

# Working Paper

**A MODEL FOR ANALYZING LAKE WATER ACIDIFICATION  
ON A LARGE REGIONAL SCALE**

**PART 2: REGIONAL APPLICATION**

Juha Kämäri  
Maximilian Posch  
Robert H. Gardner  
Jean-Paul Hettelingh

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WP-86-66

**International Institute for Applied Systems Analysis  
A-2361 Laxenburg, Austria**

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## **PREFACE**

The IIASA "Acid Rain" Project started in 1983 in order to provide the European decision makers with a tool which can be used to evaluate policies for controlling acid rain. This modeling effort is part of the official cooperation between IIASA and the UN Economic Commission of Europe (ECE).

The IIASA model currently contains three linked compartments: Pollution Generation, Atmospheric Processes and Environmental Impacts. Each of these compartments can be filled by different substitutable submodels. The submodels currently available are Energy Pathways and Sulfur Emissions, the EMEP Long Range Transport Model, Forest Soil pH and Lake Acidity. In addition, two submodels are under development: the NO<sub>x</sub> Emissions submodel and the Direct Forest Impacts submodel. The first version of the Lake Acidity submodel was presented in September 1984 in a UNESCO-IHP Workshop in Uppsala, Sweden. Since then several changes have been implemented following the advice of experts. The model structure was documented earlier in Part 1 of this paper. This part describes the application of the Lake Acidity model to numerous lake regions in Fennoscandia, as well as the sensitivity and uncertainty analysis of the model.

Leen Hordijk  
Acid Rain Project Leader

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## ABSTRACT

The International Institute for Applied Systems Analysis is developing a computer model which can be used by decision makers to evaluate policies for controlling the impact of acid rain in Europe. As part of this task, a dynamic model has been developed for describing the processes leading to acidification of surface waters. The modeling philosophy is to use a simplified approach, which is warranted for a broad geographical scope. The simulation model is constructed of several modules, each of them providing an overview of a particular aspect of lake acidification. Because of the very sparse input data available on a large regional scale, a new method is applied for estimating unknown inputs. The model is calibrated to present-day conditions by selecting input combinations from feasible ranges. Monte Carlo techniques are used to determine those combinations of inputs that produce the observed present-day lake acidity distribution, when the model is driven by a specified deposition. The ensembles obtained in the calibration procedure for each lake region are used for the scenario analysis. The usefulness of the method is compared with respect to the traditional *a priori* parameter estimation technique. Results of sensitivity and uncertainty analysis are used to compare model predictions with observed values and to indicate where changes in the distributions of model parameters will affect predictions the most.

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## **PART 2: REGIONAL APPLICATION**

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### **1. INTRODUCTION**

Numerous mathematical models have been developed that all have the potential to estimate the quality of surface water in response to varying atmospheric deposition. All models can be calibrated so that a satisfactory fit with observed data will be obtained. Different models are constructed, however, for different purposes, and therefore, models should be applied only within the limits of their applicability.

First of all, models have been developed for simulating daily variations of water quality in streams, caused by variations in deposition, as well as in catchment hydrology and meteorology (e.g. Christophersen et al. 1982). This kind of model can well be used to analyze the role and importance of catchment processes in determining the short term variation in surface water quality. It has indeed been shown that the characteristics of present-day stream water chemistry can be accounted for by incorporating only a small number of physically realistic processes. Such model however lacks long term processes, which makes it unsuitable for assessing the long term development of surface water quality.

Secondly, simplified equilibrium models have been developed, which allow the estimation of future steady-state chemical composition of lakes resulting from changes in loading of strong acids. These models are either based on observed ionic relationships in present conditions (e.g. Henriksen, 1980), or on the assumption of steady-state chemical weathering (Schnoor et al 1984). The equilibrium models are in fact easier to apply regionally, but still several difficulties remain in their application. The models do not give any information on the time span in which the steady-state condition



will be reached. Also the effect of seasonal acid surges can not be assessed by equilibrium models.

The third type of model utilizes mechanistic process oriented descriptions for hydrology, soil chemistry as well as for stream and lake water quality to provide a link between the time evolution of acidic deposition and the long term surface water acidification (e.g. Chen et al. 1983, Cosby et al. 1985a). It has been shown that the observed surface water chemistry can be reproduced by models that largely retain the simplicity of the equilibrium models but that have mechanistic process-oriented explanations in their structure (Cosby et al. 1985a, Kämäri et al. 1985b). This simplified approach also allows a theoretical basis for establishing confidence in the estimates.

To date, mechanistic models have been applied only on single catchments. Descriptions on quantitative consequences of alternative scenarios can assist in formulating policies for emission control. From a decision makers point of view, however, the behavior of a single catchment is not very interesting. The assessment should investigate broad scale aspects of alternative policy formulations, and thus analyze the behavior of as many catchments as possible. As an output, the model should produce well defined illustrative information which can easily be related to the effectiveness of the energy-emission scenario being selected.

To meet the need for regional prediction, simplified equilibrium models are being used in the U.S. integrated assessment model of the acid deposition problem (see Rubin et al. 1984). The regional distribution of lake alkalinity is represented by a three-parameter log-normal distribution. The method has been used to estimate the effect of changes in acid deposition on the mean and variance of the regional distribution (Small and Sutton 1986). The approach is similar to that by Jones et al. (1984), who have used survey information to synthesize the behavior of typical lake types of the region using the modified empirical steady-state model by Henriksen (1980) and Wright (1983). The dynamic upstream models describing the pollutant generation as well as the pollutant transport require, however, also dynamic models for describing the environmental impact to be able to give estimates on the time scales of the responses. In this paper a method is introduced for applying a simple process oriented dynamic lake acidification model on a large regional scale.

## 2. METHODS FOR REGIONAL APPLICATION

### 2.1. Method for Scenario Analysis

The regional scenario analysis assessing potential surface water impacts might be performed in two ways: 1) The catchment model can be used to analyze changes over time in the chemistry of each lake in the district. In this mode, the parameters of the model must be developed for each lake in the region by using specific catchment- and soil information (see Kämäri et al. 1985a) and the regional effects estimated by predicting the behavior of each lake in the region; or 2) The parameters of the catchment model can be regionalized by specifying the probability distribution of model parameters developed from the expected range of values for typical lakes in that region. In this study a Monte Carlo parameter estimation procedure has been adopted to develop appropriate distributions for this second approach.

The Monte Carlo method is a trial-and-error procedure for the solution of the inverse problem, i.e. for estimating the poorly known input values from the required output. In the regionalized model, the Monte Carlo method is used to determine the combinations of inputs that produce an acceptable distribution of output variables, observed in the study region. For all inputs, ranges are chosen broad enough so that any reasonable value for an input can be selected. Monte Carlo simulations are then carried out by randomly selecting a set of input values from these designated ranges and integrating the equations from 1960 on using this particular set of values. A subset of accepted input values corresponding to the actual observed present-day frequency distribution in 1980 in each lake region, is obtained.

Mathematically this procedure can be described as follows. The adopted model structure can be represented by a vector function  $f = (f_1, \dots, f_m)$ . The arguments of this function are the input and parameter values driving the model, say  $x = (x_1, \dots, x_n)$  (e.g.  $x_1$  = lake size,  $x_2$  = catchment size, ..., etc.) and time  $t$ . With  $y = (y_1, \dots, y_m)$  we denote the output of a model run, e.g. alkalinity, lake-water pH, ..., etc.

$$y = f(x, t) \quad (1a)$$

or, writing Eq.1a for each component,

$$\begin{aligned} y_1 &= f_1(x_1, \dots, x_n, t) \\ &\dots \\ &\dots \\ y_m &= f_m(x_1, \dots, x_n, t) \end{aligned} \quad (1b)$$

Instead of taking fixed input values  $x$  and running the model once to obtain the output (prediction) at time  $t$ , one allows the input values to vary within an interval,  $x_k^{\min} \leq x_k \leq x_k^{\max}$ ,  $k = 1, \dots, n$ , where the lower and upper bounds are estimated from the catchment characteristics of the region studied. To put it precisely, each input parameter is randomized with a distribution  $p_k$ ,  $k = 1, \dots, n$  obeying

$$p_k(x_k) = 0 \quad \text{if } x_k < x_k^{\min} \quad \text{or } x_k > x_k^{\max} \quad (2a)$$

and  $\int_a^b p_k(x) dx$  is the probability that  $x_k$  lies in the interval  $[a, b]$ . Obviously

$$\int_{x_k^{\min}}^{x_k^{\max}} p_k(x) dx = 1 \quad \text{for } k = 1, \dots, n \quad (2b)$$

The frequency distributions  $p_k$  represent the distribution of the parameters  $x_k$  in the region as close as possible. In case of a poorly known input parameter a uniform distribution over  $[x_k^{\min}, x_k^{\max}]$  is chosen, where the boundaries are wide enough to encompass any feasible value in the region under consideration.

To be able to apply the Monte-Carlo procedure the distribution of the output values  $y$  at a certain point in time  $t_1$ , say  $q_l$ ,  $l = 1, \dots, m$ , have to be known from measurements; i.e. we know

$$\int_{y_l^{\min}}^{y_l^{\max}} q_l(y) dy = 1 \quad \text{for } l = 1, \dots, m \quad (3)$$

For the description of the procedure used to solve the inverse problem, i.e. to determine the input parameter distributions for projections, we consider only one output value  $y$  (i.e.  $m = 1$ ; say lake-water pH) and furthermore we assume that the measured distribution at  $t_1$  is a discrete one ( $I$  ... number of classes,  $\eta_i$  ... class boundaries)

$$q(y) = \begin{cases} q_i & \text{for } \eta_{i-1} < y \leq \eta_i \quad i=1, \dots, I \\ 0 & \text{else} \end{cases} \quad (4a)$$

with

$$\sum_{i=1}^I q_i (\eta_i - \eta_{i-1}) = 1 \quad (4b)$$

and

$$\eta_0 = y^{\min} \quad \text{and} \quad \eta_I = y^{\max} \quad (4c)$$

(the index 1 on  $q$  has been dropped for convenience.) Actually, the assumption of a discrete distribution is not very stringent, since a) measurements are always given as histograms, and b) any continuous distribution can be approximated by a discrete one.

In order to derive "acceptable" input parameter distributions the model is run many times, each time with a new randomly selected input vector  $x$ , where the random selection is performed according to the distributions  $p_k$ . Let  $P = \{x^{(1)}, \dots, x^{(N)}\}$  be the set of these random vectors  $x$  and  $Q = \{y^{(1)}, \dots, y^{(N)}\}$  the set of output values of these runs at time  $t_1$ . These  $N$  output values are classified according to the classes defined in Eq.4a. Let  $N_i$  be the number of realizations with  $\eta_{i-1} < y \leq \eta_i$  with  $y \in Q$  (clearly  $\sum_i N_i = N$ ). Monte-Carlo runs are performed until  $N_i \geq N_0 q_i$  for all  $i = 1, \dots, I$ , where  $N_0$  is a preselected number of runs to be accepted. In this way a subset  $Q_0 = \{y_1, \dots, y_{N_0}\}$  of  $Q$  is selected<sup>3</sup>, so that there are  $N_0 q_i$  output values with  $\eta_{i-1} < y \leq \eta_i$  ( $i = 1, \dots, I$ ) with  $y \in Q_0$ . To this subset  $Q_0$  corresponds a subset  $P_0 = \{x_1, \dots, x_{N_0}\}$  of  $P$  of accepted input vectors  $x$ . From this set of accepted input vectors "new" input parameter distributions  $p_k^0$ ,  $k = 1, \dots, n$  can be derived; and these distributions are used for projections, i.e. for computing  $y$ -values for  $t > t_1$ .

Assuming that the set of input values obtained in the calibration is representative of real catchments in the study region, this ensemble can be used for the scenario analysis of the response of lake systems to different patterns in acidic deposition.

## 2.2. Method for Sensitivity and Uncertainty Analysis

Several programs which have been specifically developed for efficient Monte Carlo sampling of model parameters (Gardner et al. 1983) and the analysis of statistical relationships between parameters and predictions (Gardner and Trabalka, 1985) were adapted to IIASA's computers and applied to the lake model, Region 1 of Finland. These programs are linked together in a system called PRISM. PRISM has been extensively applied to a variety of models and environmental assessment problems (e.g. Gardner and Trabalka 1985, Bartell et al. 1983, Hoffman and Gardner 1983, Hoffman, Gardner and Bartell 1986).

PRISM is composed of three parts:

<sup>3</sup> Note that  $y_i$  is the  $i$ -th value of the set  $Q$ , not the  $i$ -th component of a vector  $y$ .

- (1) PRISM1 produces a set of model parameters from pre-specified distributions and correlations;

For each of the  $n$  input parameters of  $\mathbf{x}$ , the type of frequency distribution, the mean, the standard deviation, the minimum- and the maximum values are read. The range of values of the input parameters is such that the number of intervals equals the number of parameter sets to be used for the simulations, here  $N$ . This ensures the  $N$  segments to be equally distributed over the entire value range for every parameter. This is done by means of a matrix containing  $N$  sets of  $n$  normal random numbers, which are ranked from one to  $N$ . The ranks are used to denominate the  $N$  segments within every parameter value range.

By specifying a variance-covariance matrix, the vectors  $\mathbf{x}$  may be independently selected and correlated thus obtaining correlations of ranks of parameter values. As a matter of fact, by pre-specifying a correlation between two parameters, a correlation of the ranks of the final output values will be produced. In PRISM1, a procedure recommended by Iman and Conover (1982), has been implemented to reduce the sampling errors associated with the Monte Carlo estimation of correlations to a minimum.

PRISM1 may be used to perform a sensitivity analysis by varying all the input parameters by one percent of their mean value or perform an uncertainty analysis by specifying probability distributions for each parameter (Gardner, 1984).

- (2) PRISM2 runs the model to obtain the unique set of predictions associated with each parameter set, that has been obtained from PRISM1. PRISM2 is in fact an interface between the output of PRISM1, the lake model and PRISM3.
- (3) PRISM3 finally provides a statistical characterization of the variability of the model output and estimates the statistical relationships between model parameters and model predictions. For each model output the arithmetic mean, the variance, the standard deviation, the coefficient of variation and the geometric mean are computed. Secondly a listing of correlations between and among the model parameters and responses, above a user selected threshold, is provided. Lastly a stepwise regression analysis, using a standard FORTRAN package (IMSL 1980), is performed in PRISM3 between model responses and model parameters thus providing an order of importance of the set of input parameters (see Gardner, et al. 1983 for program documentation and Gardner and Trabalka 1985 for details of the statistical methods).

PRISM has been used to analyze the behavior of the RAINS lake model for input data of Region 1 of Finland, results of which are discussed in the next chapter.

### 3. MODEL ANALYSIS

#### 3.1. Model Parameters and their Distributions

A series of Monte Carlo simulations were performed to (1) estimate the effect that uncertainties in model parameters have on model predictions and (2) define the changes in parameter distributions which may be necessary to match the model predictions with measured values. Information concerning parameter sensitivities and distributional changes is important because it provides a means of evaluating the suitability of model simulations to represent a particular region of the landscape and a means of identifying those variables for which additional data will most improve model results.

The regional version of the lake model requires that the input of parameters be specified as probability distributions. However, the statistical descriptors of these distributions (e.g. mean, variance, etc.) are generally unknown. The reasons for this uncertainty are the lack of adequate data for all the regions, the uncertainties associated with those observations or experiments that are available, and uncertainties and errors associated with the process of extrapolating data to a regional level. For each parameter, these uncertainties have been taken into account by specifying a distribution whose range of values is large enough to include all possible parameter values.

The model under study contains as a total about 50 parameters, input variables, driving forces or initial conditions, which have to be estimated on the basis of rather uncertain *a priori* information. All these inputs will, for simplicity, be called parameters in the following. Some parameters have been lumped so that the number of parameters included in the evaluation is 44. These parameters and their definitions are listed in Table 1.

In principle, in order to define ranges or frequency distributions for parameters it is required that all such inputs are physically meaningful and measurable so that those ranges can be found. In our case, we had information to prespecify frequency distributions for nine parameters: AREAL, RATCL, LDEPT, SOILT, SLOPE, SIBRC, CEC, BASEA, FCAP. The meteorologic parameters, TEM01 to TEM12 and PRE01 to PRE12, reflected the spatial variability within the region of concern of long-term means of monthly air temperature and precipitation. The ranges for these prespecified distributions are listed in Section 4.1. All other parameters were given quite wide ranges. The allowable ranges were either based on the conjecture of the regional range of variation of the parameter, implying that the minimum and maximum of the existing conditions were estimated, or on the mean value, obtained from the literature, around which a feasible range was assumed.

Table 1: Model parameters used in sensitivity and uncertainty analysis.

No	Name	Definition*	Explanation
1	AREAL	$A_l$	Lake surface area
2	RATCL	$A_l / A_c$	Ratio of lake area to catchment area
3	LDEPT	$z$	Lake depth
4	SOILT	$z_A + z_B$	Total soil thickness (sum of A and B layers)
5	SLOPE	$S$	Mean surface slope
6	SIBRC	$b\tau_g$	Silicate buffer rate
7	CEC	$CEC_{tot}$	Total cation exchange capacity
8	BASEA	$BC_{CE,A} / CEC_{tot}$	Base saturation of A-layer
9	PCAP	$\theta_f$	Soil moisture content at field capacity
10	INPH	$pH$	Measured pH in 1980
11-22	TEM01,...,TEM12	$T_1, \dots, T_{12}$	Monthly mean air temperature
23-34	PRE01,...,PRE12	$P_1, \dots, P_{12}$	Monthly mean precipitation
35	STFAC	$\psi$	Factor of deposition on forest vs. open land
36	BASEB	$BC_{CE,B} / CEC_{tot}$	Base saturation of B-layer
37	FSAT	$\theta_s$	Soil moisture content at saturation
38	RZO	$z_o$	Depth of lake mixing layer
39	EPSEV	$c$	Evapotranspiration coefficient
40	TLOW	$T_s$	Threshold temperature for snow
41	THIGH	$T_r$	Threshold temperature for rain
42	MELTR	$\beta$	Melting rate coefficient
43	CALC	$K_H K_1 p \omega_2$	Lumped equilibrium constant for inorganic carbon species
44	COND	$K_s$	Hydraulic conductivity at saturation

\*Definitions as given in Kämäri et al. (1985b).

### 3.2. Model Sensitivity and Uncertainty

A sensitivity- and an uncertainty analysis have been performed on data of Region 1 of Finland. The input format needed to perform an uncertainty analysis is displayed in Table 2 for ten parameters that proved to be the most important as determined by the sensitivity and uncertainty analysis given in Table 3.

Estimates of the differential sensitivity (Tomovic and Vukobratovic 1972) of model predictions to changes in the model parameters can be estimated by Monte Carlo methods when the variance of all parameters is set to 1% of their nominal value (Gardner 1984). This numerical estimate of sensitivity is useful because it measures the direct effect of each parameter on model results without the effect of nonlinearities in the model and interactions between parameters confounding the analysis.

Table 3 presents the results of the sensitivity analysis with the ranking of parameter importance (column 1) based on the proportion of model variability explained by that parameter (column 2). Model predictions are most sensitive to SOILT, with this parameter explaining over 35% of the variability in predicted 1980 pH levels. Predictions are less sensitive to BASEB and SIBRC with these parameters explaining 15% and 14%, respectively, of the

Table 2: Descriptions of the Statistical Distributions, the mean, the standard deviation, the coefficient of variation (C.V.), the minimum and the maximum for 10 of 44 Model Parameters.

Name	Distribution Type	Mean	Standard Deviation	C.V.	Minimum	Maximum
SOILT	uniform	2.6	1.4	53	0.2	5.0
BASEB	uniform	0.45	0.029	6	0.4	0.5
SIBRC	histogram	0.0034	0.0014	41	0.0017	0.0083
MELTR	normal	0.0021	0.0032	152	0.0	0.37
EPSEV	normal	0.0039	0.00058	15	0.002	0.0053
FCAP	histogram	0.23	0.092	40	0.22	0.4
RATCL	uniform	8.5	3.8	44	2.0	15.0
COND	uniform	332.	192.	58	0.0	665.0
LDEPT	histogram	7.7	8.4	110	0.8	100.0
BASEA	histogram	0.28	0.28	97	0.005	1.0

total variability. Parameters MELTR, EPSEV, FCAP and COND explain less than 10% of the variability of results. The remaining 38 parameters are relatively unimportant, affecting model predictions by less than 1%.

Table 3 also lists the results of the uncertainty analysis (columns 3 and 4). The differences between the sensitivity and uncertainties are primarily due to the large differences in variability of a few parameters. Table 1 shows that SOILT has a moderately large coefficient of variation (53%) and this combined with a high sensitivity results in SOILT producing over 58% of the variance in predicted pH levels in 1980. Differences in the relative variability of BASEB and SIBRC also explains why their effect on model uncertainty is not the same as their sensitivities. Although BASEB and SIBRC have similar sensitivities, SIBRC is more than six times as variable as BASEB (Table 2). The result is that over 9% of the uncertainty in model predictions is due to SIBRC, while BASEB causes less than a 1% change in model results. The sensitivities of RATCL, LDEPT and BASEA are all relatively small (<1%), but when combined with rather large uncertainties, these parameters explain from 3% to 4% of the variability in the predicted pH levels. The regression statistics that these results are based on show that the direct effect of parameter variability can explain over 80% of the variability in model results ( $R^2=0.81$ ). Thus, nonlinear behavior of the model and interactions among the parameters causes less than 20% of the total variance of estimated 1980 lake pH levels.

The estimates of the percent effects for SOILT and SIBRC given in column 4 of Table 3 indicate the possible improvement in predictions which might result from reductions in the variability of these two parameters. For instance, a 50% reduction in the variability of SOILT will cause the variability in predicted pH levels in 1980 to drop by at least 25%, while the same degree of improvement in SIBRC would improve model estimates by less than



**Table 3:** Results of sensitivity and uncertainty analysis for 10 model parameters. The ranks given in columns 1 and 3 are based on the magnitude of the effect of that parameter on predicted pH values in 1980. The percent contributed by each parameter is estimated from multiple regression methods as: (partial sum of squares / total sum of squares \* 100). Sensitivities are determined by simultaneous variation of all 44 parameters by 1% of the mean value (Table 2). Values for the uncertainty analysis are determined by simultaneous variation of parameters from prespecified frequency distributions (Table 2). Values less than 1% are not shown.

Name	Sensitivity		Uncertainty	
	Rank	Percent	Rank	Percent
SOILT	1	35	1	58
BASEB	2	15	21	
SIBRC	3	14	2	9
MELTR	4	8	37	
EPSEV	5	8	6	
FCAP	6	3	34	
RATCL	20		3	4
COND	7	3	16	
LDEPT	18		4	3
BASEA	13		5	3

5%. Thus, further improvements (i.e. reductions in uncertainties) of other parameters will have relatively little effect on results unless the variability of SOILT and SIBRC are reduced.

### 3.3. Comparison of Simulation Results with Measurements

The data from measurements of pH in 303 lakes in Region 1 of Finland in 1980 provides the basis for evaluation of model results and adjustment of a few parameters which most affect model predictions. We developed a systematic procedure to use this information which involves: (1) determination of the statistical characteristics of the measured pH levels; (2) development of *a priori* criteria for comparing simulations and data and retaining the subset of simulations which satisfy these criteria; (3) examination of the distributional characteristics of parameters associated with this subset of simulations; (4) estimation of new statistical distributions for parameters identified by sensitivity and uncertainty analysis to be important in predicting pH levels in 1980; and (5) comparison of the results of a new series of Monte Carlo simulations against the original data to evaluate the degree of improvement.

This process of selecting the best subset of simulations (termed "filtering" in the sequel) is based on the rationale that model simulations which begin in 1960 and produce unsatisfactory results in 1980 (i.e. fail to meet the pre-established criteria) should not be used to make future predictions of effects of sulfur deposition. However, the information provided by the subset of accepted simulations may provide a means of reducing the variances of critical parameters and thus reducing the uncertainty associated with the model results. Although all 44 parameters will show some change in the statistics of their distributions as a result of the filtering process, we restrict our interest to those parameters which have been shown to be important (i.e. SOILT and SIBRC, Table 3).

Table 4: Statistical summary of lake pH values in 1980. The first column of pH values was estimated from measurements of 303 lakes in Region 1 of Finland. Column 2 gives the statistical characteristics of predicted pH values for 1980 based on 500 Monte Carlo iterations with 44 parameters subject to random variation (Table 2). The third column gives the statistical characteristics of those simulations (104 out of 500) which satisfied the filtering criteria. The final column shows the statistical characteristics of 100 simulations with modified values for the parameters SOILT and SIBRC (Table 5).

Statistic	Actual distribution	Simulation results	After filtering	Results with new parameters
Mean	5.8	6.0	5.8	5.6
Std. Dev.	0.69	1.2	0.9	1.3
C.V.	12.	20.	15.	22.
Minimum	4.0	3.8	4.0	3.9
2.5 %tile	4.4	3.99	4.2	3.9
25 %tile	5.3	4.7	5.2	4.2
50 %tile	5.9	6.5	5.8	6.0
75 %tile	6.4	7.0	6.3	6.8
97.5%tile	6.9	7.4	7.3	7.5
Maximum	7.1	7.7	7.7	7.4

Column 1 of Table 4 presents the statistical characteristics of the 303 lake samples. The mean value of measured lake pH was 5.8 with a coefficient of variation of 12%. The minimum and maximum pH level for these observations is 4.0 and 7.1, respectively. We selected five intervals between these limits to empirically characterize the frequency distribution of measured pH values. The limits of each interval were set so that the relative frequencies were approximately equal (the limits were 4.0 to 5.1, 5.1 to 5.6, 5.6 to 6.0, 6.0 to 6.4 and 6.4 to 8.0 with observed frequencies of 0.21, 0.19, 0.20, 0.20 and 0.20, respectively). Before the simulations were performed, two criteria of comparison were developed from this data: (1) the simulations must produce pH levels in 1980 that lie within the range 4.0 to 7.1;

and (2) the relative frequencies of the subset of satisfactory simulations must match those of the data.

Five hundred Monte Carlo simulations were performed and the results compared with these criteria. Column 2 of Table 4 presents the statistical characteristics of these simulations before filtering. The agreement between model results and data is quite good with the mean value slightly higher (6.0 vs. 5.8) and the variance of the simulations somewhat larger than that of the data (1.2 vs. 0.69). Application of the first criterion resulted in the elimination of 13 simulations out of 500, i.e. 3% were rejected because they were outside the limits established by the data. The application of the second criterion revealed that the relative frequency of predicted pH values was uneven with only 4% of the simulations falling between 5.1 and 5.6, while 19% of the measured values fall into this interval. The adjustments necessary to obtain the desired frequency distribution requires the rejection of 383 additional simulations. The statistical characteristics of the final 104 filtered simulations (Column 3 of Table 4) show that the application of these criteria resulted in an improvement in the mean and reduction in the variance as well as a general improvement in the lower percentiles of the pH distribution.

Table 5: Comparison of the statistical characteristics of SOILT and SIBRC before and after the filtering procedure. The columns indicated with "before" give the statistical characteristics of SOILT and SIBRC used to generate 500 Monte Carlo simulations. The columns indicated with "after" are the statistical characteristics of the subset of simulations (104 out of 500) which satisfied the filtering criteria.

<b>Statistic</b>	<b>SOILT before</b>	<b>SOILT after</b>	<b>SIBRC before</b>	<b>SIBRC after</b>
Mean	2.6	2.3	0.0033	0.0031
Std. Dev.	1.4	1.3	0.0014	0.0014
C.V.	53.0	53.9	41.0	45.0
Minimum	0.20	0.24	0.0017	0.0017
2.5%tile	0.32	0.36	0.0017	0.0017
25 %tile	1.4	1.25	0.0024	0.0022
50 %tile	2.6	2.2	0.0031	0.0028
75 %tile	3.8	3.5	0.0038	0.0034
97.5%tile	4.9	4.6	0.0076	0.0077
Maximum	5.0	4.7	0.0083	0.0073

The changes in statistical characteristics of SOILT and SIBRC as a result of the filtering process are slight (Table 5) with reduction by 12% in the mean of SOILT as the most evident effect. The consequences of these changes in SOILT and SIBRC were determined by using the statistics shown in Columns 2 and 4 of Table 5 as an input for a new set of Monte Carlo simulations. The results (Column 4 of Table 4) show a 7% reduction in the mean of

the predicted 1980 pH levels, as compared to the original simulations (Column 2 of Table 5), and a slight improvement of the overall distribution of simulated pH values. It is apparent that the general fit of the model to the data of Region 1 is rather good and, in spite of the elimination of 75% of the simulations by the filtering criteria, the process does not dramatically improve the results. However, it is also clear, that adjustments to SOILT and SIBRC, although slight, do achieve the desired result. Additional information from actual measurements for these two key parameters would be desirable to further reduce the uncertainties associated with the lake model.

The capability of the model, driven without filtering parameters out of the prespecified parameter distributions (see Table 2), to produce observed regional lake acidity patterns varies from region to region. This tendency is demonstrated in Figure 1, in which the measured pH distributions for all five Finnish lake regions are displayed side by side with the pH distributions that were obtained from 100 20-year Monte Carlo runs using prespecified parameter distributions as sources of inputs. The results in Figure 1 suggest that for some regions there was better *a priori* information for the inputs than for others. For all regions it seemed, however, that the model output adequately covered the whole range of observations. This in turn suggested that the prespecified parameter distributions were defined broad enough so that any realistic combination of parameters could be sampled in the Monte Carlo runs.

#### 4. REGIONAL APPLICATION

##### 4.1. Data

No calibration would be necessary if it was known that the model accurately represented the behavior of the catchment and if the *a priori* information on the shape of the distributions for all parameters, initial conditions and catchment characteristics was correct. The model would produce reliable distributions of the projections. The data, however, available on a large regional scale like Europe is characterized by a high degree of heterogeneity and generalization. The results of the analyses show that for some regions the observed lake pH distribution could quite easily be generated, but for some regions, there was substantial difference between the simulations and the measurements. Therefore, to enable more credible input combinations to be generated, a formal approach was formulated for filtering out the undesired inputs (see Section 2). This filtering procedure resulted in a rejection of a number of those random ensembles of parameters that are produced too frequently with the prespecified input frequency distributions. This procedure changes the shape of the input distributions to more accurately reflect the information available from available observations.

The above initialization of the model for scenario analysis, that is scaling up the catchment model to a regional level, has several preparatory steps. First of all, ranges or distributions for unknown parameters were selected. In the estimation procedure, best available information and best

guesses for the input distributions were used as a starting point. Then for the model output, a target distribution was specified on the basis of a large number of water quality observations. Finally, the filtering procedure was applied. To start with, frequency distributions were selected independently for the following twelve input and output parameters.

1. *Lake surface area* in Fennoscandia (Finland and Scandinavia) can vary anywhere from close to zero to over thousand  $km^2$ . Usually a freshwater reservoir is termed a lake only if its surface area exceeds  $0.01 km^2$ .
2. *Lake catchment area to lake surface area ratio* provides an estimate for the proportion of precipitation and air pollutants being deposited directly on the lake surface. The ratio can range from 1.2 to several hundreds, being, however, most commonly between 2. and 15.
3. *Mean lake depth* is a morphometric parameter that for individual lakes can be determined from bathymetric maps. Lake volume ( $V_l$ ) is calculated from the mean lake depth simply by  $V_l = z \cdot A_l$  (see Table 1). The mean lake depth can have a large range of variation, but in Fennoscandia it usually ranges from 1 m to 100 m.
4. *Mean catchment soil thickness* is used to determine the volumes of the two soil reservoirs, and the capacities of the soil buffering processes. It is in most areas of Fennoscandia in the order of a few meters to a few tens of meters.
5. *Mean surface slope of the terrestrial catchments* vary from even terrains ( $0. m m^{-1}$ ) to terrains varying in altitude, undulating catchments ( $10. \dots 20. m m^{-1}$ ), and finally to mountainous catchment areas with steep slopes ( $>30. m m^{-1}$ ).
6. *Silicate buffer rate*, i.e. the weathering rate of the silicate minerals depends on the rock type as well as on the physico-chemical conditions in soil. Literature values for the long-term silicate weathering rate range from  $0.02$  to  $0.2 eq m^{-3} yr^{-1}$ .
7. *Total cation exchange capacity* refers to the maximum capacity of positively charged cations the soil can adsorb to its negatively charged colloids or mineral particles. Cation exchange capacity thus depends largely on the texture as well as on the humus content of the soil, being in the order of  $10. eq m^{-3}$  for coarse sandy soils and several hundreds  $eq m^{-3}$  for clay.
8. *Base saturation* determines the fraction of the total cation exchange capacity being occupied by base cations ( $Ca^{2+}, Mg^{2+}, K^+, Na^+$ ). The top layers of silicate soils are usually within the range of 0.05 to 0.15. Deeper layers have higher base saturations.
9. *Field capacity*, i.e. the amount of water the soil can retain against the pull of gravity, is a function of soil properties. Depending on the type of soil, values can range from  $0.02 m m^{-1}$  for sandy soils to  $0.30 m m^{-1}$  for clays.
10. *Climatic mean of monthly air temperature* is determined by a long-term average observed in the study region. Depending on the location within the region the long-term mean temperature can have a variation of 20 %.

11. *Climatic mean of monthly precipitation* is determined by a long-term average observed in the study region. Depending on the location within the region the long-term mean precipitation can vary by 25 %.
12. *Lake pH and alkalinity* are used as output state variables, which provide information on the acidification status of the lake. These variables are commonly measured in the survey programs. Lake pH, being the negative logarithm of the hydrogen ion concentration, can range in natural waters from 3.5 to 10. Lake alkalinity in surface waters usually has values between  $-0.1$  and  $2.0 \text{ meq l}^{-1}$

A large number of water quality observations has become available in national survey programs investigating the present extent of lake acidification. At present, lake survey information has been implemented for the use of regional modeling from two Nordic countries, Finland and Sweden. From Finland, data from 9000 lakes from years 1975 - 1984 was made available by the National Board of Waters, Water Quality Data Bank. The lake pH information was divided into five parts to form lake acidity distributions for five individual distinct lake regions. In Sweden, an extensive survey was conducted in 1980 and reported by Johansson and Nyberg (1981). The lake pH and alkalinity distributions were given separately for each of the 24 provinces in Sweden. These data groups were aggregated at IIASA to form six lake regions each of them receiving more or less homogeneous deposition. The lake regions considered in this application are displayed in Figure 2.

The frequency distributions of lake surface area and lake mean depth for Sweden were obtained from the Swedish Lake Register of the Swedish Meteorological and Hydrological Institute (SMHI). For Finland, this information was provided by the Hydrological Office of the Finnish National Board of Waters. An inventory, determining the number and the size distribution of lakes in the whole of Finland, was completed in 1985 (E. Kuusisto, National Board of Waters; forthcoming). The total number of lakes in Finland (larger than  $500 \text{ m}^2$ ) was counted to be 187,888.

The initial cation exchange capacities as well as the soil base saturation were assigned distributions for all lake districts both in Finland and Sweden based on the FAO-UNESCO soil map of the world (FAO-UNESCO 1974). The soil map also provided information on the distributions of typical surface slopes, which also is an input to the model. A frequency distribution for the soil moisture content at field capacity was formulated on the basis of the texture classes obtained from the soil map.

A geological map (UNESCO 1972) was used for assigning distributions for the weathering rate of the silicate parent material. The same classification of different rock types into weathering rate classes was applied as in Kauppi et al. (1985). Ranges for the mean monthly temperature and precipitation of each district were derived from climatic data of about 200 observation stations in Europe, North-Africa and West-Asia (Müller 1982). The minimum and maximum monthly values for each district were obtained by interpolating the observed mean monthly values over the whole of Europe. The ranges used, therefore, reflect the climatic variability within the region.

For the mean catchment soil thickness and for the ratio of lake area to catchment area there was not enough *a priori* information available to allow any detailed distributions to be formulated. These input variables were designated ranges broad enough so that any reasonable value for an input could be selected from the rectangular distributions. All other parameters were assigned constant values since, based on the model analysis above, they do not significantly affect the output.

The prespecified frequency distributions for parameters as well as the distributions obtained as a result of the filtering for one region in Finland are displayed in Figure 3. In Figure 3a the corresponding cumulative frequencies are shown. The greatest difference between the *input* and the *output* distributions could be observed in the case of the mean catchment soil thickness. It illustrates the main result of the sensitivity analysis that the soil thickness is important in determining the behavior of catchments. This result can also be seen in Figure 4 where the output frequency distribution for the mean catchment soil thickness is presented for all regions in Finland. The output distributions differ from the prespecified rectangular distributions for all Finnish lake regions.

#### 4.2. Scenario Analysis

The purpose of the model development has been to apply it as a part of a larger structure, the Regional Acidification Information and Simulation (RAINS) model. The RAINS model attempts to structure the scientific information about the acidification problem in a form usable to decision-makers. The model provides a tool for assisting policy-makers in their evaluation of air pollution control strategies, for acidification in Europe.

In this way the regional lake acidification model is turned into a device for examining the impact of policies on an environmental system. Multiple simulations of different policy alternatives will give information on the effectiveness of chosen policy options. Each simulation represents a set of assumptions on the energy development and on the measures taken to control emissions. A consistent set of assumptions (a policy set) is here called an energy-emission scenario and the type of analysis is termed scenario analysis.

After scaling the lake acidification model up to a regional level and having obtained a set of accepted parameter vectors with the filtering procedure, the obtained ensembles can be used for future simulations. The regionalized model is now applicable for providing estimates of the time patterns of regional lake acidification for any energy-emission scenario and year between 1980 and 2040. The model is run through the period of 60 years separately for each predefined lake region. An estimate of the lake pH or lake alkalinity frequency distribution for either spring or summer is produced as the output.

In the following, two example scenarios produced by the energy-emission submodel of RAINS, are compared. The two examples are only intended to demonstrate the model behavior as well as the model output. No conclusions can be drawn about the effectiveness of the selected control strategies.

From 1960 until 1980 the two constructed energy-emission scenarios were identical. The historical deposition pattern obtained on basis of these energy-emission trends was used as a driving force for the filtering procedure. For the whole time span, covered by the model, the scenarios assumed the same rates of energy development as defined by the latest estimates of the International Energy Agency (IEA 1985). From 1980 on, however, the scenarios departed so that the 'base' scenario did not assume any pollution controls, whereas, the 'low' scenario assumed effective measures taken for the control of sulfur emissions. These controls were defined as 1) pollution control devices on all power plants and 2) fuel cleaning in the domestic energy sector (see Alcamo et al. 1985). The time development of total sulfur emissions for the two scenarios is displayed in Figure 5.

By the year 1980, lake acidification has been reported to be an observed phenomenon practically throughout Finland and Sweden. In the worst acidified areas, viz. in the west-coast of Sweden over 30 % of the total number of lakes are acidified having measured summer pH values lower than 5.0. In southern Finland, the pH of the water is below 5.0 in less than 10 % of the lakes. In spring, when the annual minimum pH in the surface waters occurs, the acidity of the lakes is even greater. Because of this, the spring pH can be considered as a reasonable indicator of the risk of damage in aquatic life due to lake acidification. The frequency distributions for the lake pH in spring 1980, used as the starting state of acidification for the scenarios, are shown in Figure 6.

The results of the model runs using the two scenarios show a clear difference in the resulting spring pH values for example for the year 2010 (Figure 7). When the 'base' scenario was used as the input, acidification tended to continue, and the frequency distributions for the spring pH showed a shift towards the lower end of the distribution. However, with the 'low' scenario, the model resulted in a slight improvement of the situation. This shift in the frequency distributions towards higher pH values implied that the deposition had lowered so much that for some lakes the alkalinity production exceeded the deposition, and consequently, the model estimated a recovery.

More precise figures for the time development of the regional lake acidity are given in Table 6. The table compares the two scenarios in the selected reference years. A critical pH of 5.0 is taken as the reference value, because this represents a high risk of damage to aquatic life. The estimates of the time pattern of the percentage of all lakes with a spring pH below the selected value showed that first by the year 2010 there was a recovery in most lake regions if the 'low' scenario was assumed. In Region 1 of Finland 3.9 percentpoints of the lakes recovered (from 18.5 to 14.6 percent) and in the southern region of Sweden a recovery of 6.7 percentpoints was thus obtained. This recovery evidently had to do with the reduction in the strong acid load so that for part of the catchments the alkalinity generation is estimated to exceed the acid load. The results in Table 6 show that under the low sulfur deposition scenario some regions become more acidic after year 2010 because of the cumulative long-term processes in soil chemistry (In Region 1 of Finland an increase of 3.9 percentpoints can be noted between 2010 and 2030). The deposition rate of strong acids had still exceeded the weathering rate of silicate minerals in soils, and soil acidification had proceeded, increasing the acid load from the uppermost soil



layers.

When the 'base' scenario was used as the driving force, there was a clear ongoing lake acidification process occurring in the regions of higher sulfur deposition, southern Finland and southern Sweden. For Lapland (Region 5), deposition was calculated to remain in such low levels even with the 'base' scenario that no drastic effects on the lake water chemistry was predicted (1.9 percent of the lakes in Region 5 of Finland have a pH below 5.0 throughout the reference years).

Table 6: Percentage of lakes in Finland and Sweden having spring pH-values lower than 5.0, for the two example scenarios.

Region	1980	pH less than 5.0					
		1990		2010		2030	
		Base	Low	Base	Low	Base	Low
<b>Finland</b>							
1	19.4	21.4	18.5	29.1	14.6	32.0	18.5
2	5.9	7.9	6.9	7.9	5.9	8.9	5.9
3	2.0	5.9	1.9	9.8	2.9	9.8	2.9
4	5.7	5.7	5.7	10.4	3.8	13.2	4.7
5	1.9	1.9	1.9	1.9	1.9	1.9	1.9
<b>Sweden</b>							
1	12.5	14.4	12.5	20.2	5.8	24.0	5.8
2	41.2	43.1	41.2	50.0	35.3	52.0	35.3
3	16.4	15.4	15.4	20.2	10.6	24.0	10.6
4	11.4	14.3	11.4	22.9	11.4	28.6	12.4
5	2.9	3.9	3.9	4.9	4.9	6.8	4.9
6	2.9	3.9	2.9	3.9	2.9	4.9	2.9

## 5. DISCUSSION

Uncertainty inherent in environmental modeling is inevitable. It seems unlikely that any complex environmental system can be well described in the traditional physicochemical sense (Hornberger and Spear 1981). The credibility of the models results is, however, a key issue in using mathematical models for decision making. An essential aspect of the credibility is how well the user of the model understands the uncertainty. The evaluation of the lake acidification model of RAINS uncertainties and sensitivities has been performed using the PRISM framework.

In regional applications, there remains uncertainty in the accuracy of the data in two levels. First, measurements from the study area, forming the input data used, always include some measurement error. The second level has to do with the interpretation of the regional properties. Measurements can only be viewed as samples of the regional system under consideration. It is definitely impossible to sample every one of the catchments in Europe. The aggregation and interpretation of aggregated information together limit the utility of regional data as such. In some cases measurements are

completely missing and the inputs have to be chosen from the best possible experts opinion or even guesses. A filtering procedure has been used in order to restrict unrealistic input ranges from producing an unrealistic output.

The regional application itself forms an additional source of uncertainty, which in fact may result in systematic errors. When determining the input ensembles that produced acceptable distributions for output variables, a fixed historical deposition pattern from 1960 to 1980 was assumed. If this deposition pattern was altered, a new different set of inputs might be obtained from the allowable ranges. Besides the historical deposition pattern, also the shortness of the calibration period (20 years) forms a possible source of error.

The results of the evaluation of parameters of the regional lake water acidification model show that, in spite of large uncertainties for some key parameters, the model seems to provide a good representation of measured pH levels in Region 1, Finland. The analyses point out that in order to improve the results and reduce the uncertainties associated with different scenarios, efforts should be made to accurately define the input distributions for the most critical parameters; the mean catchment soil thickness (SOILT) and the weathering rate (SIBRC) in the region. Relatively little emphasis has been given to these two properties that together largely determine the long-term behavior of the catchments. Current research is, however, continuously expanding our knowledge on them and we expect to be able to incorporate more realistic *a priori* distributions in the future.

The information provided by the sensitivity and uncertainty analysis can be used, moreover, as a basis for further development of the model. Processes associated with parameters which proved to be relatively unimportant, can be aggregated and the model simplified. There is good reason to use annual or semiannual time steps to describe weather patterns rather than to use the current finer resolution of monthly temperature and precipitation. These weather variables account for the hydrology and thus for the seasonal variation in acidity, but they have no apparent effect on the long-term development of the catchment.

Acidification models assessing long-term responses are extremely difficult to verify. Strict validation of these types of models requires long time series records to determine whether the model estimates match the observed catchment responses. Unfortunately very few, if any, such records exist. The question whether the long term responses estimated by the model are true projections of real systems' responses remains therefore uncertain (cf. Cosby et al. 1985a,b) Given the best available data and using parameter values that are within the ranges appropriate for natural soils in Finland and Sweden, our model seems to produce plausible results. The validation process in the case of a model examining long-term chemical changes has to be viewed as a stepwise process of gaining credibility. Ultimate validation can never be established. Instead, uncertainty involved in both the model structure and the model application can be assessed. That aspect deserves a concentrated research effort in the future.

The filtering procedure for finding an acceptable subset of parameter combinations is by no means a final solution to the problem how to deal with uncertain and unknown regional input data. The technique using *a priori* criteria to select a satisfactory subset of model simulation resulted in some improvements in the predicted results. We intend to continue these investigations with data from other regions in Scandinavia in order to produce reliable parameter estimates for each lake region and develop a strategy to aggregate parameters for use with a simplified model structure. These parameters will then provide the basis for estimating the expected effects on lakes and associated uncertainties of different deposition scenarios of the RAINS model.

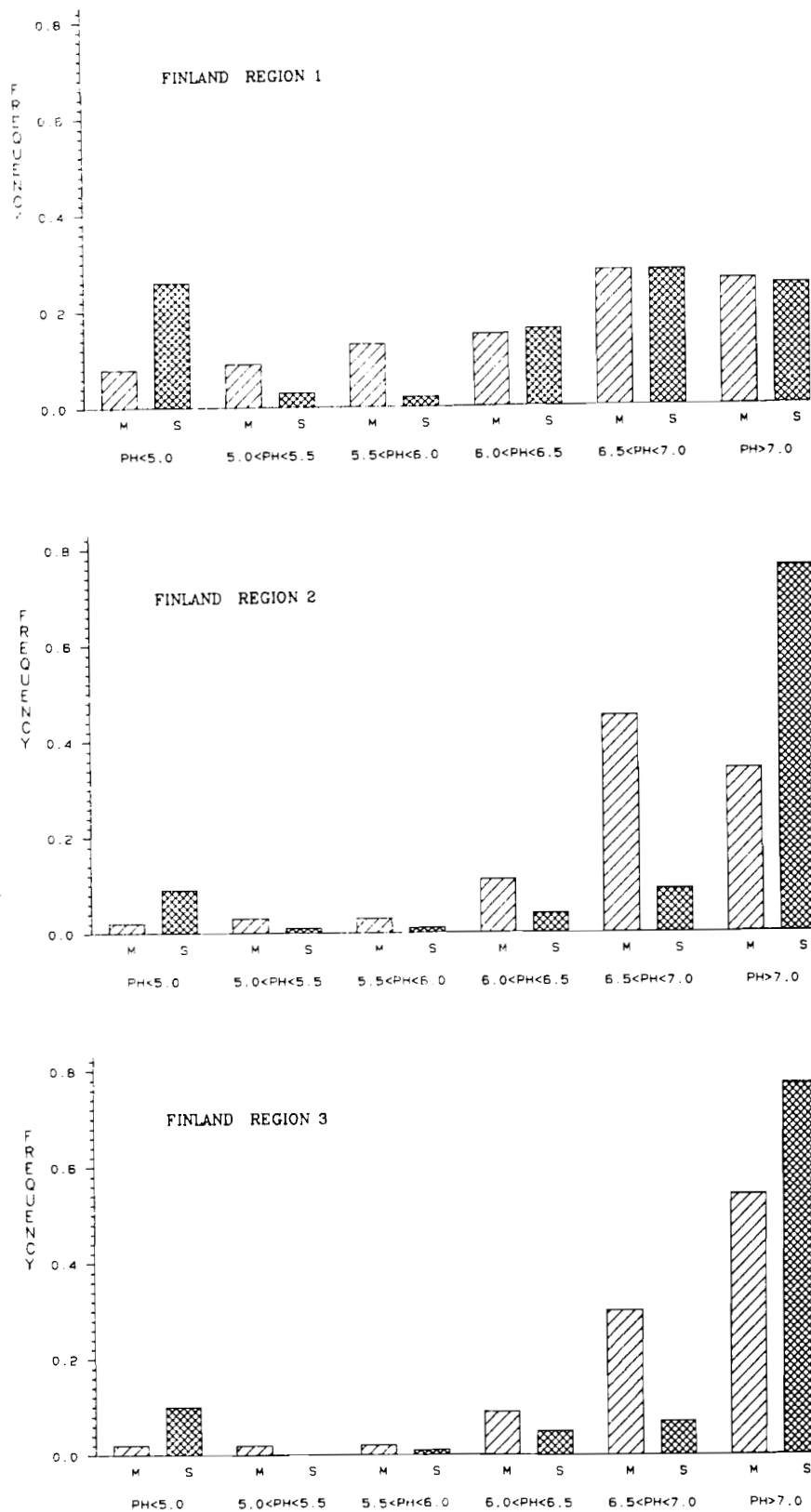


Figure 1: Measured (M) and simulated (S) lake pH distributions for 1980 in the five Finnish lake regions run with pre-specified input distributions.

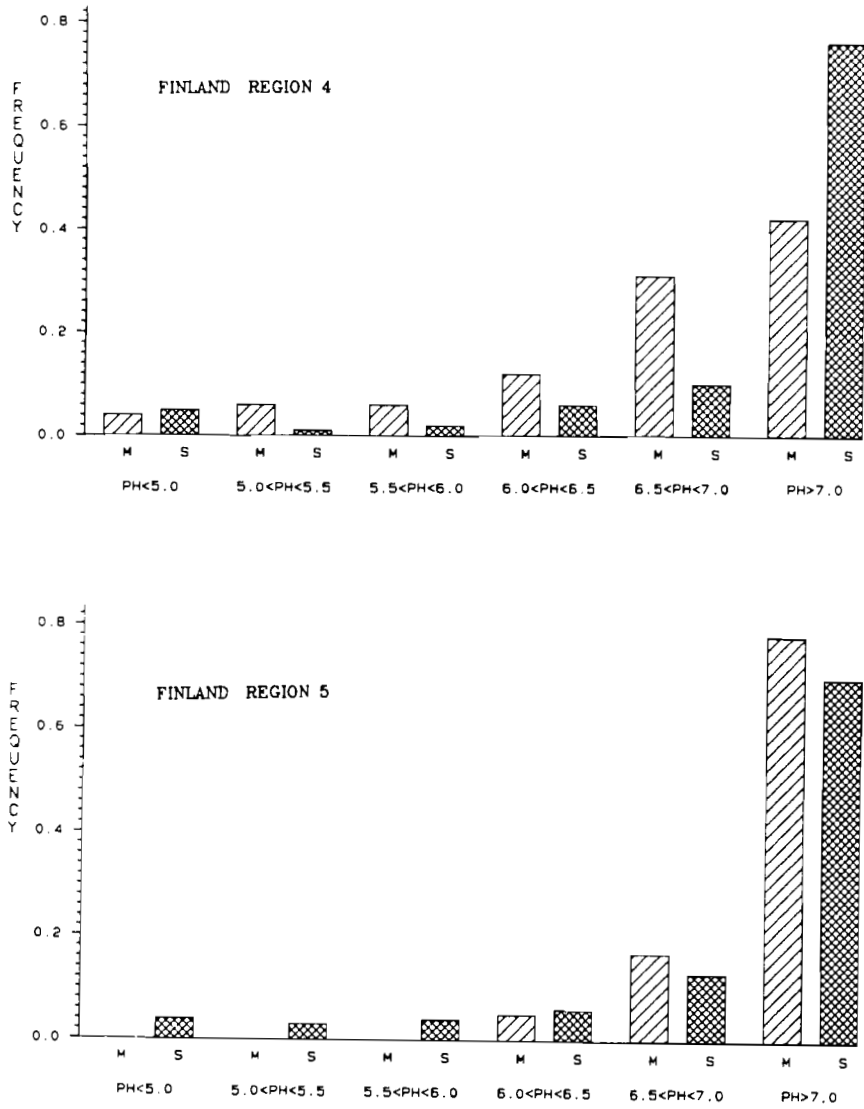


Figure 1: continued .....

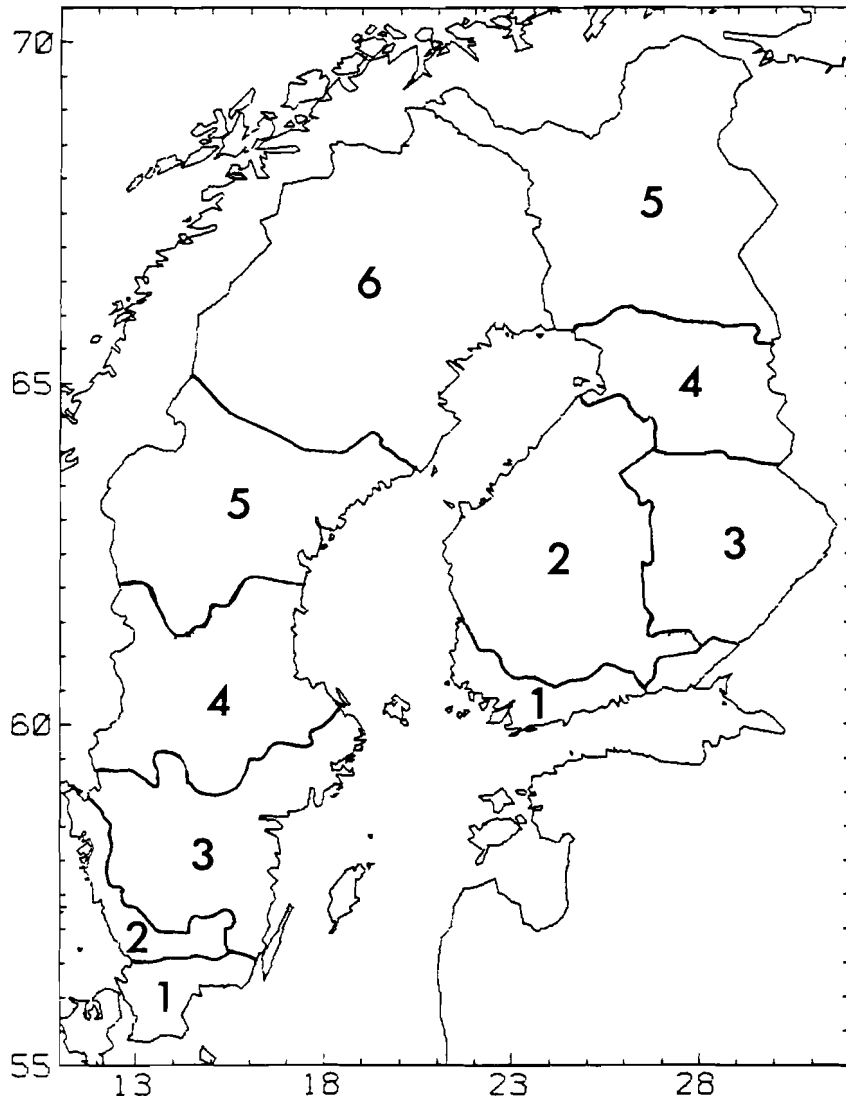


Figure 2: Geographical location of the lake regions in Finland and Sweden.

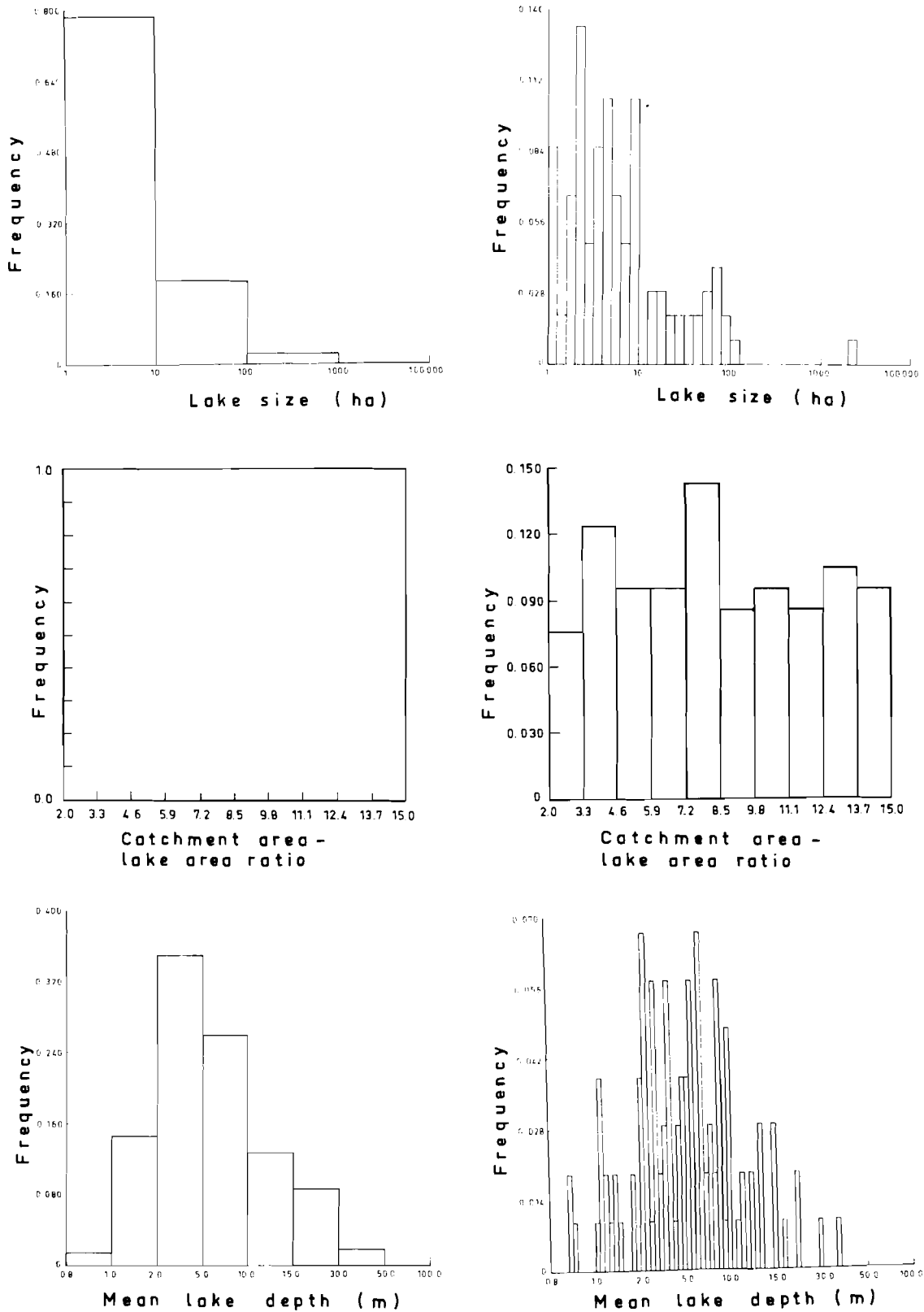


Figure 3: Input (left column) and output distributions (right column) for the nine input parameters of Region 5 in Finland sampled with the filtering procedure.

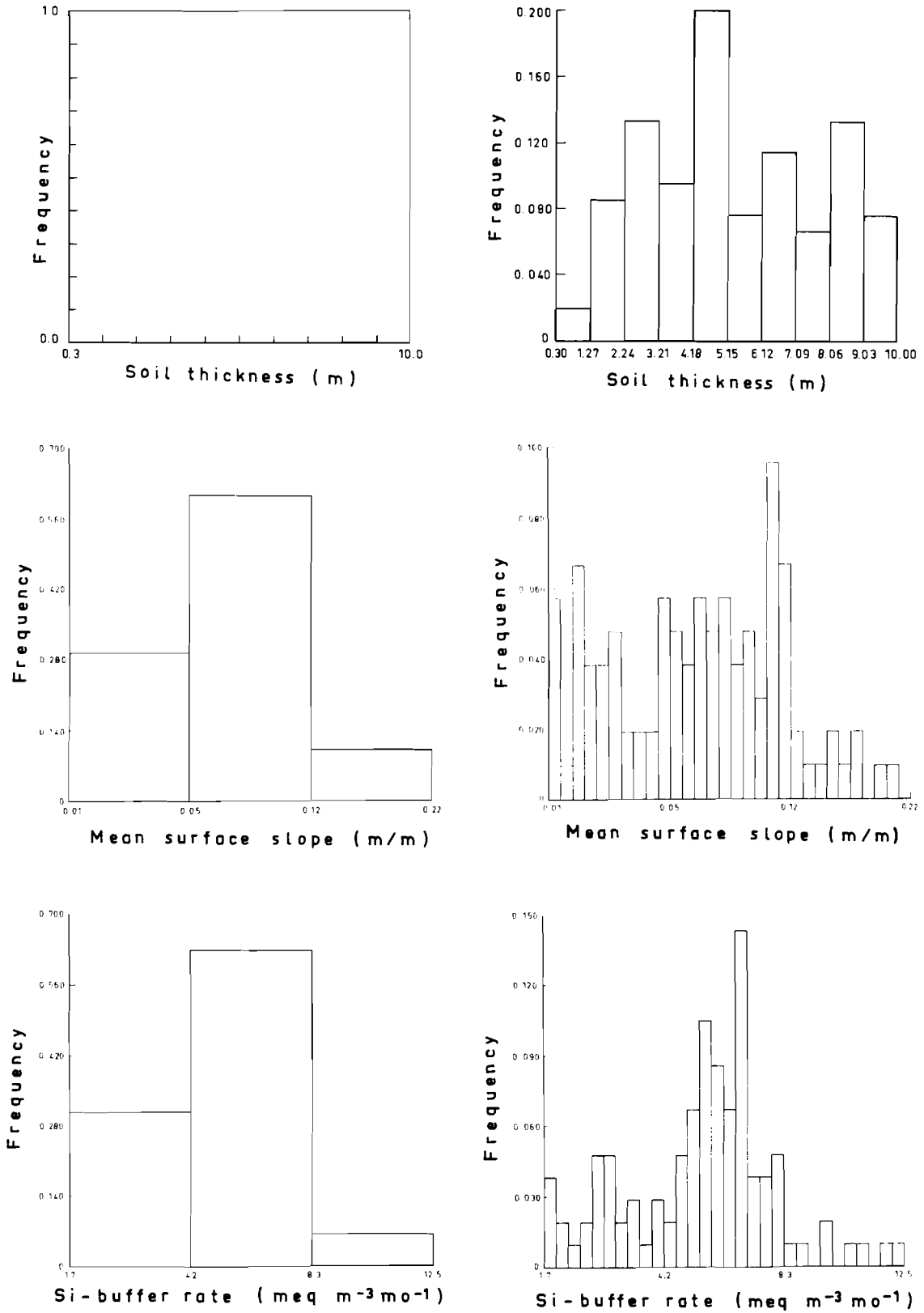


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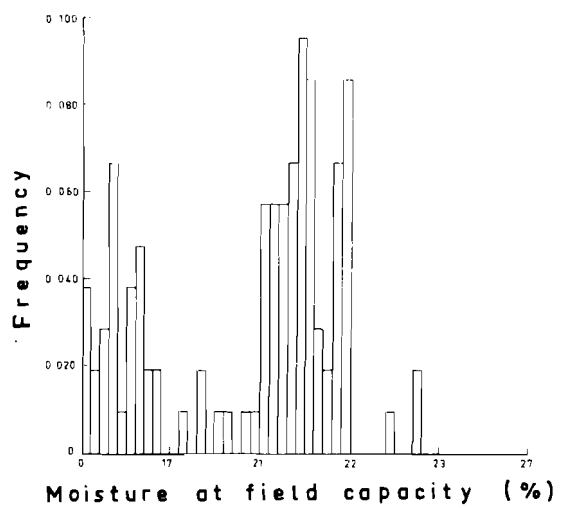
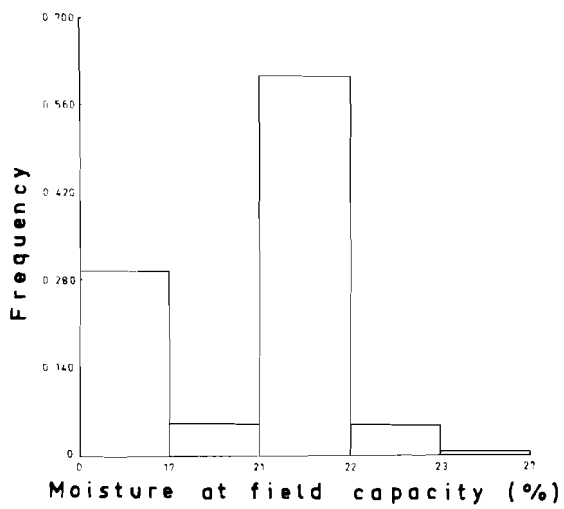
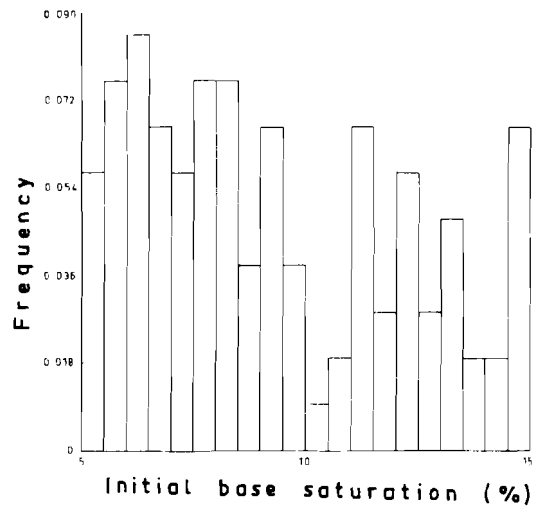
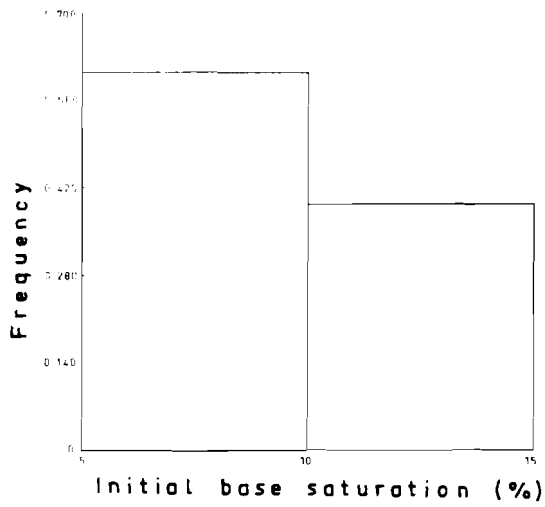
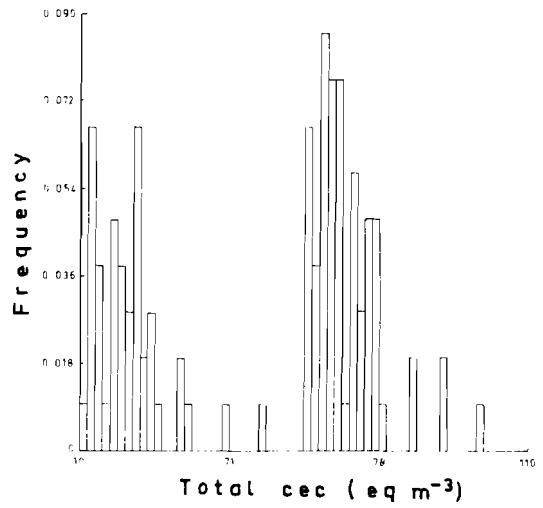
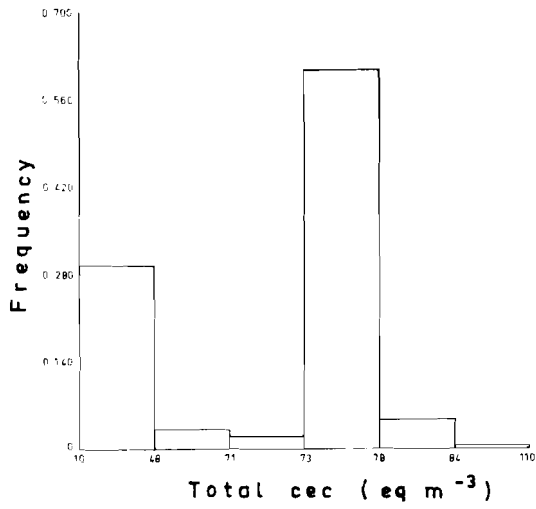
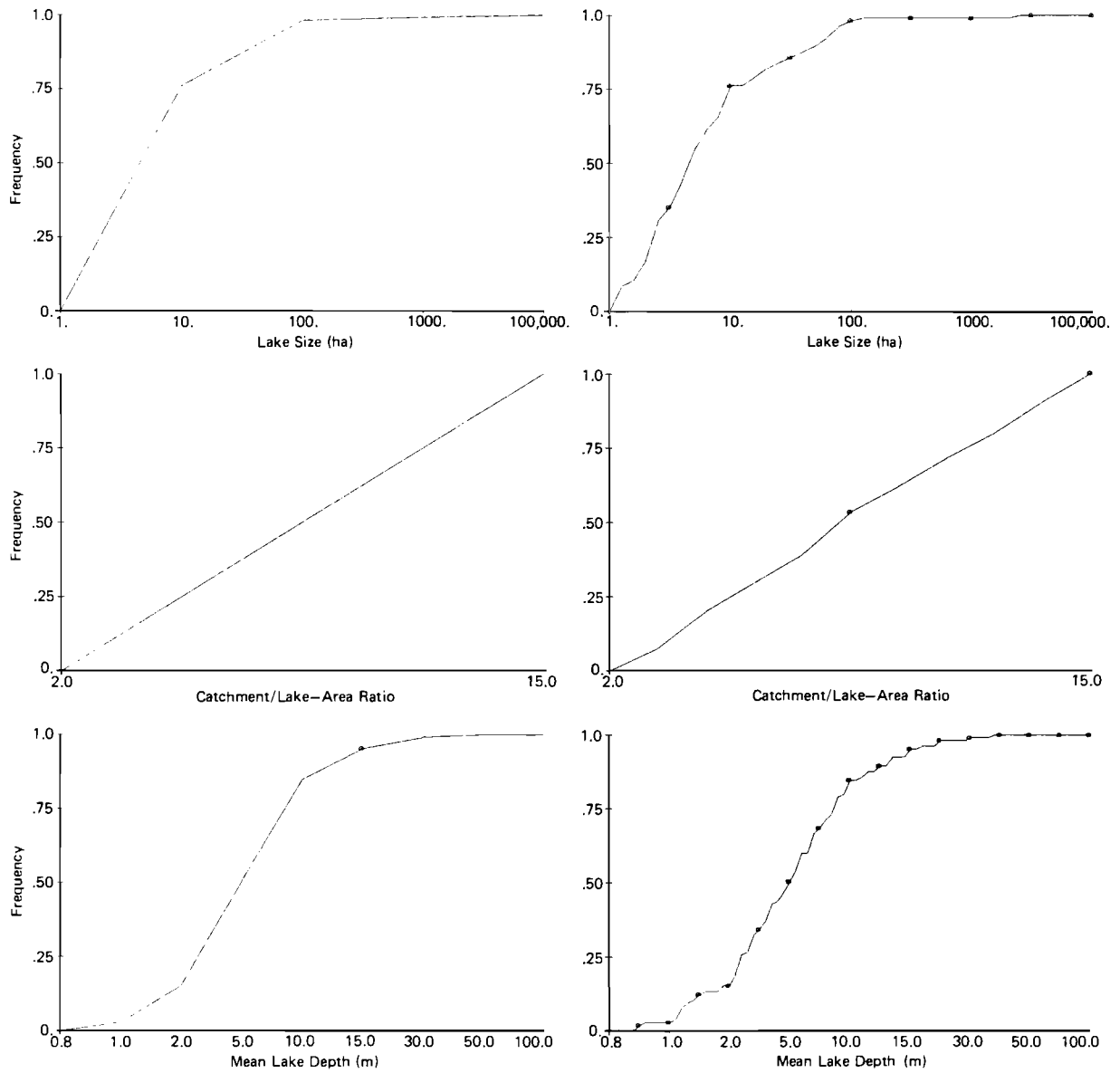


Figure 3: continued .....



**Figure 3a.** Input (left column) and output cumulative distributions (right column) for the nine input parameters of Region 5 in Finland sampled with the filtering procedure.

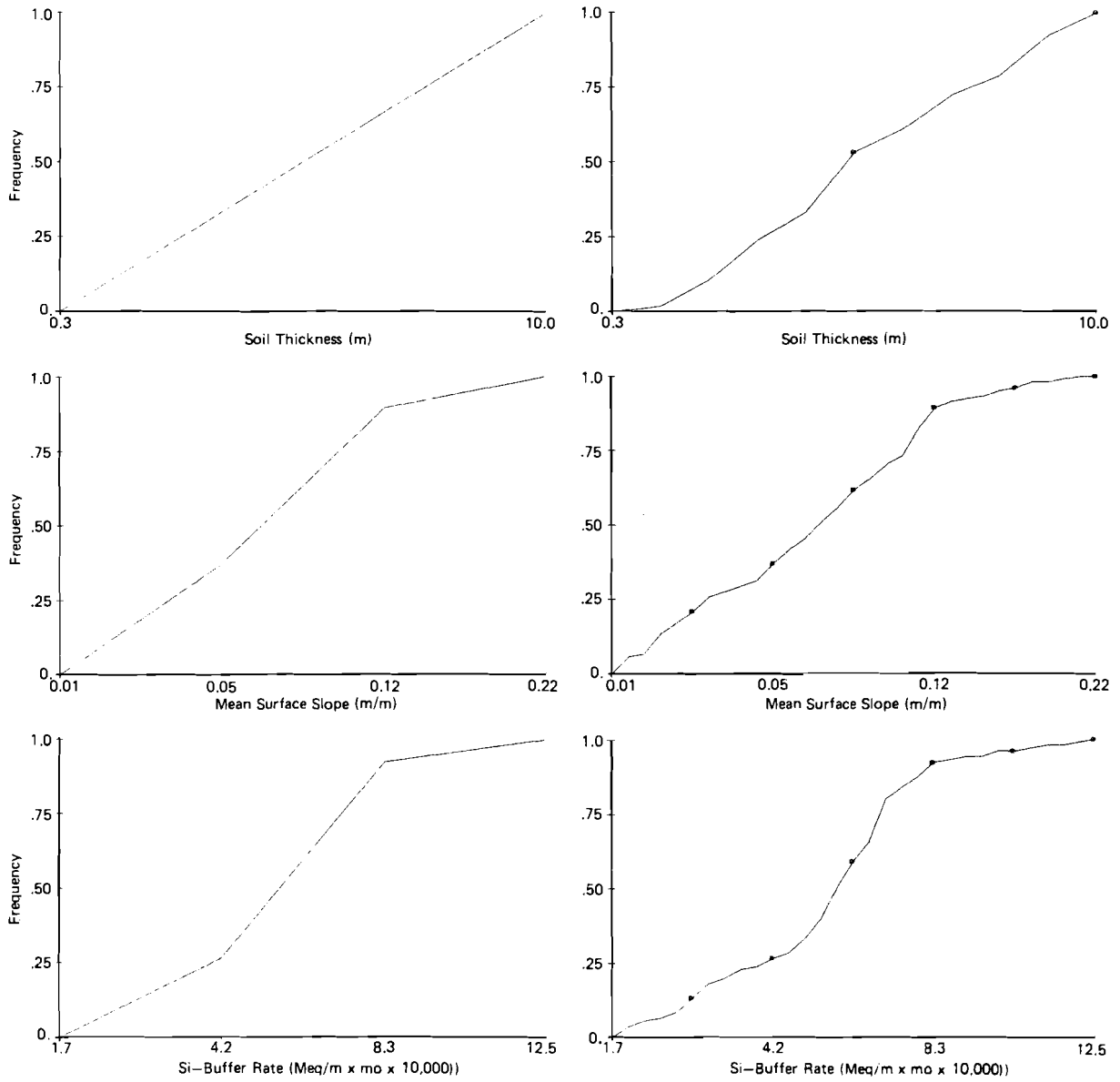


Figure 3a. continued ....

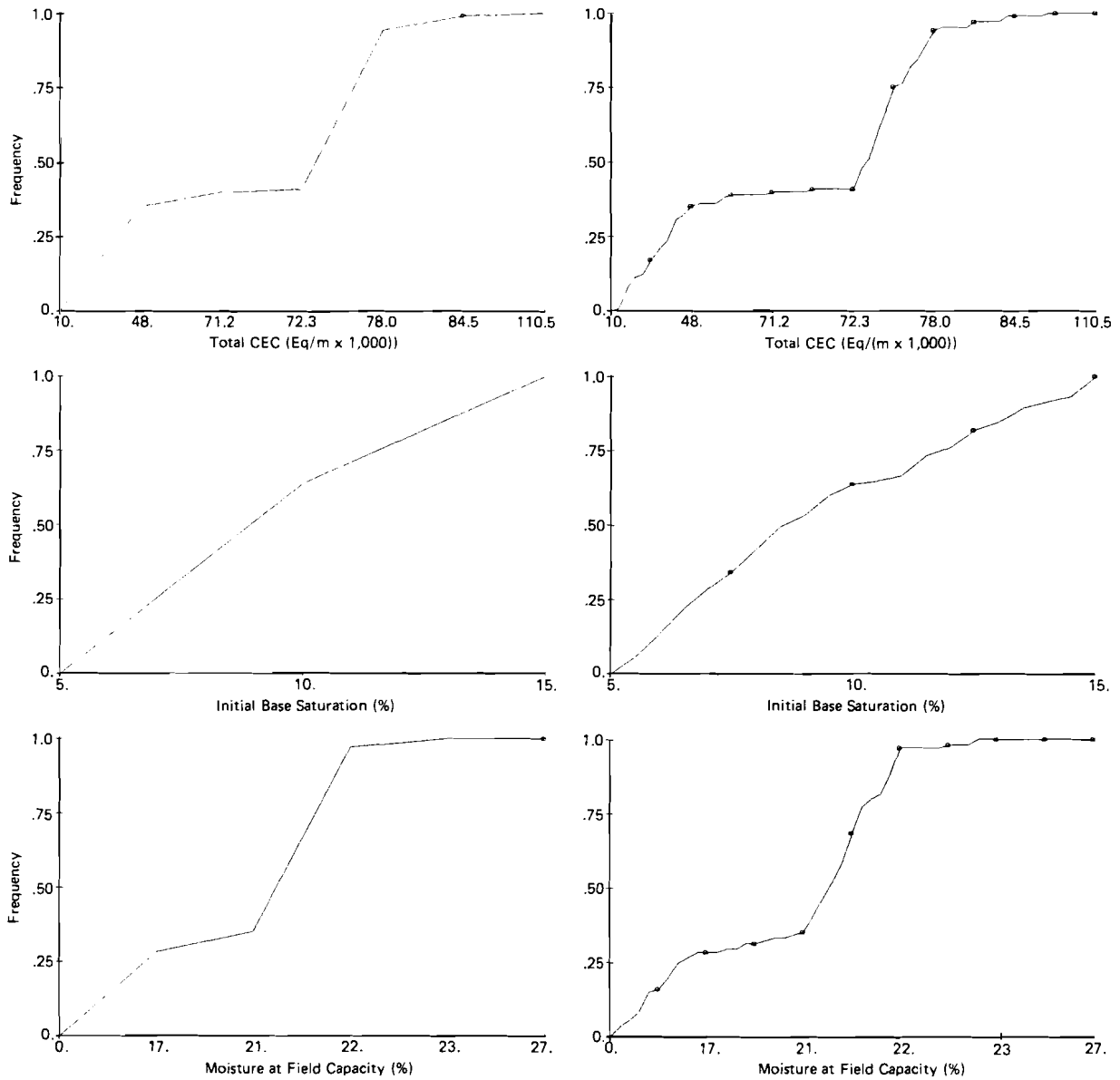


Figure 3a.

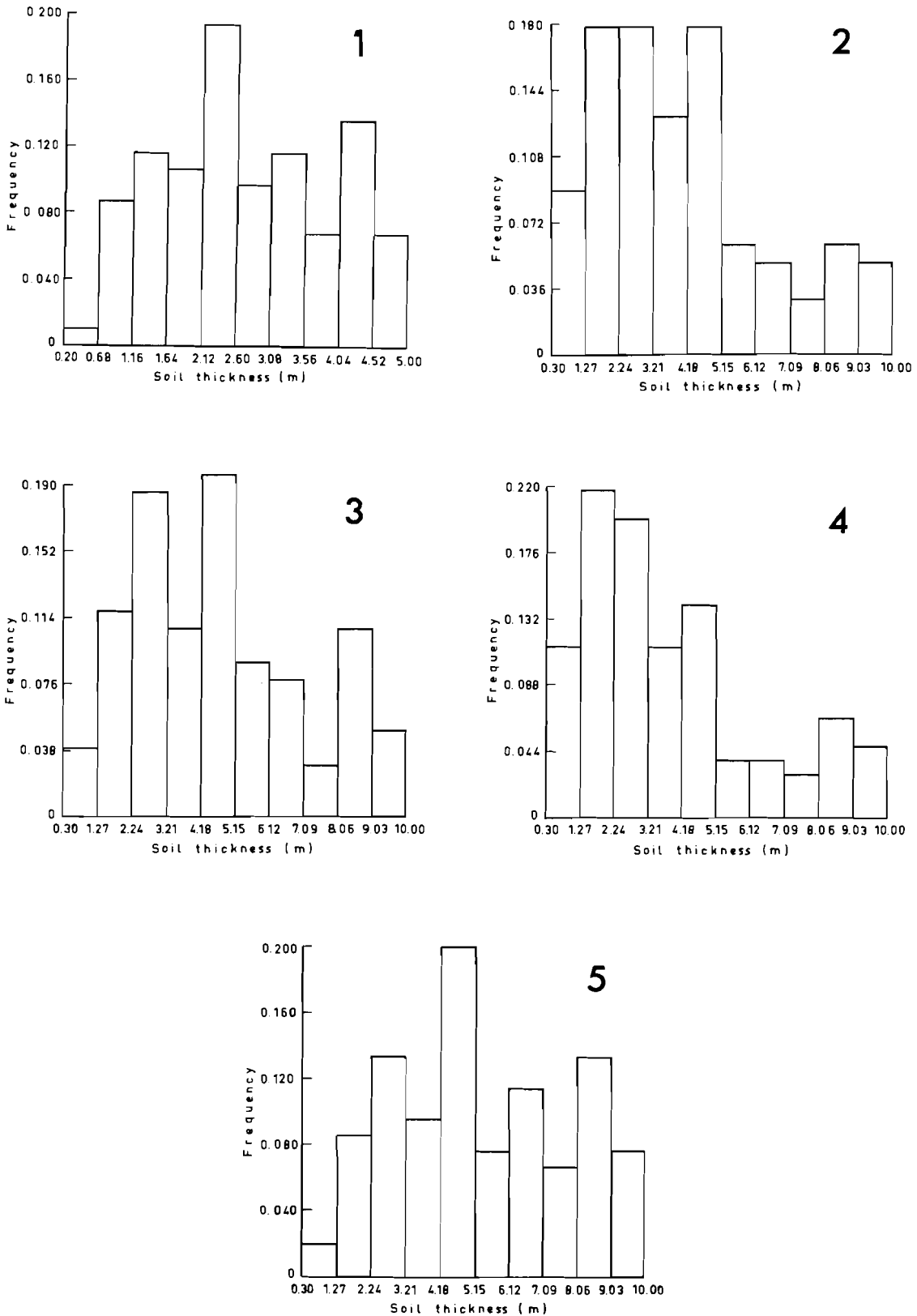


Figure 4: Output distributions of soil thickness in the five Finnish lake regions obtained with the filtering procedure.

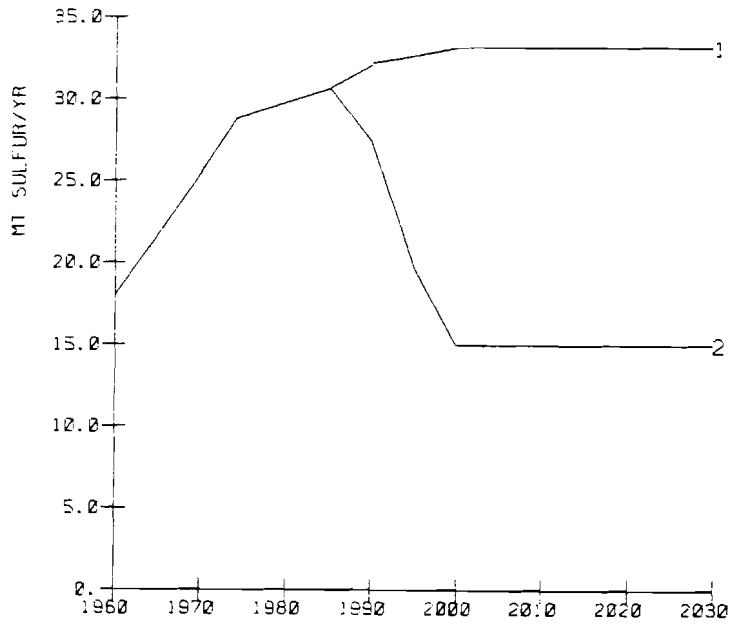


Figure 5: Total sulfur emissions in Europe for the 'base' and 'low' emission scenarios.

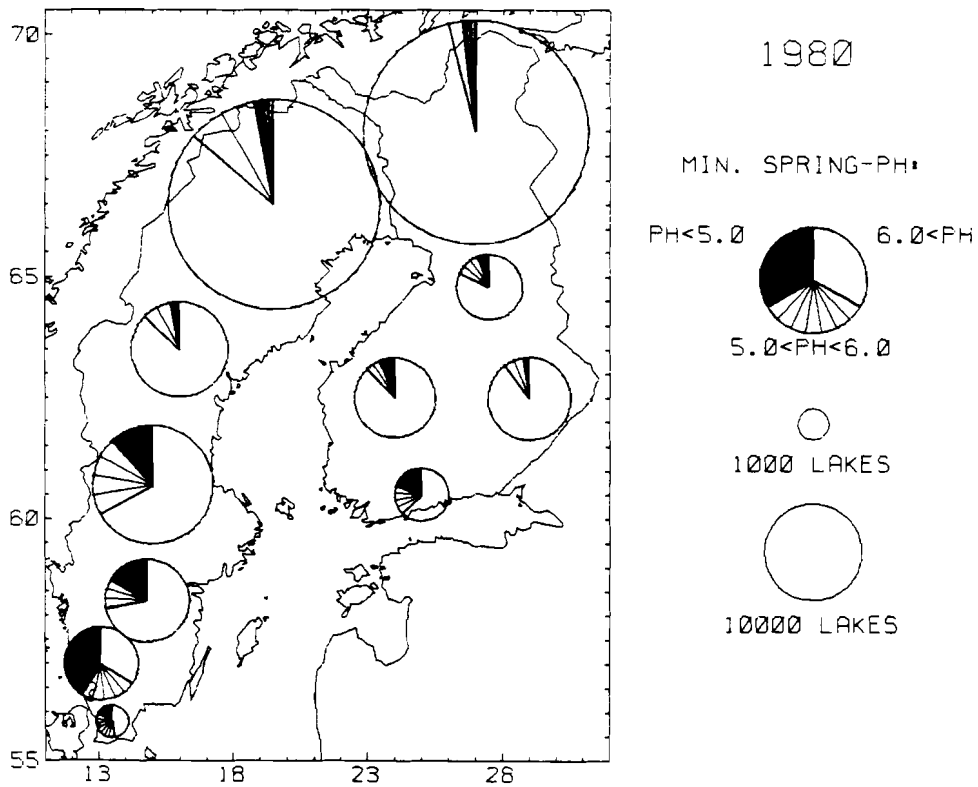


Figure 6: State of lake acidification in Finland and Sweden in 1980. The area of the circles is proportional to the number of lakes in the respective regions.

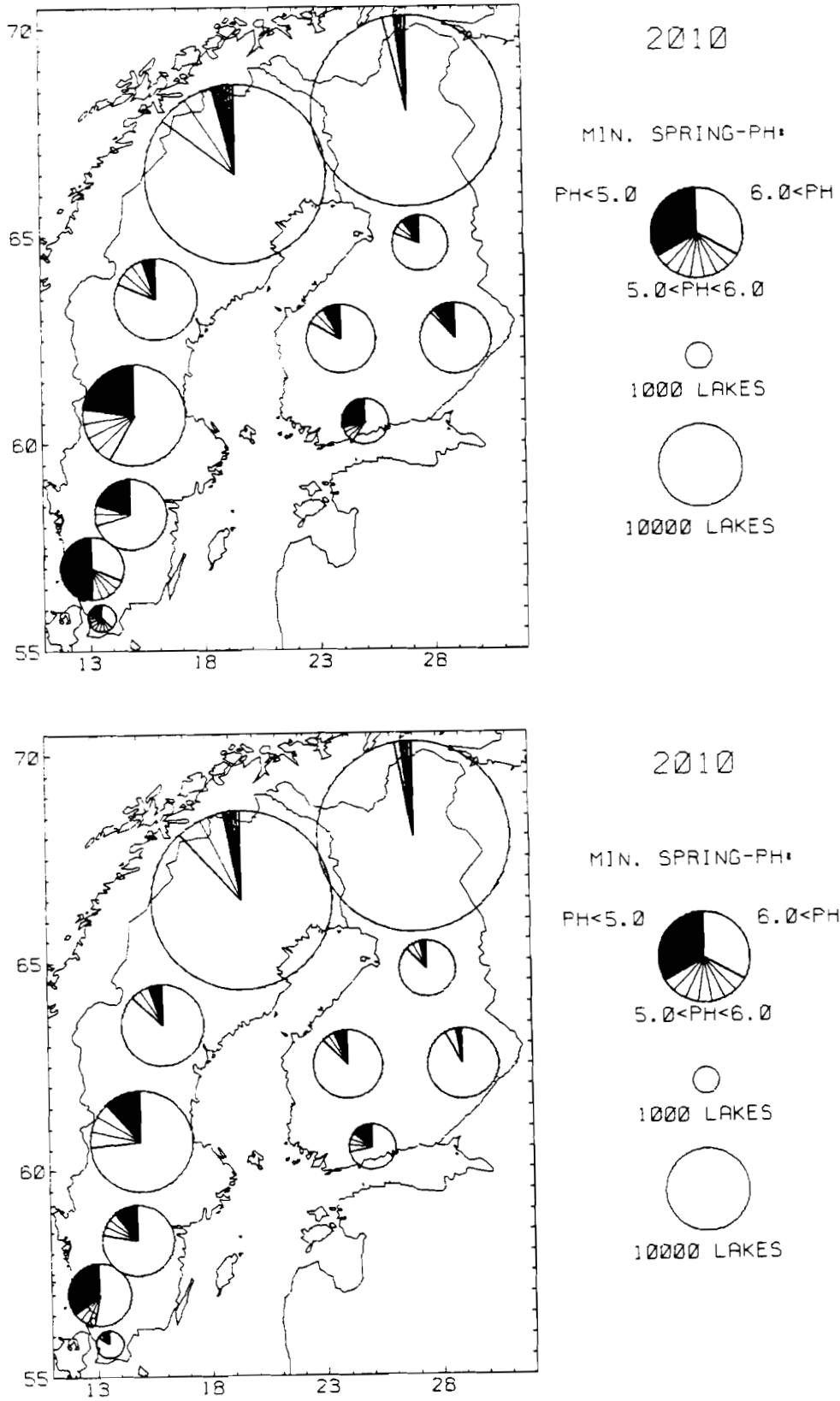


Figure 7: State of lake acidification in Finland and Sweden in the year 2010 assuming the 'base' (top) and 'low' (bottom) sulfur emission scenario.

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