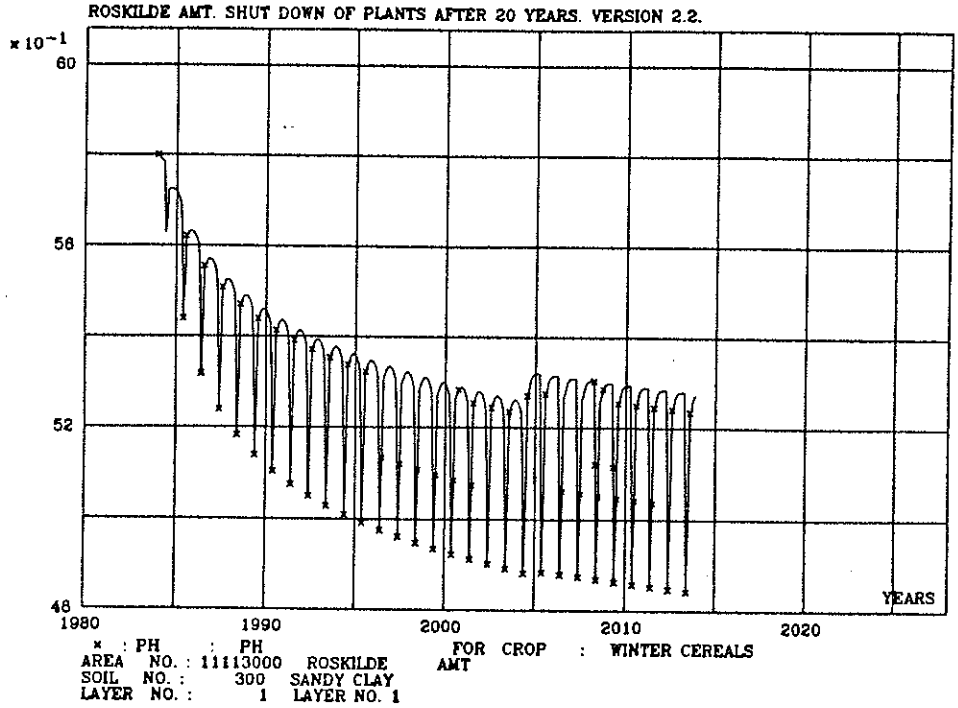


Fig. 5a. The variation in pH in the upper layer of the soil type, sandy clay when winter cereals are growing upon it.

APPENDIX B

Table 1b. Start values for basis test calculations.

```
        STARTVARIABLES FOR SOIL TYPE NO.  400 : TEST SOIL
  **************************************************************

VARIABLE/SOIL LAYER                    1              2              3              4

WATER CONTENT IN MM.            60.00000       90.00000      150.00000      300.00000
START PH                         7.00000        7.00000        7.00000        7.00000
BASE SATURATION              1.11708E-08    1.11708E-08    1.11708E-08    1.11708E-08

ION CONCENTRATIONS :

  14   CADMIUM               2.80000E-09    2.80000E-09    2.80000E-09    2.80000E-09
   1   HYDROGEN              1.11340E-07    1.11340E-07    1.11340E-07    1.11340E-07
   2   SULPHATE              7.48000E-04    7.48000E-04    7.48000E-04    7.48000E-04
   3   CALCIUM               2.67000E-03    2.67000E-03    2.67000E-03    2.67000E-03
   4   CHLORIDE              2.92171E-03    2.92171E-03    2.92171E-03    2.92171E-03
   5   POTASSIUM             2.56000E-05    2.56000E-05    2.56000E-05    2.56000E-05
   6   MAGNESIUM             2.47000E-04    2.47000E-04    2.47000E-04    2.47000E-04
   7   SODIUM                5.65000E-04    5.65000E-04    5.65000E-04    5.65000E-04
   8   AMMONIUM              4.29000E-06    4.29000E-06    4.29000E-06    4.29000E-06
   9   NITRATE               1.36000E-03    1.36000E-03    1.36000E-03    1.36000E-03
  10   BICARBONATE           6.51289E-04    6.51289E-04    6.51289E-04    6.51289E-04
  11   CARBONATE             2.90891E-07    2.90891E-07    2.90891E-07    2.90891E-07
  12   LIME                  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  13   GYPSUM                0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00

PERMANENT ADSORBED ION CONCENTRATIONS :

  14   CADMIUM               3.35726E-08    3.35726E-08    3.35726E-08    3.35726E-08
   1   HYDROGEN              0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   2   SULPHATE              3.96311E-06    3.96311E-06    3.96311E-06    3.96311E-06
   3   CALCIUM               7.71218E-02    7.71218E-02    7.71218E-02    7.71218E-02
   4   CHLORIDE              0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   5   POTASSIUM             2.78303E-05    2.78303E-05    2.78303E-05    2.78303E-05
   6   MAGNESIUM             2.37816E-03    2.37816E-03    2.37816E-03    2.37816E-03
   7   SODIUM                6.14223E-04    6.14223E-04    6.14223E-04    6.14223E-04
   8   AMMONIUM              4.09966E-06    4.09966E-06    4.09966E-06    4.09966E-06
   9   NITRATE               0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  10   BICARBONATE           0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  11   CARBONATE             0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  12   LIME                  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  13   GYPSUM                0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00

VARIABLE ADSORBED ION CONCENTRATIONS :

  14   CADMIUM               2.51793E-09    2.51793E-09    2.51793E-09    2.51793E-09
   1   HYDROGEN              0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   2   SULPHATE              0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   3   CALCIUM               5.78414E-03    5.78414E-03    5.78414E-03    5.78414E-03
   4   CHLORIDE              0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   5   POTASSIUM             2.08727E-06    2.08727E-06    2.08727E-06    2.08727E-06
   6   MAGNESIUM             1.78362E-04    1.78362E-04    1.78362E-04    1.78362E-04
   7   SODIUM                4.60667E-05    4.60667E-05    4.60667E-05    4.60667E-05
   8   AMMONIUM              3.07475E-07    3.07475E-07    3.07475E-07    3.07475E-07
   9   NITRATE               0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  10   BICARBONATE           0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  11   CARBONATE             0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  12   LIME                  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  13   GYPSUM                0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
```

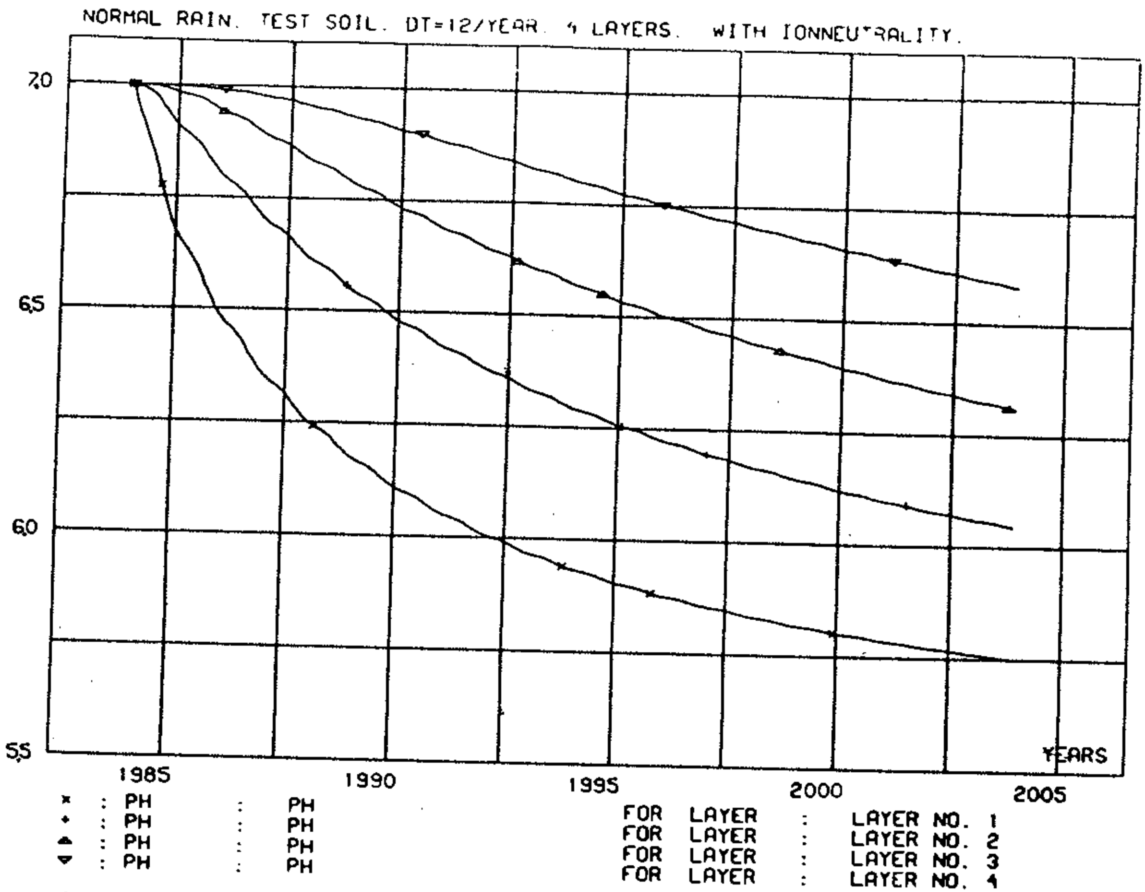


Fig. 1b. pH in a test soil.

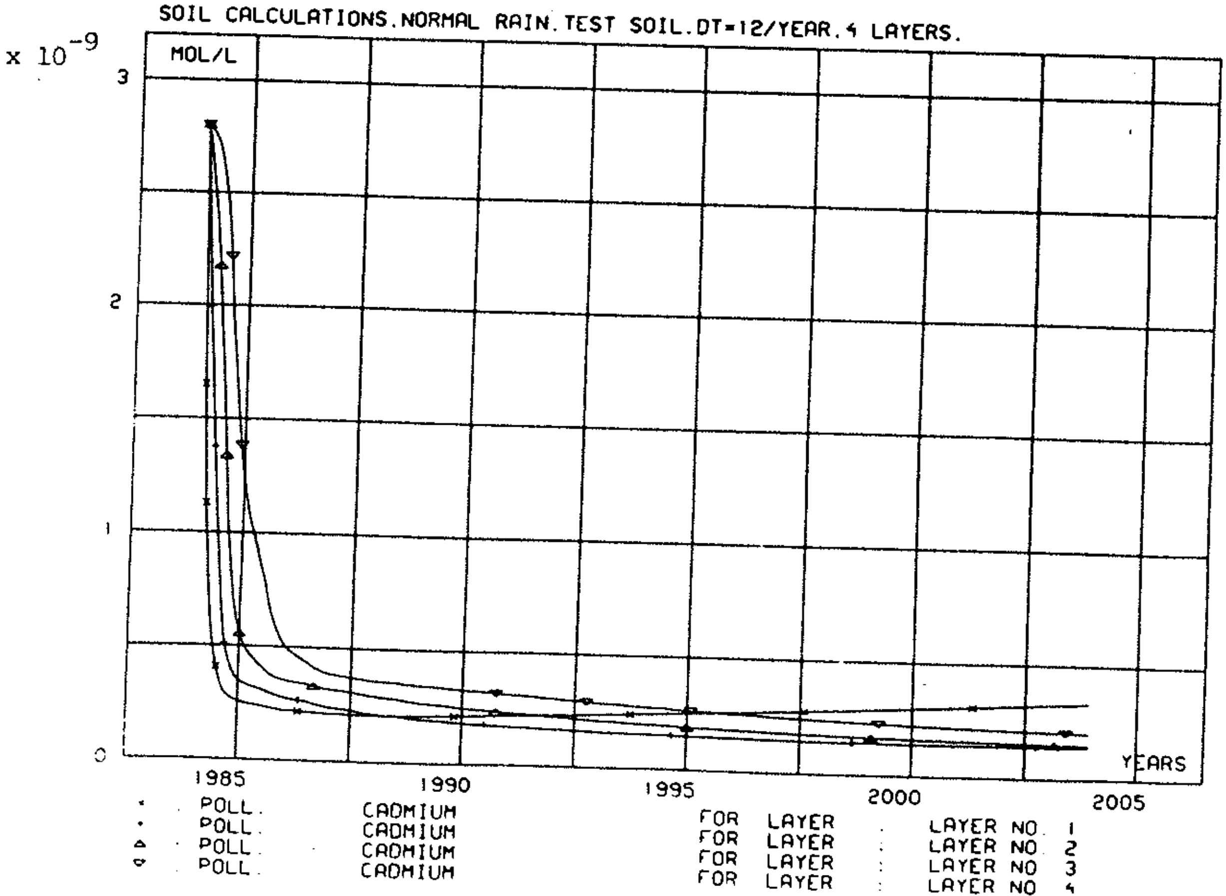


Fig. 2b. Dissolved cadmium in a test soil.

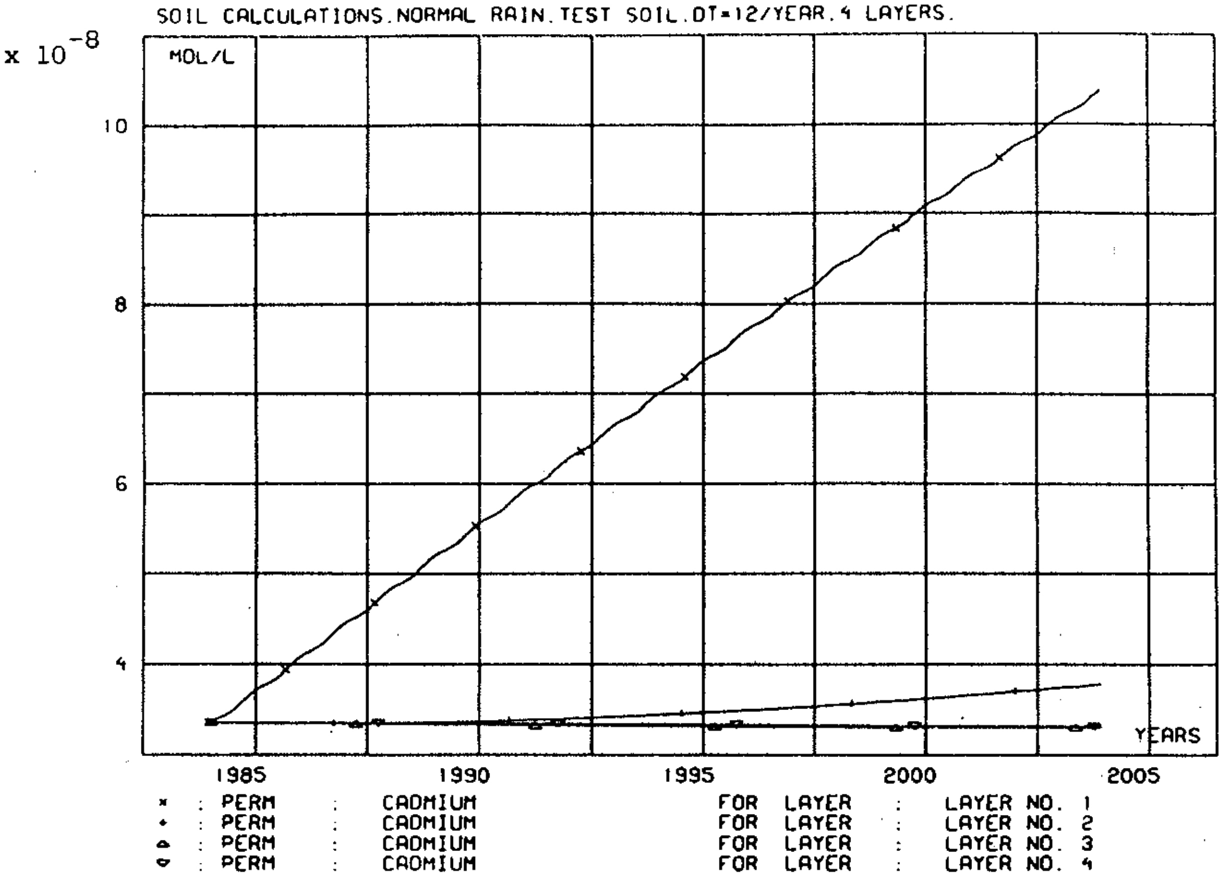


Fig. 3b. Permanent adsorbed cadmium in a test soil.

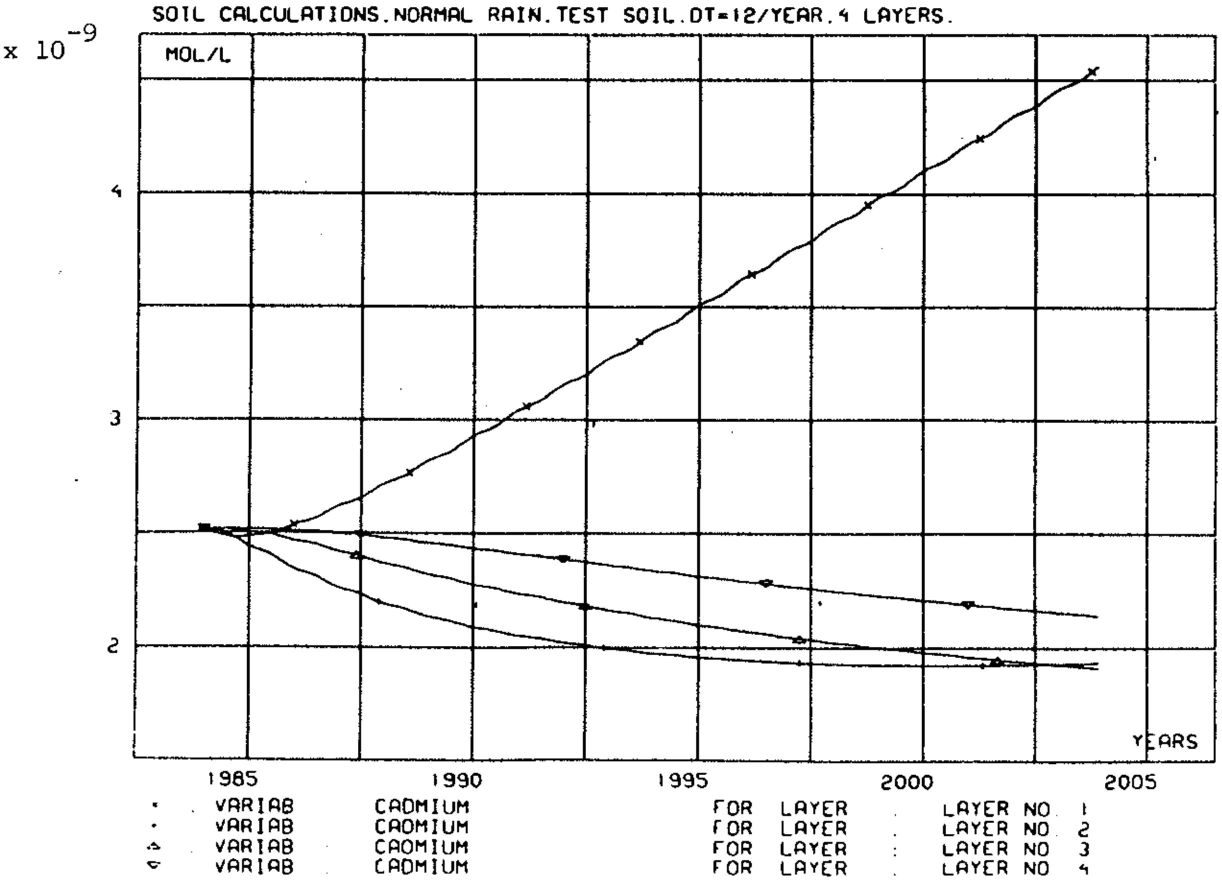


Fig. 4b. Variable adsorbed cadmium in a test soil.

APPENDIX C

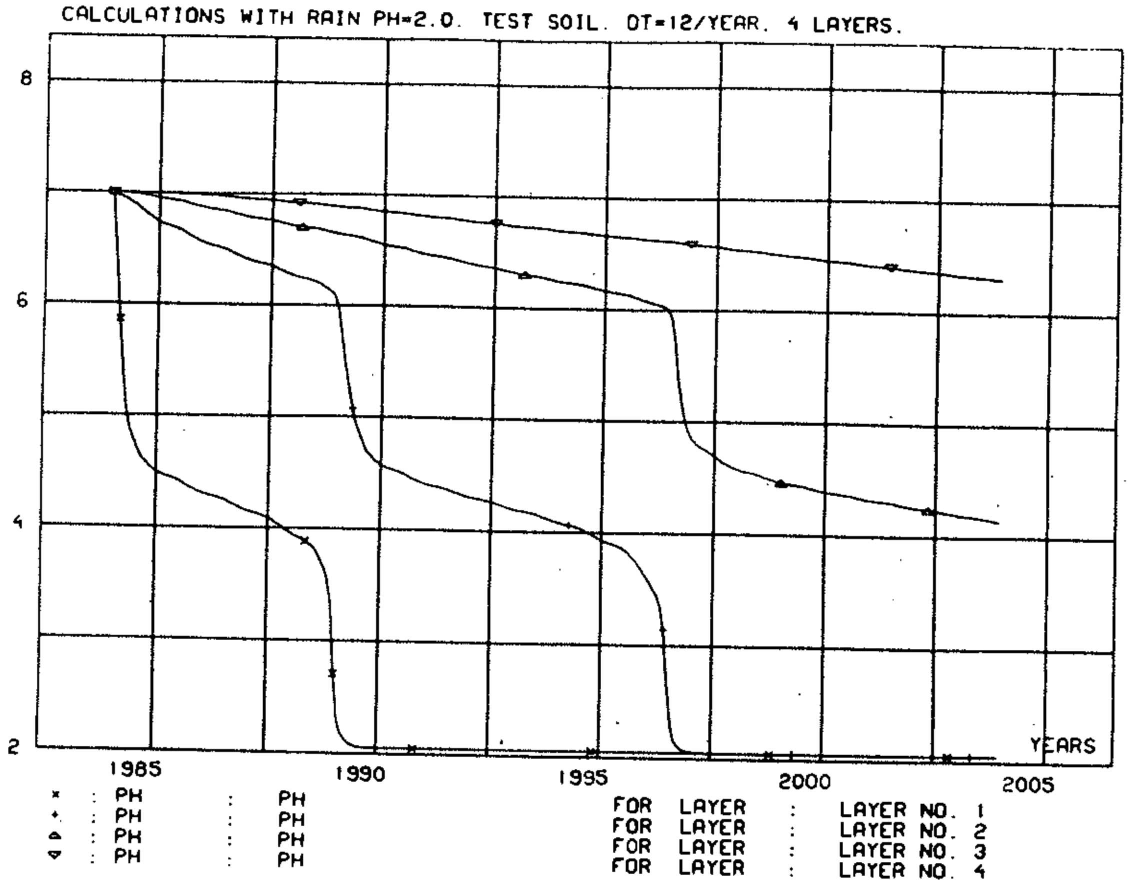


Fig. 1c. pH development in a test soil for pH=2 in rainfall.

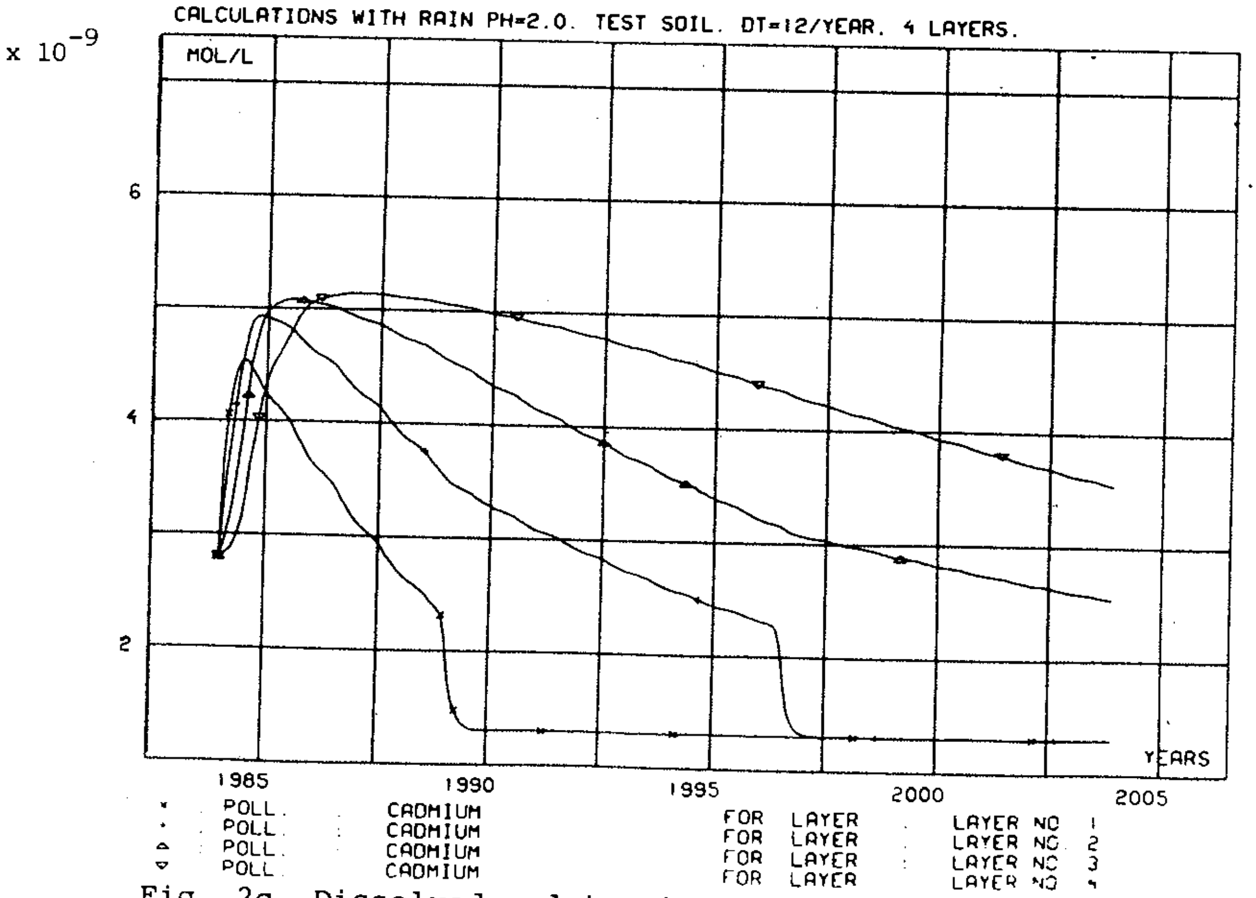


Fig. 2c. Dissolved cadmium in a test soil for pH=2 in rainfall.

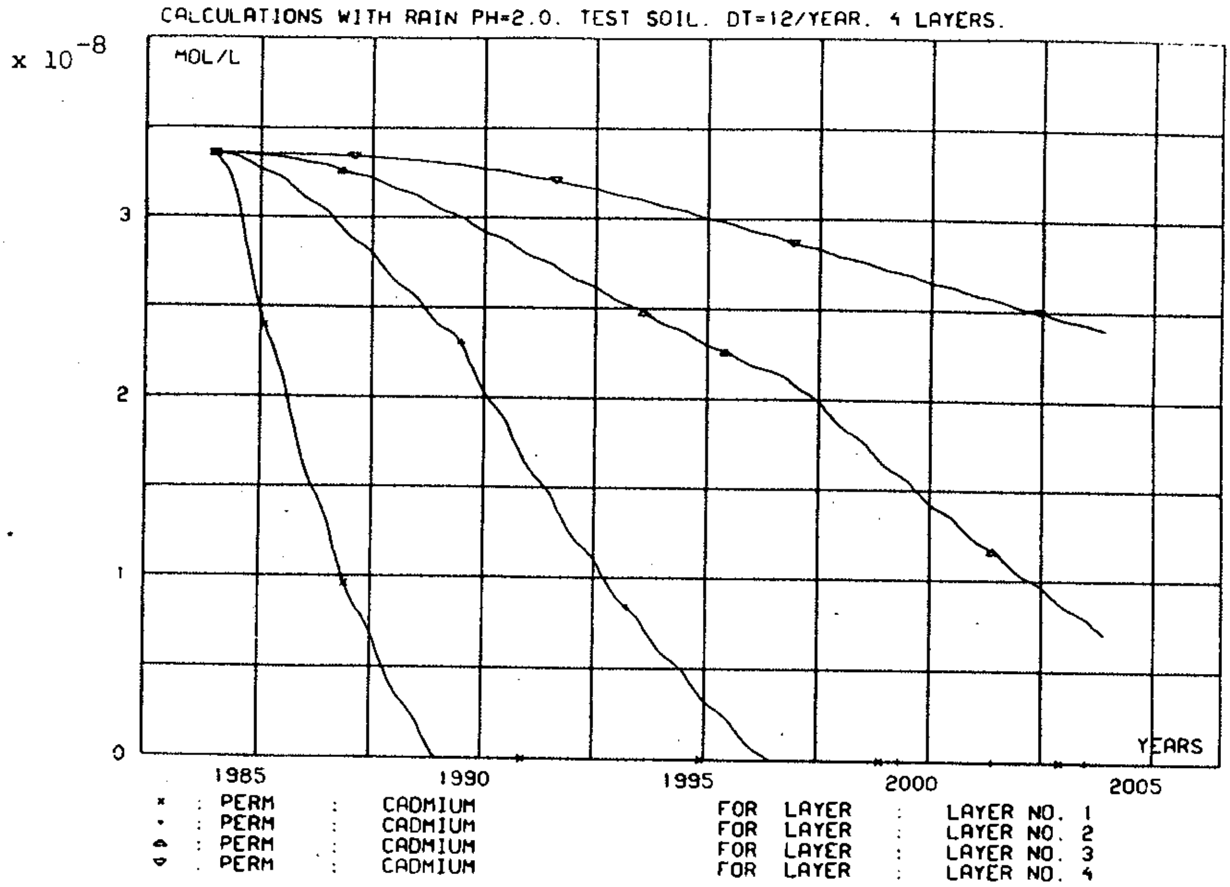


Fig. 3c. Permanent adsorbed cadmium in a test soil for pH=2 in rainfall.

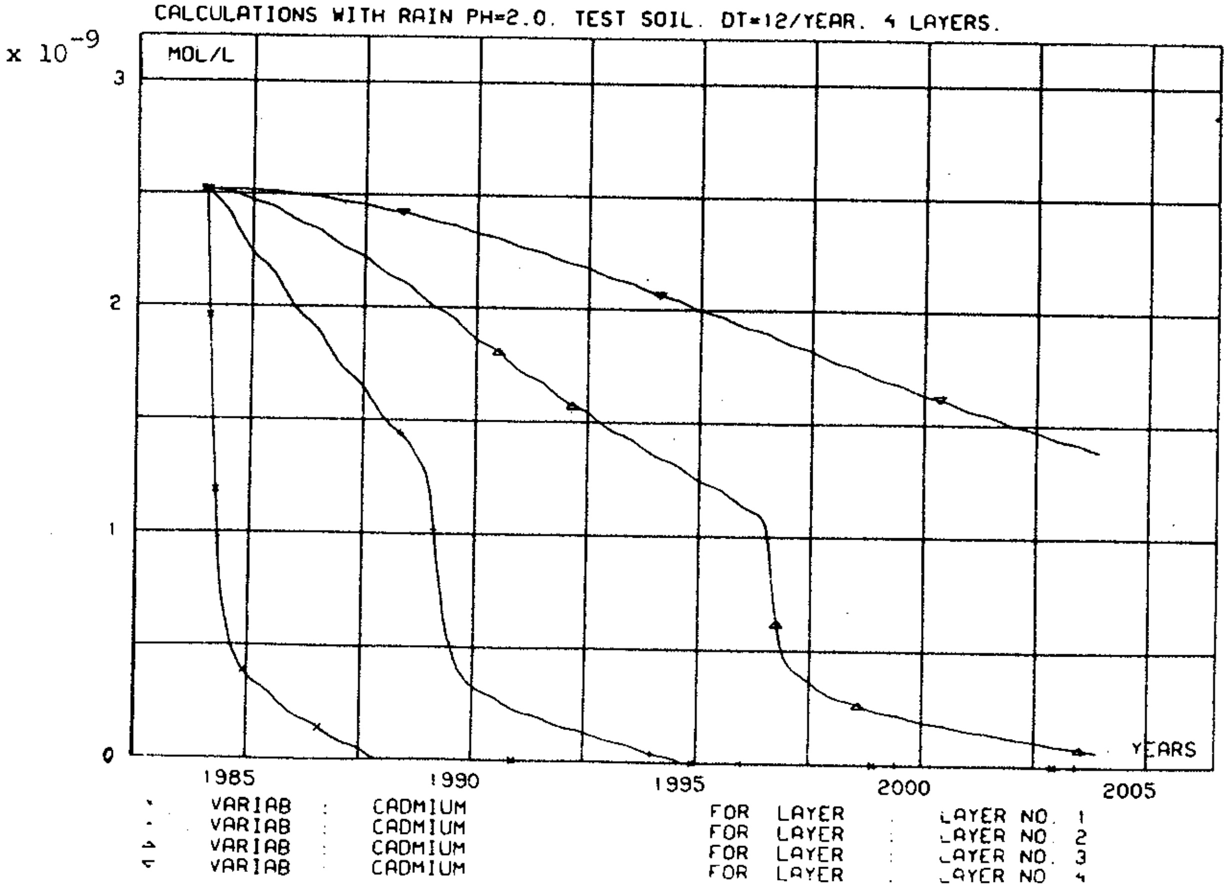
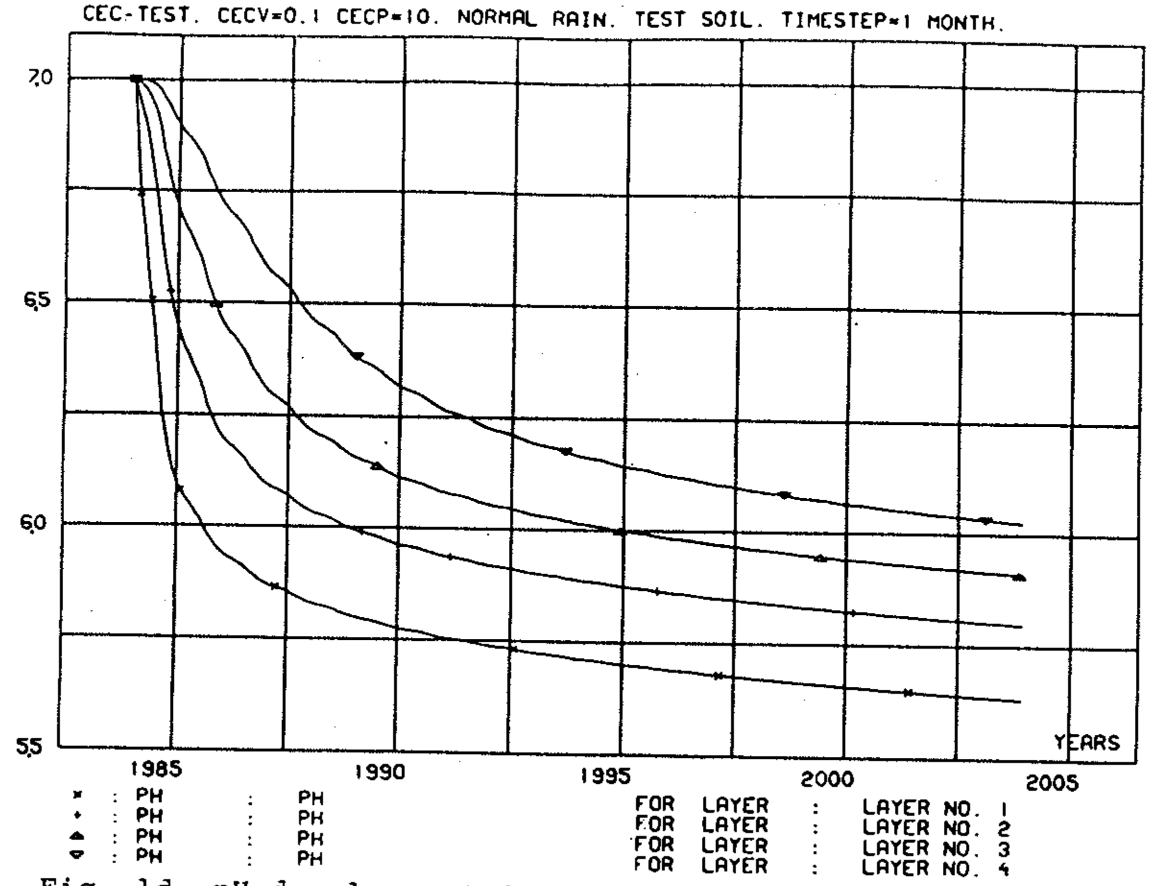
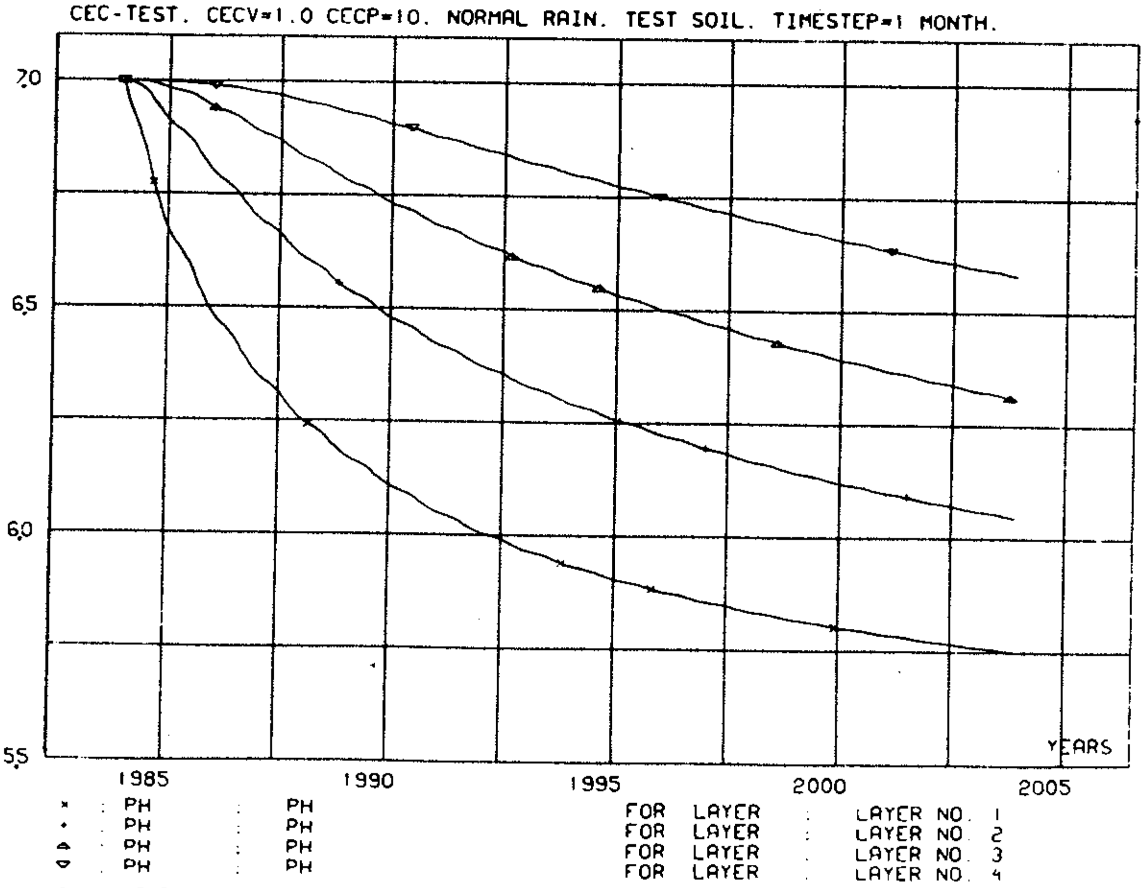


Fig. 4c. Variable adsorbed cadmium in a test soil for pH=2 in rainfall.



<u>Fig. 1d</u>. pH-development in a test soil for variable cation exchange capacity = 0.1 meq/100 g.



<u>Fig. 2d</u>. pH-development in a test soil for variable cation exchange capacity = 1.0 meq/100 g.

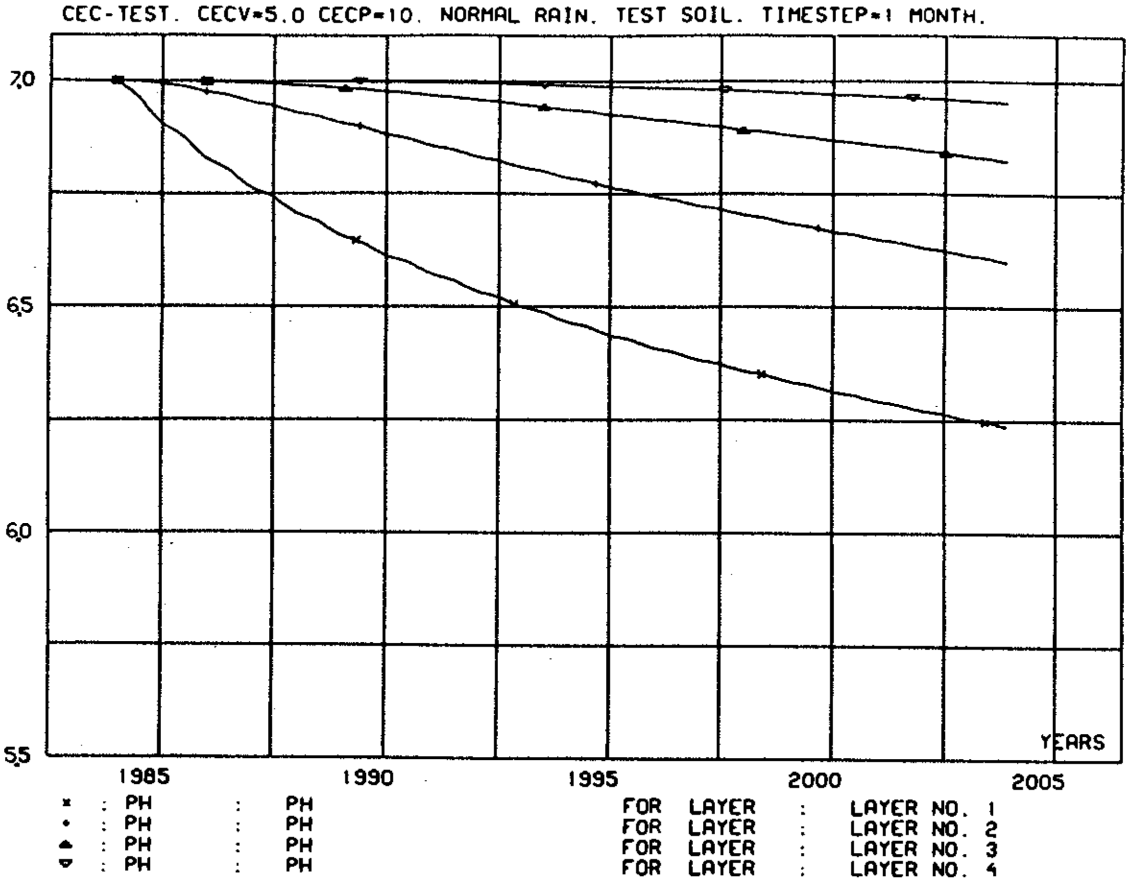


Fig. 3d. pH-development in a test soil for variable cation exchange capacity = 5.0 meq/100 g.

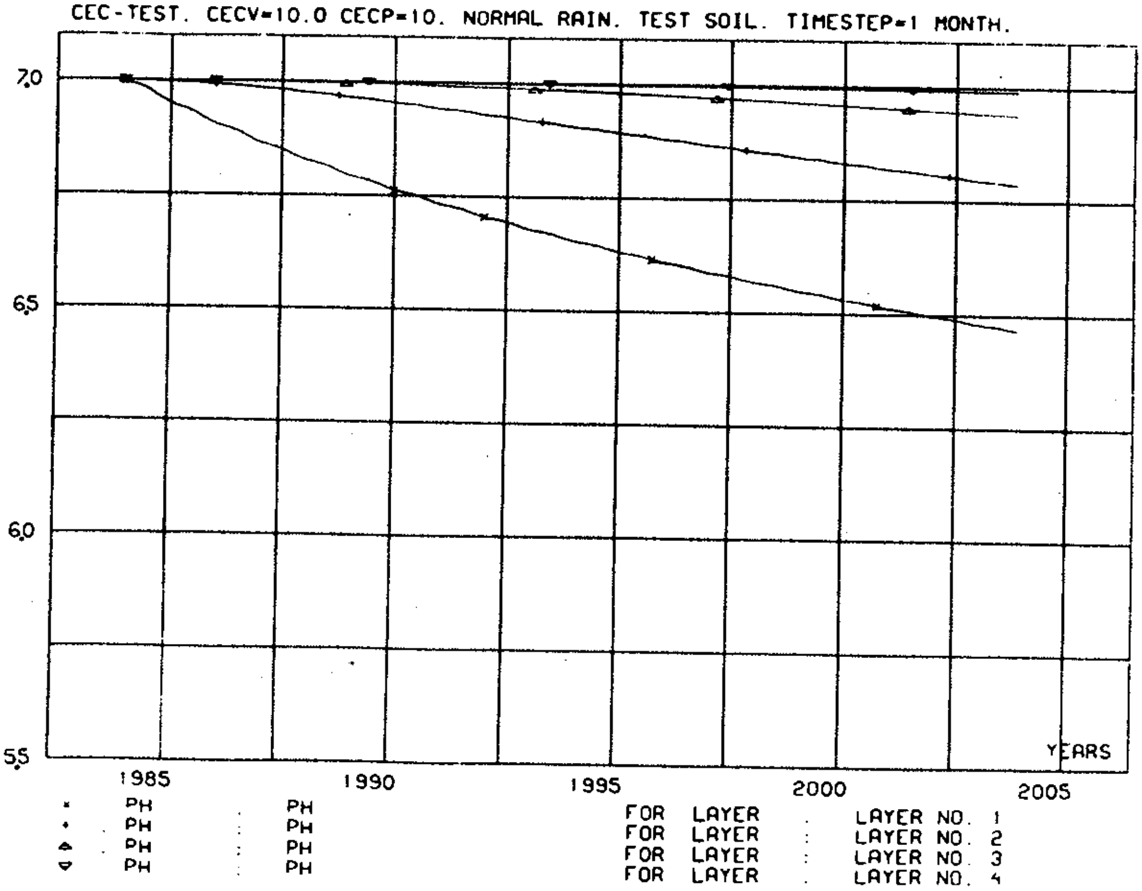


Fig. 4d. pH-development in a test soil for variable cation exchange capacity = 10 meq/100 g.

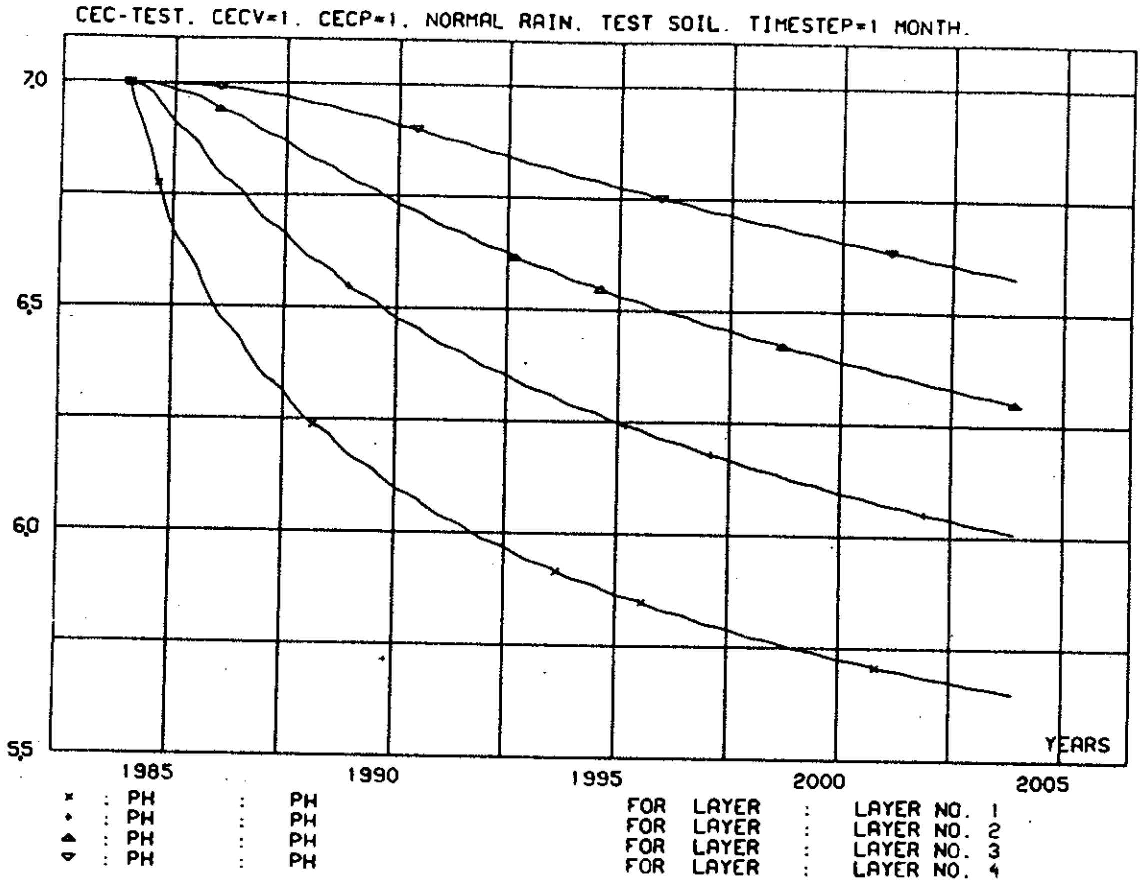


Fig. 5d. pH in a test soil for permanent cation exchange capacity = 1. meq/100 g.

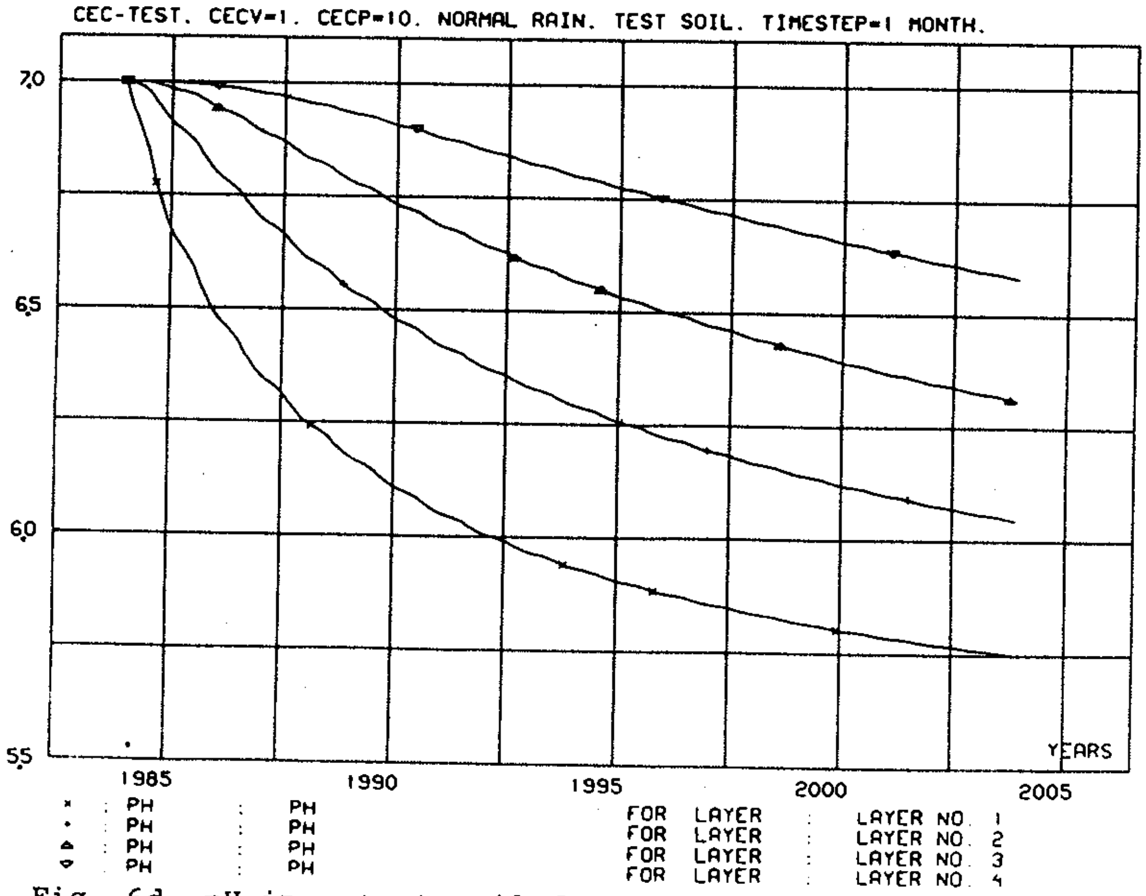


Fig. 6d. pH in a test soil for permanent cation exchange capacity = 10 meq/100 g.

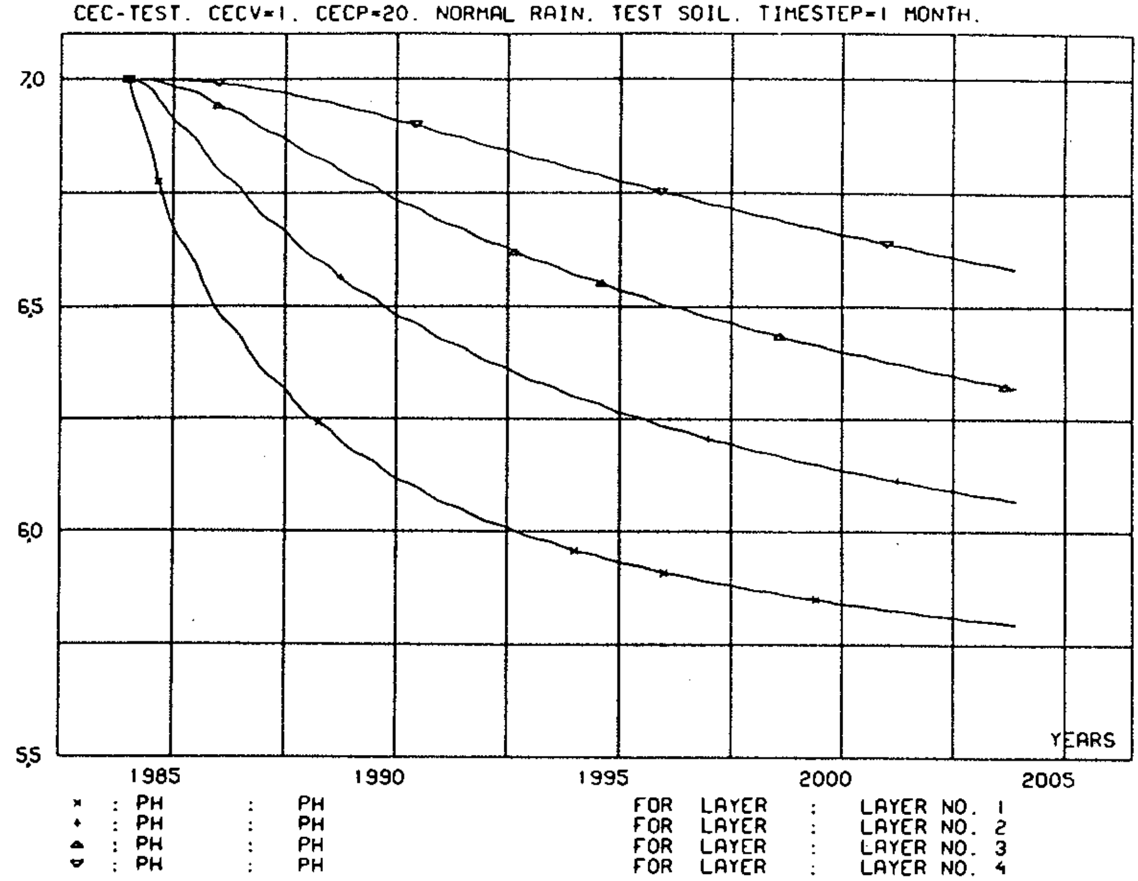


Fig. 7d. pH in a test soil for permanent cation exchange capacity = 20 meq/100 g.

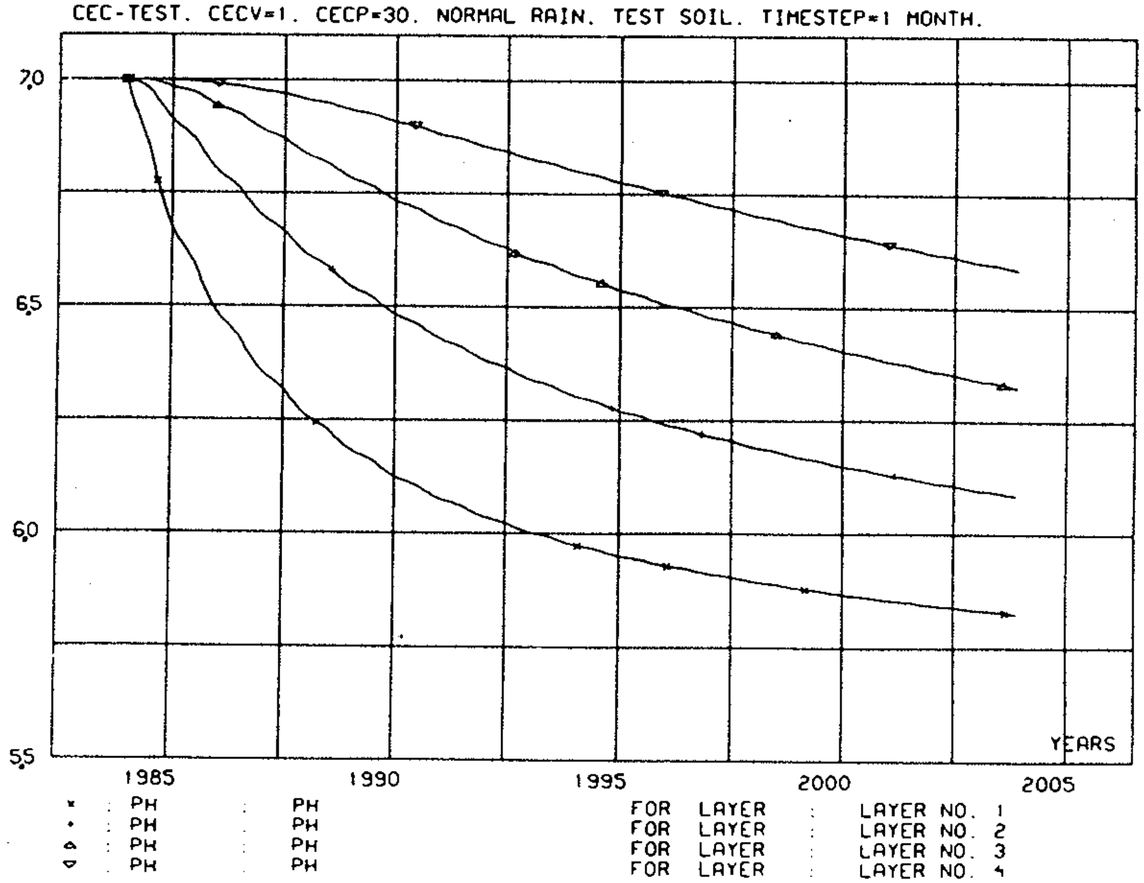


Fig. 8d. pH in a test soil for permanent cation exchange capacity = 30 meq/100 g.

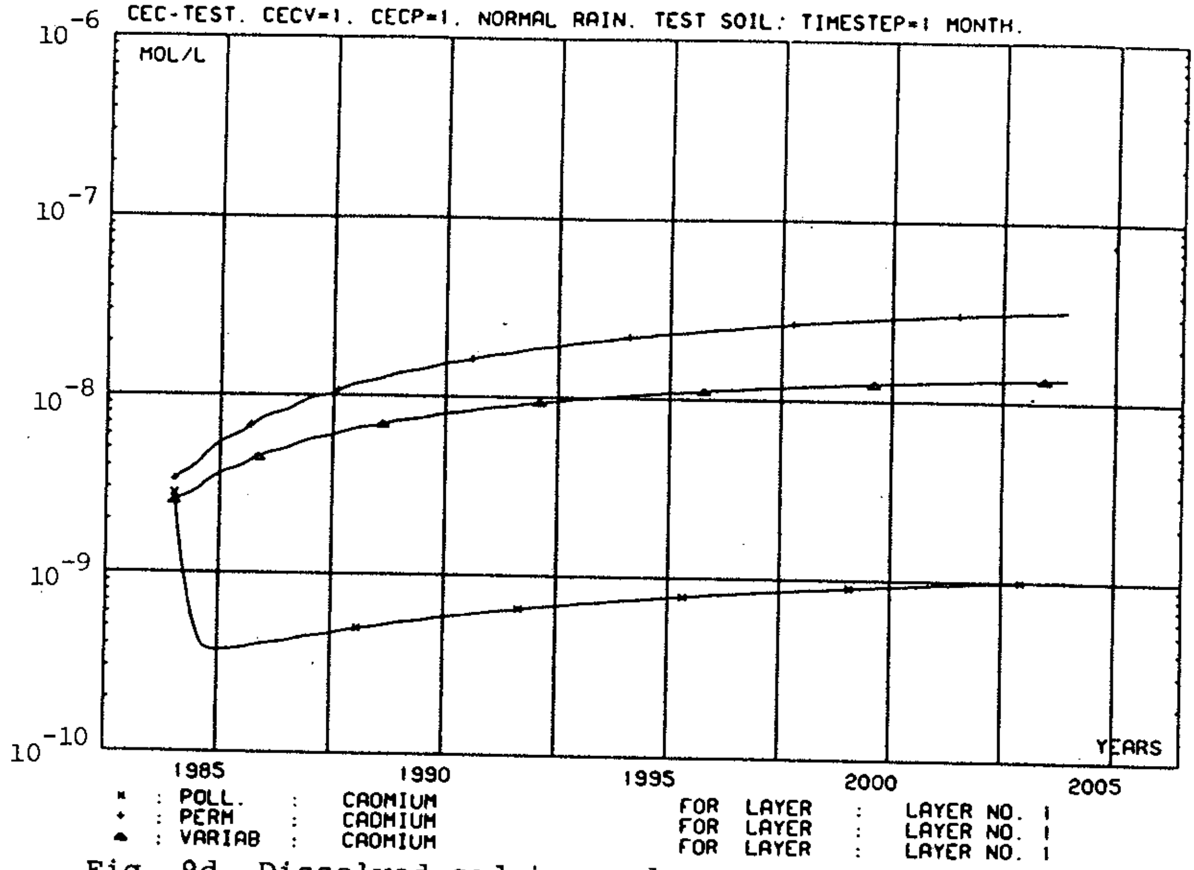


Fig. 9d. Dissolved cadmium and permanent and variable adsorbed. cadmium for permanent cation exchange capacity = 1. meq/100g.

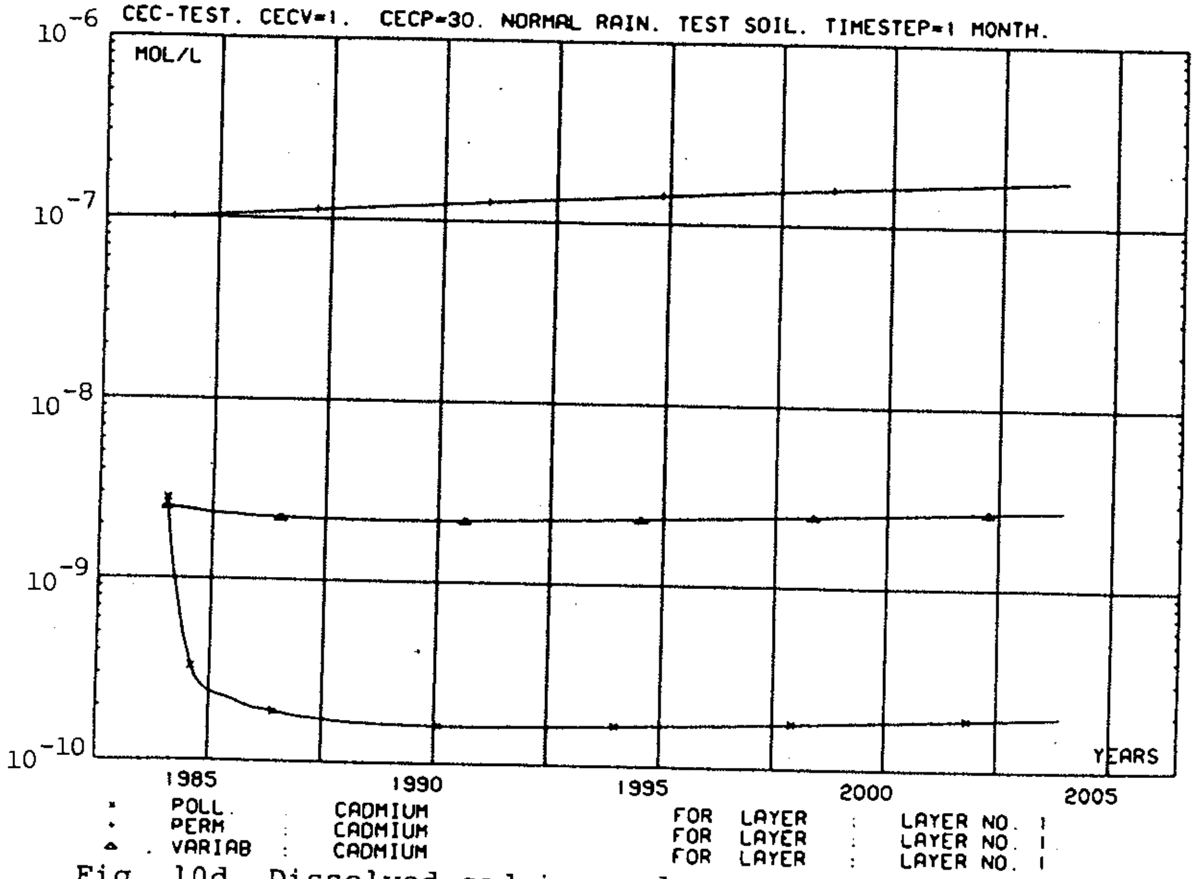


Fig. 10d. Dissolved cadmium and permanent and variable adsorbed cadmium for permanent exchange capacity = 30 meq/100 g.

APPENDIX E

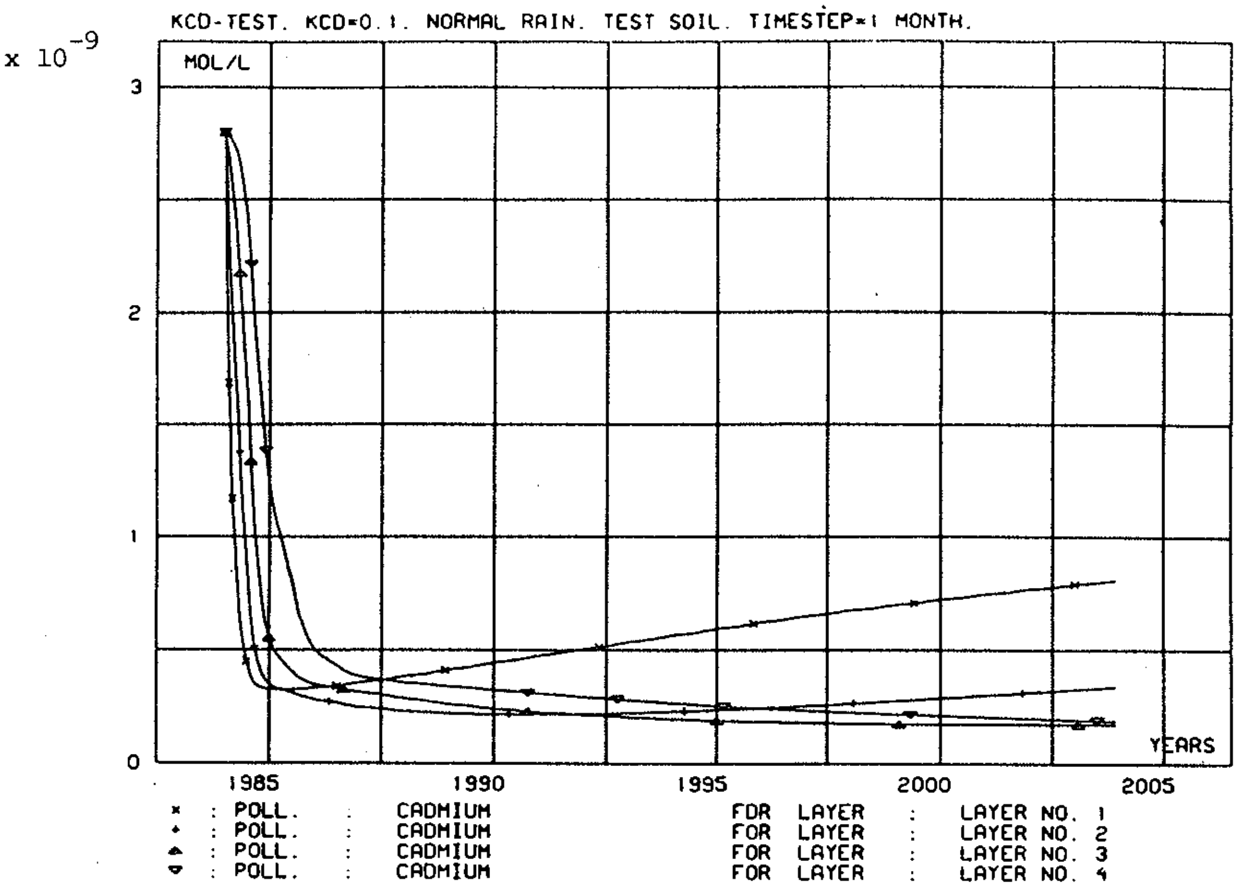


Fig. 1e. Dissolved cadmium for K_{CD} = 0.1.

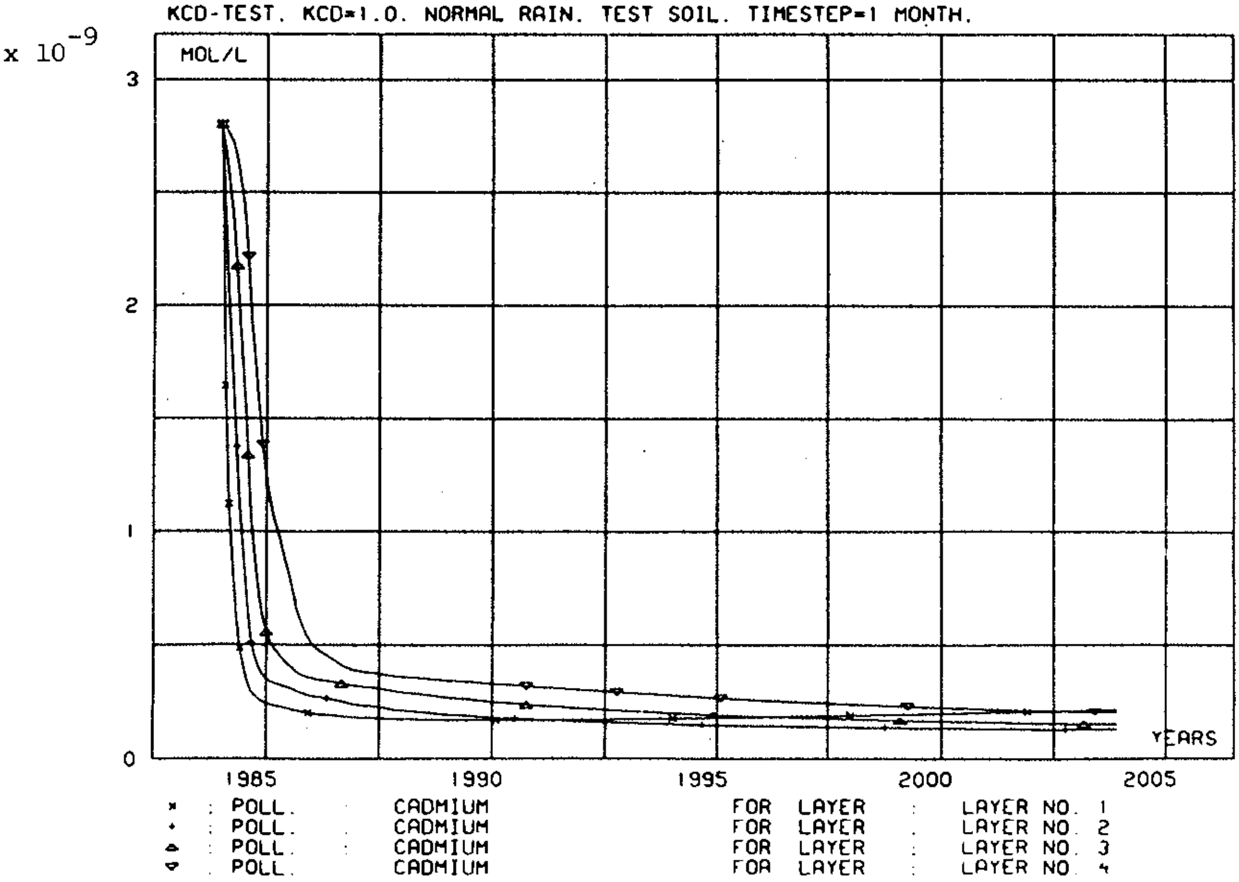
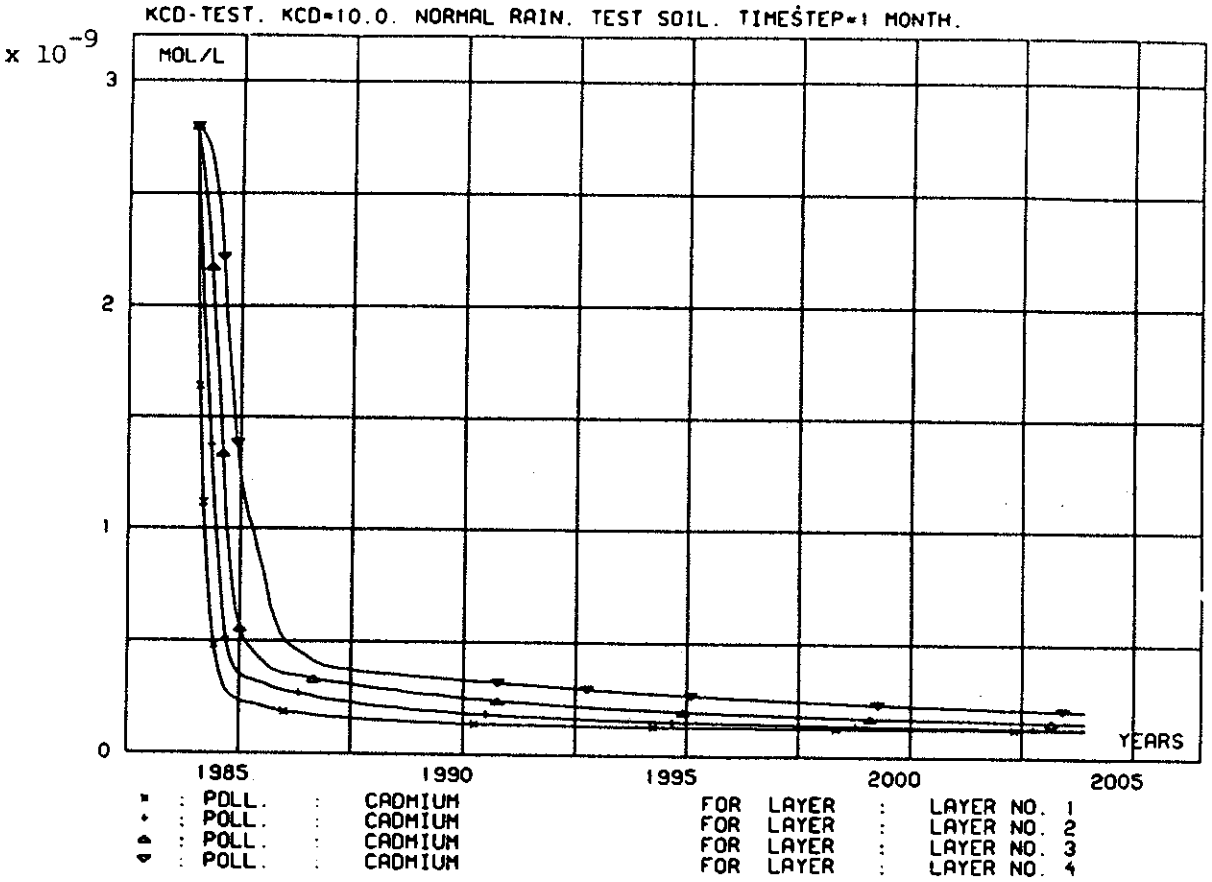


Fig. 2e. Dissolved cadmium for K_{Cd} = 1.0.



<u>Fig. 3e</u>. Dissolved cadmium for $K_{Cd} = 10.0$.

APPENDIX F

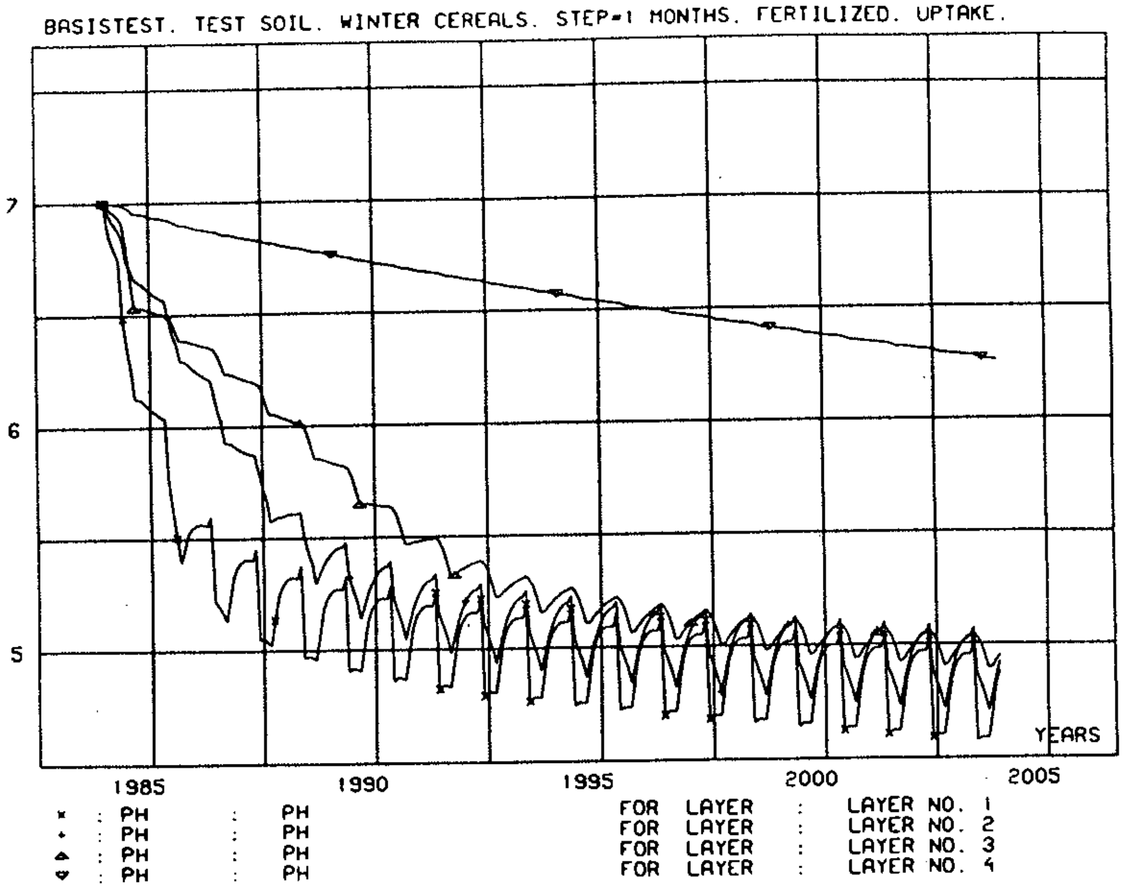


Fig. 1f. pH in a test soil with crops.

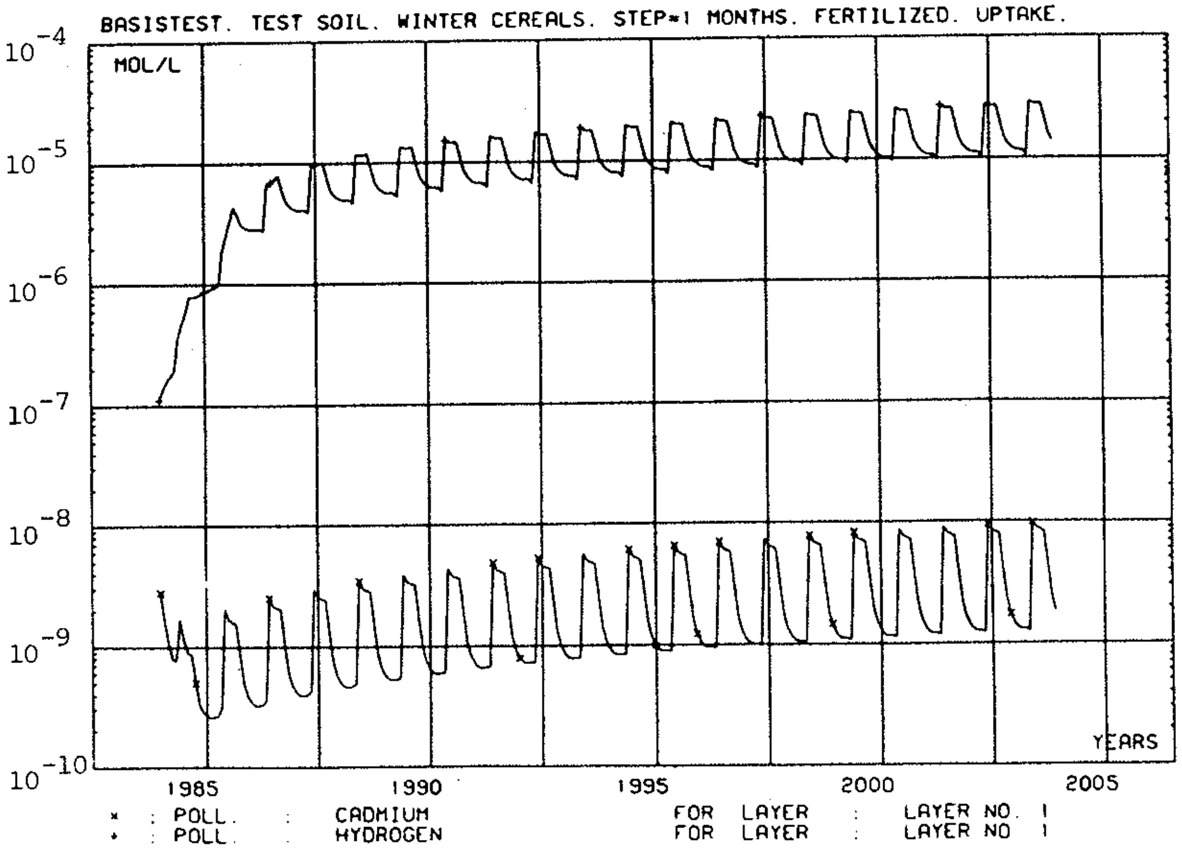


Fig. 2f. Dissolved cadmium and proton concentration in a test soil with crops.

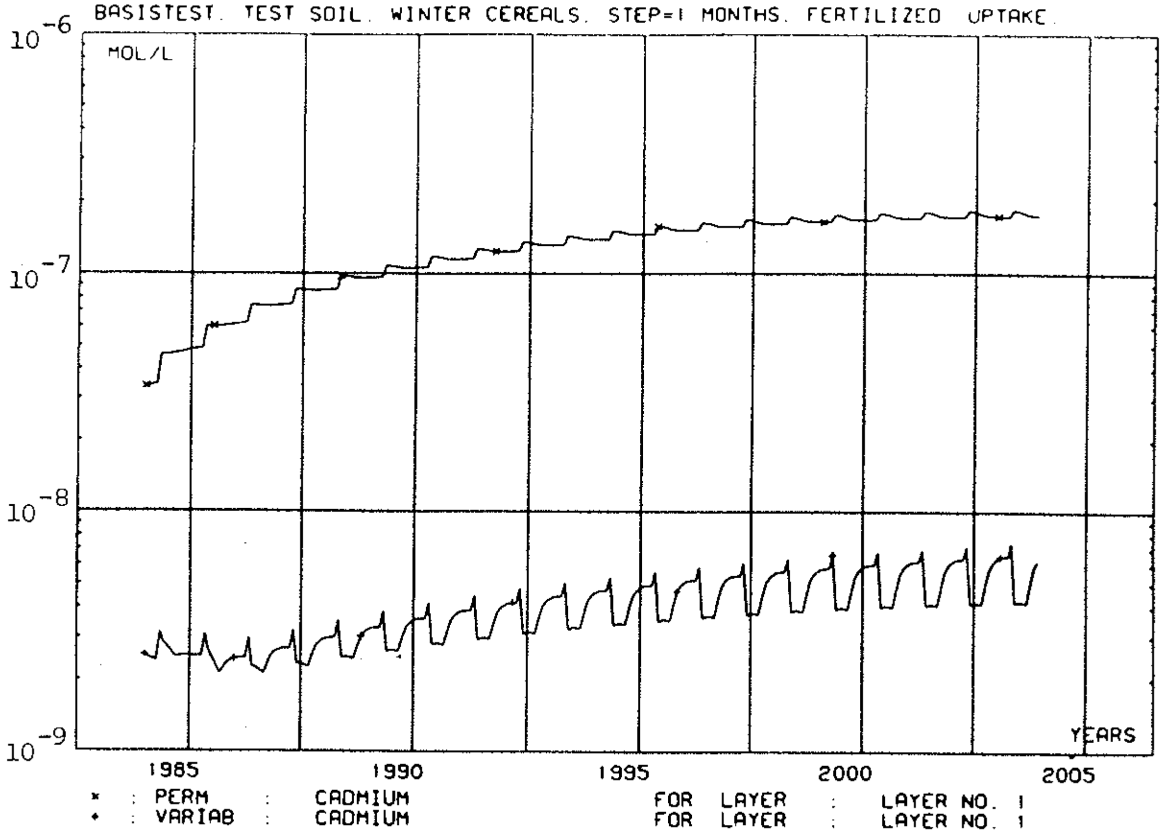


Fig. 3f. Permanent and variable adsorbed cadmium in a test soil with crops.

Tryk: Grafisk Service Center, Risø.

Risø National Laboratory **Risø - M -** 2501

Risø - M - 2501

Title and author(s) ILLUSTRATION OF THE PRESENT CAPABILITIES OF THE ECCES PROGRAM SYSTEM Brian Christensen, Peer Bo Mortensen and Torben Petersen	Date Department or group Energy Technology Group's own registration number(s)
44 pages + tables + illustrations	
Abstract	Copies to

This report describes the status of the development of the ECCES program system. The capabilities of the model are described together with the results of a scenario calculation. Furthermore a series of calculations are shown in order to demonstrate some phenomena concerning the soil chemistry and plant models.

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