

Sensitivity analysis of the surface water acidification model ILWAS in the saturated and unsaturated zone

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ABSTRACT The ILWAS model was developed for the Electric Power Research Institute (EPRI) to predict the effect of acid deposition on surface water chemistry. This paper summarizes a sensitivity analysis conducted for the ILWAS model. The important variables in ILWAS were identified in an application of the model to the Panther Lake watershed in the Adirondack Mountains in the state of New York. The sensitivity analysis was found to be useful in eliminating the least sensitive hydrologic and chemical variables, thus simplifying the task of calibration of the model.

INTRODUCTION

To better understand the acidification process in a watershed, scientists have developed physically based mathematical models which quantify the linkage between atmospheric deposition and stream water quality (e.g. Chen *et al.*, 1983; Christophersen *et al.*, 1982; Cosby *et al.*, 1985). The ILWAS (Integrated Lake-Watershed Acidification Study) model developed by Chen *et al.* (1983) is, at the present, the most comprehensive simulator. However, ILWAS requires extensive information on watershed physical and chemical characteristics which limits its use. Sensitivity analysis enables the identification of the important parameters in the model which require precise data. Less sensitive parameters can then be approximated by using the information in the literature or can be estimated by experience (Chang *et al.*, 1986). Consequently, a sensitivity analysis was performed to simplify the ILWAS model by using data collected for the Panther Lake watershed in the Adirondack region of the state of New York.

THE ILWAS MODEL

The ILWAS (Integrated Lake-Watershed Acidification Study) was funded by the Electric Power Research Institute from 1977 to 1984. ILWAS was an interdisciplinary, multi-institutional study of three forested watersheds (Panther, Woods, Sagamore) in the Adirondack Mountains of New York State. Details of the model including its formulation were presented by Gherini *et al.* (1983) and by Goldstein *et al.* (1985). The following paragraphs give a brief overview of the model structure.

The ILWAS model conceptualizes a spatially heterogeneous watershed system in subcatchments, stream segments and lake(s). Each subcatchment contains compartments representing the canopy, the snowpack, and the soil

layers. The lake is divided into horizontally mixed layers to allow for calculation of temperature and water quality profiles. Basically, the model is composed of a hydrologic module and a chemical module, both split into a number of submodels. The hydrologic module routes precipitation from the vegetative canopy to lake outlet. It includes 1) interception and evapotranspiration; 2) snowpack and snowmelt simulation; 3) overland flow; 4) subsurface water movement; 5) stream and lake routing.

The chemical module calculates the pH, the concentrations of alkalinity, the major cations (Ca^{2+} , Mg^{2+} , K^+ , Na^+ , and NH_4^+) and anions (SO_4^{2-} , NO_3^- , Cl^- , and F^-), monomeric aluminum and its organic and inorganic complexes, organic acid analogues and dissolved inorganic carbon. It simulates 1) the canopy processes of accumulation and throughfall of wet and dry deposition, exudation, and wash-off; 2) the snowpack processes of ion-accumulation and ion-leaching; 3) the soil processes of cation exchange, anion adsorption, mineral weathering, CO_2 exchange, and organic matter decomposition; 4) the chemical equilibria occurring in the aqueous phase. A schematic and processes summary of the ILWAS model are given in Fig. 1.

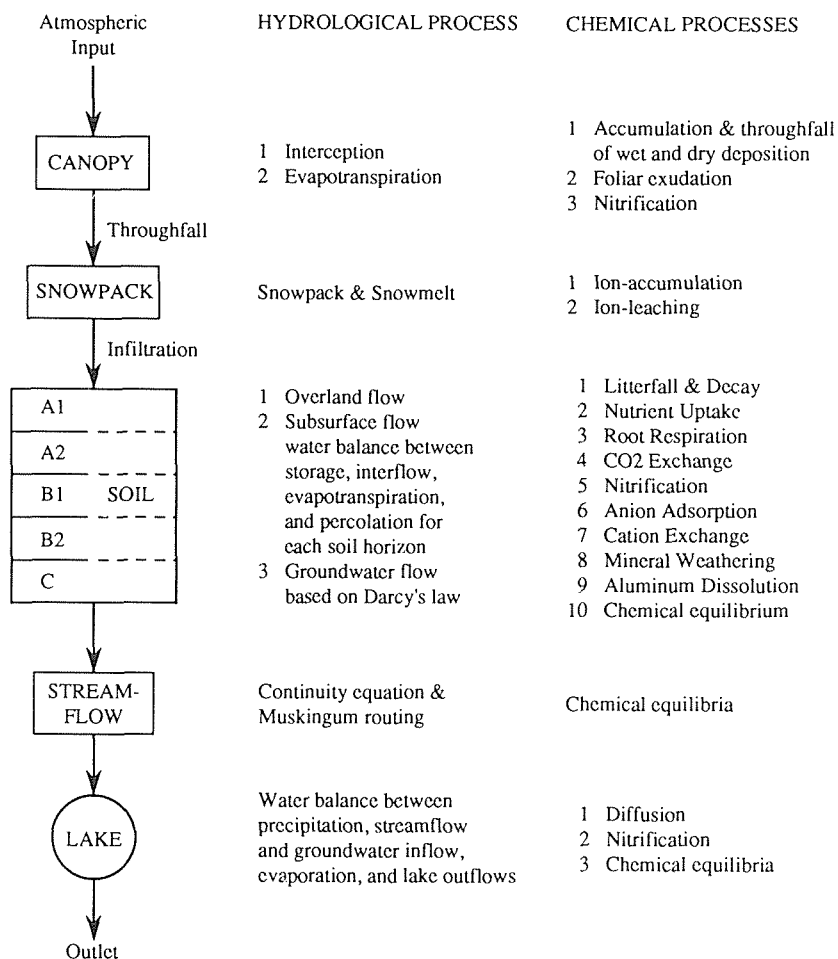


FIG. 1 Schematic and Major Processes of the ILWAS Model.

Because of its complexity, the ILWAS model requires extensive input data. For complete simulation, five input source files need to be read including control variables, lake-watershed characteristics, rate coefficients, meteorological data, and precipitation and air quality data.

SENSITIVITY ANALYSIS

The sensitivity of the ILWAS model to parameter variations was estimated as follows. First, the variable whose effect on the system response was to be estimated was selected and a reasonable range of values was defined for this variable. Next, the model was run for several values of this variable within the selected range. The simulated system responses were then examined. If the system responses showed a large variation, the selected input variable was defined as a sensitive variable. The sensitivity analysis was performed by using the Panther Lake watershed data (August 1978 to August 1981). The lake outlet hydrogen ion concentration was taken as the principal model output for evaluating the effects of changes in external input variables and internal watershed variables.

External input variables

The external input variables included six meteorological variables (precipitation, temperature, atmospheric pressure, cloud cover, dewpoint temperature and wind speed). The results show that precipitation and temperature are the most sensitive input variables, and other meteorological variables are not sensitive. A result obtained from this analysis on monthly data is shown in Fig. 2 (a and b).

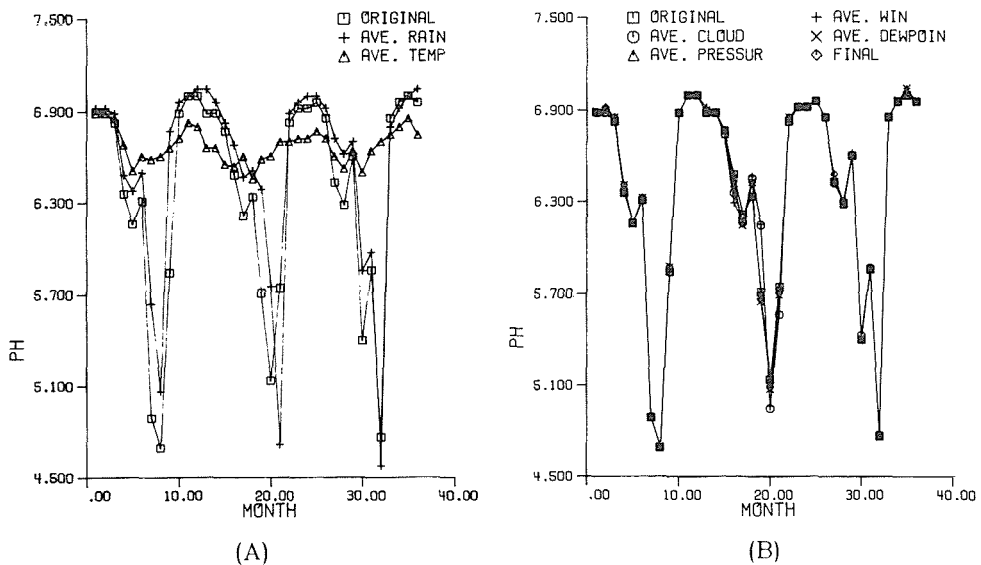


FIG. 2 Lake outflow pH as a function of time. Symbols indicate pH values obtained with monthly meteorological variables used by Chen *et al.* (1983) (ORIGINAL), with average annual value of indicated variable, and with the simultaneous use of four mean annual variables (FINAL).

It is evident (Fig. 2b) that the average value (of observed values over 3 years) of one or all of the insensitive meteorologic variables does not affect the pH value of the lake outflow very much. These 4 insensitive variables (atmospheric pressure, cloud cover, wind speed and dew point) only affect the lake evaporation rate. Consequently, if the watersheds do not have lakes, these 4 variables would not affect the result at all.

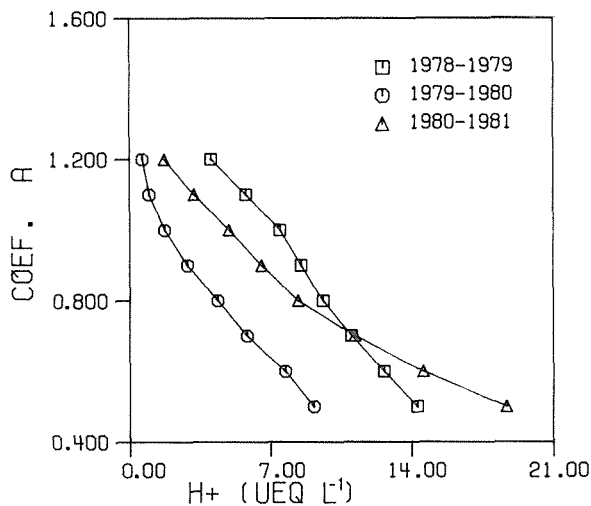


FIG. 3 Effect of changes of total soil depth on lake outflow H^+ concentration. The existing soil depth is multiplied by the coefficient A shown in the ordinate.

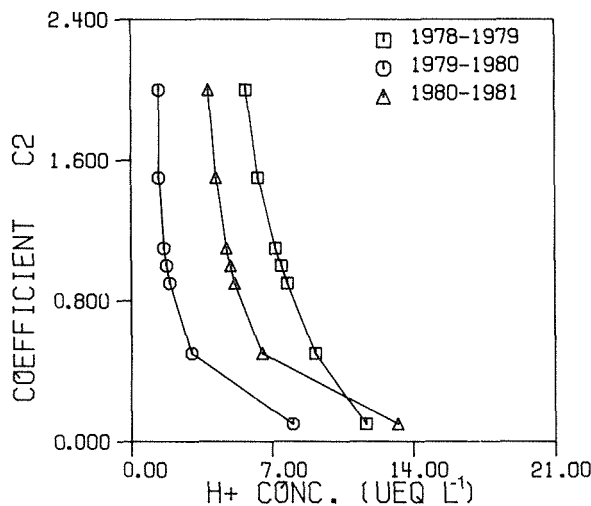


FIG. 4 Effect of vertical hydraulic conductivity on basin outflow H^+ concentration. The actual hydraulic conductivity if multiplied by the coefficient C2 shown in the ordinate.

Internal watershed variables

Because of the great number of parameters (more than 130) in the several compartments comprising the model, it is impractical to conduct a sensitivity analysis of all of them. However, some parameters in each compartment of the model are obviously key parameters because they influence or control others. For example, the plant type in the canopy, soil depth and the infiltration rate in the soil compartment, snowmelt rate in the snowpack compartment, and watershed slope in the surface flow are important parameters. With the most important parameters in each compartment selected, each of these parameters was changed individually and the ILWAS model simulation was performed. Finally, the results were compared to determine which compartment had the most effect on the lake outlet hydrogen ion concentration or pH value. The following results were obtained.

Soil compartment

The sensitivity analysis of the soil component was performed in 4 parts: a) the effect of the total depth, b) the effect of the thickness of each individual soil layer, c) the effect of reducing the number of soil layers and d) the effect of the hydraulic conductivity on lake outflow acidity. The depth of each layer appears explicitly in the water balance equation:

$$A_j Z_j \frac{d\theta_j}{dt} = A_j P_{j-1} - A_j E_{pj} - P_j A_{j+1} - L_j \quad (1)$$

where

A_j	= area of layer j (cm^2)
Z_j	= thickness of layer j (cm)
θ_j	= volumetric water content of layer j
P_{j-1}	= percolation from layer j-1 into layer j
E_{pj}	= evapotranspiration from layer j (cm s^{-1})
L_j	= lateral flow from layer j ($\text{cm}^3 \text{s}^{-1}$)

The depth of each of the five layers was multiplied by a coefficient varying from 0.40 to 1.20, all other parameters were kept constant, and likewise the hydraulic conductivity of all 5 soil layers was multiplied by a coefficient varying from 0.1 to 2.0, all other parameters being kept constant. It is seen that the soil compartment has a large acid buffering capacity and demonstrates the most significant effect on the pH value of the basin outflow. In the Panther Lake watershed, as the total soil thickness increases, the acidity of lake outflow decreases (Fig. 3).

With increased vertical hydraulic conductivity, more water can percolate through deep soil, so the basin outflow becomes less acidic (Fig. 4).

Surface slope

The principal variable affecting the overland flow is the slope of the surface as the surface runoff is calculated from:

$$L_o = \frac{1}{n} W (D - D_o)^{5/3} S^{1/2} \quad (2)$$

where

- L_o = surface runoff ($\text{cm}^3 \text{s}^{-1}$)
 D = depth of water (cm),
 D_o = max. detention storage (cm)
 n = Manning's roughness coefficient
 S = slope

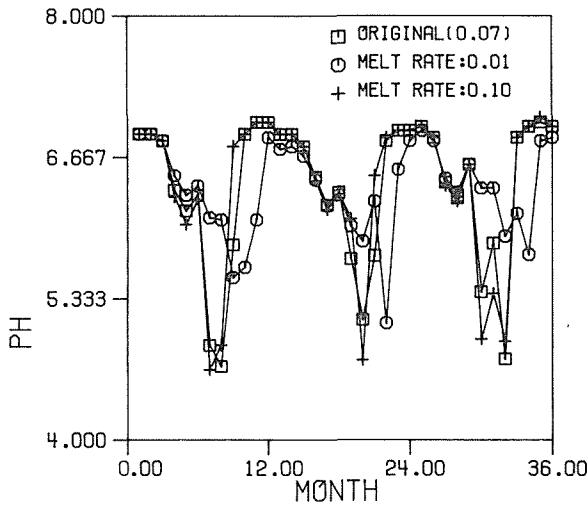


FIG. 5 Lake outflow pH for different snowmelt rate coefficients. From these results, it is seen that a small α value (0.01) results in underestimation of the acidity peak and in a delay of its occurrence. The amplitude of the acidity peak is overestimated by a high α value (0.1).

The slope also appears in the expression for the lateral flow in the saturated soil layers:

$$L_j = K_j W S Z_{sj} \quad (3)$$

where

- L_j = the lateral flow from layer j
 K_j = the saturated hydraulic conductivity of layer j (cm s^{-1})
 W = the subcatchment width (cm)
 S = hydraulic gradient
 Z_{sj} = effective saturated depth

The effect of changing the surface slope on the H^+ concentration in basin outflow is an increase in the acidity of the outflow as the slope decreases. As the value of the slope approaches 0.5 times the original slope, H^+ concentration in outflow eventually increased to $18 \mu\text{eq l}^{-1}$ from an original value $7.47 \mu\text{eq l}^{-1}$ for the first simulation year.

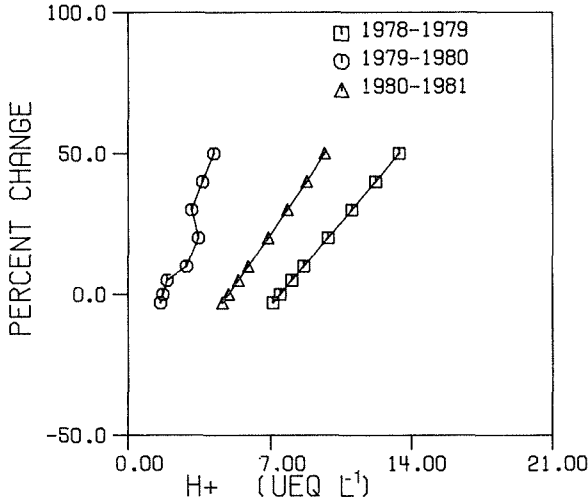


FIG. 6 Outflow H^+ concentration as a function of percent change of coniferous forest cover to deciduous forest cover.

Snowmelt

The snowmelt is estimated by the following relationships

$$M_o = \alpha (T - T_s) [0.4 + \sin (0.0087 \beta)] \quad (4)$$

$$M_r = 0.0039 (T - T_s) P_T \quad (5)$$

where

- M_o = air temperature-induced melting rate in open areas (cm day^{-1})
- M_r = rain-induced melting rate, (cm day^{-1})
- α = rate coefficient ($\text{cm day}^{-1} \text{ } ^\circ\text{C}^{-1}$)
- T = mean basin air temperature ($^\circ\text{C}$)
- T_s = incipient snow formulation temperature ($^\circ\text{C}$)
- β = aspect of the subcatchment (degrees measured clockwise from the North)
- P_T = throughfall rate (cm day^{-1}).

Panther Lake outflow exhibits sharp peaks of acidity during spring snowmelt. Several values of the snowmelt rate coefficient were investigated and the results are shown in Fig. 5.

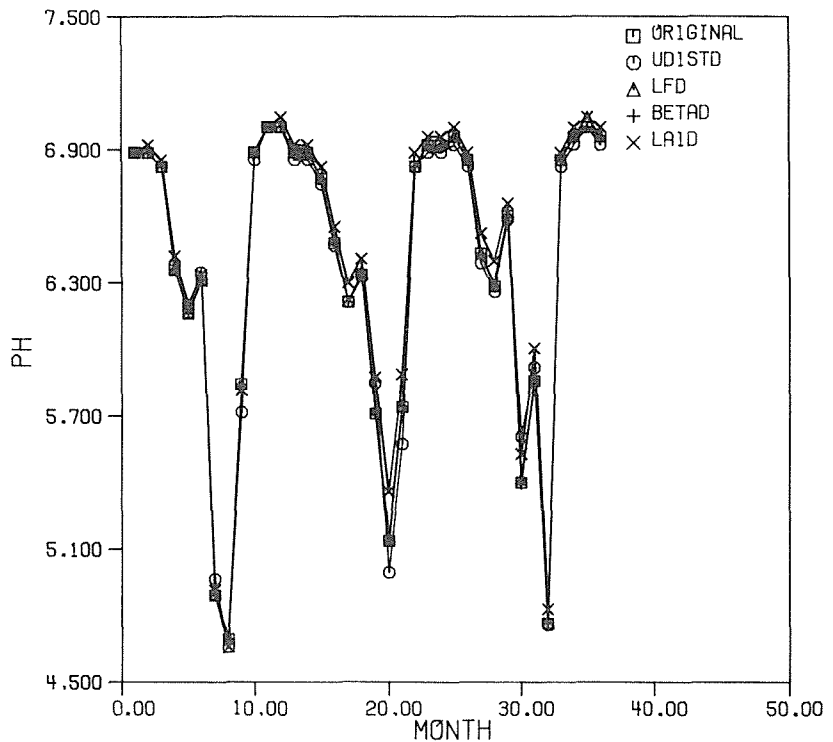


FIG. 7 Outflow pH using annual average values for four deciduous parameters. UD1STD is uptake of trees; LFD is litter fall rate; BETAD is foliar exudation rate; LAID is leaf area index.

Canopy

The forest cover on Panther Lake watershed includes 75% hardwood (dominated by beech and maple), 14% mixed forest, 10% lowland coniferous forest and 1% wetland. The deciduous forest is thus the dominant species for this watershed. For deciduous canopy the acidity of the throughfall decreases with the leaf area index because of the important leaf exudation. In contrast, the coniferous canopy is particularly efficient in the collection of dry deposition, and because of higher leaf area index the coniferous canopy gives higher fluxes of all ionic species. To test the hypothesis that the canopy controls, in part the watershed outflow acidity, the proportion of coniferous cover was decreased to 3% and increased up to 50%.

The canopy compartment demonstrated a smaller effect than other compartments. As the watershed vegetation type was changed from deciduous to coniferous, the basin outflow becomes acidic (Fig. 6); however, this change was not significant compared to the changes brought about by varying the soil depth or the watershed slope.

The sensitivity analysis was also performed to determine if an accurate determination of several monthly canopy parameters is necessary. The results obtained by using annual average values of the canopy parameters are not significantly different from those obtained using monthly values (Fig. 7).

CONCLUSIONS

The conclusions from the sensitivity analysis are:

- (a) the amount of cloud cover, atmospheric pressure, wind speed, and dewpoint are not important meteorological inputs and can be replaced by yearly average values or by empirical equations;
- (b) the soil buffering capacity demonstrates significant effect on the pH value of the basin outflow.

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