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Foreword

The paper is a result of a joint effort by the System and Decision Sciences (SDS) Program and and Transboundary Air Pollution (TAP) Project in the Environment Program. It links the up-to-date optimization techniques developed by SDS with the soil acidification model of TAP. The methodology for optimized stratagies was proposed to reduce soil acidification in Europe brought about by the long-range atmospheric transport of air pollutants.

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Contents

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1 Introduction

The emphasis of the model is on the transboundary aspect of air pollution in Europe with the aim to find cost effective environment policies for Europe. The model will be imbedded in the IIASA Regional Acidification Information and Simulation (RAINS) model. The spatial coverage of RAINS is all of Europe, and the time horizon begins in 1960 to permit checking of historical calculations, and extends to 2040 to allow examination of long-term consequences of control strategies. In this work we concentrate on soil acidification, which is an important link between air pollution and damage to the terrestrial and aquatic environment. The ability of soil to buffer acid deposition is a key factor in regulating the long-term surface and groundwater acidification. Soil acidification has also been related to forest die-back via its effect in the tree root zone. This work is concentrating on the finding of cost effective pollution control satisfying environment constrains, such as pH-value in forest soils.

2 Atmospheric Transport

Since the typical residence time of SO_2, NO_x and NH_3 in the atmosphere is in the order of one to two days, emissions from one European country are often deposited in another country. The transport model computes sulfur, nitrogen and ammonia deposition in Europe depending upon the emissions in each country, and then sums the contributions from each country with a background contribution to get deposition at any grid location. This model consists of a transfer matrix based on a Lagrangian model of long range transport of air pollutants in Europe, developed under the Cooperative Program for Monitoring and Evaluation of Long Range Transmission of Air Pollutions in Europe (EMEP). This model accounts for the effects of winds, precipitation, and other meteorological and chemical variables [3]

$$x_{lj}(t) = \sum_{i=1}^{I} \alpha_{ilj}(w)E_{ij}(t, u_{ij}) + b_{lj}; \qquad l = 1, \ldots, L; \quad t = 1, \ldots, T; \quad j = 1, \ldots, 3, \quad (1)$$

l is an index of location;

1

L is an amount of location points;

j is a pollutant number ($j = 1$ for SO_2; $j = 2$ for NO_x; $j = 3$ for NH_3);

i is a number of emitting country;

I is an amount of considered countries;

t is a number of time interval (in this model time interval corresponds to a year);

T is a time interval described by the model (number of years);

x_{lj} is the deposition of pollutant j in location point l;

u_{ij} is a control vector;

$E_{ij}(t, u_{ij})$ is an emission of the gas j from the country i at the time t;

$\alpha_{ilj}(\omega)$ is a transportation coefficient from the country i to the location point l for the gas j;

ω is a random vector describing uncertainty in the transportation coefficient;

b_{lj} is a background contribution at location l of pollutant j.

3   Soil Model

Below we give equations for the soil part of the model. A detailed description of the chemical equations for the soil part of the model can be found in the paper [5]. Here we give only brief comments to the equations.

3.1   Input equations

The atmospheric depositions (see equation (1)) are used to get the net input of cation NH_4^+ and strong acid anions (SO_4^{2-}, NO_3^-).

First the NH_4^+ and NO_3 are corrected by the net uptake of N by the vegetation. We introduce a help variable x_{l4} which sums up the total available N

$$x_{l4}(t) = x_{l2}(t) + x_{l3}(t) + k_1(z_{l4}(t-1) + z_{l5}(t-1)),\qquad(2)$$

here k_1 is a field capacity; $z_{l3}, z_{l4} z_{l5}$ are equivalent concentrations of $SO_4^{2-}, NO_3^-, NH_4^+$ ions in soil water.

A part of the deposited ammonia $x_{l3}(t)$ changed to nitrate (nitrification) and is added to the NO_3^- deposition

$$x_{l5}(t) = x_{l2}(t) + k_3 x_{l3}(t) , \tag{3}$$

where k_3, $0 \le k_3 \le 1$ is a nitrification factor. NO_3^- input to the system is computed by substracting a fraction of N-uptake of vegetation

$$x_{l6}(t) = \begin{cases} \max\{0, x_{l5}(t) - k_4(x_{l5}(t) + k_1 z_{l4}(t-1))/x_{l4}(t)\} , & \text{if } x_{l4} \ne 0 , \\ 0 , & \text{if } x_{l4} = 0 , \end{cases} \tag{4}$$

k_4 is potential N-uptake of the plants. The maximum in the above equation ensures that the N-uptake can not be bigger than the available N. Parallel calculations are made for NH_4^+

$$x_{l7}(t) = (1 - k_3)x_{l3}(t) , \tag{5}$$

$$x_{l8}(t) = \begin{cases} \max\{0, x_{l7}(t) - k_4(x_{l7}(t) + k_1 z_{l5}(t-1))/x_{l4}(t)\} , & \text{if } x_{l4} \ne 0 , \\ 0 , & \text{if } x_{l4} = 0 . \end{cases} \tag{6}$$

The input of AL^{3+}, BC^{2+} are discussed later. We introduce a new help variable x_{l9} representing the sum of charges available for chemical reaction in the soil, this is the linking variable between input equation end soil model

$$x_{l9}(t) = z_{l3}(t) + z_{l4}(t) - z_{l5} , \tag{7}$$

where the total amount of ions $(SO_2^{2-}, NO_3^-, NH_4^+)$ is computed by mass balance equations

$$SO_4^{2-} : \quad z_{l3}(t) = k_{13}(k_1 z_{l3}(t-1) + x_{l1}(t)) , \tag{8}$$

$$NO_3^- : \quad z_{l4}(t) = k_{13}(k_1 z_{l4}(t-1) + x_{l6}(t)) , \tag{9}$$

$$NH_4^+ : \quad z_{l5}(t) = k_{13}(k_1 z_{l5}(t-1) + x_{l8}(t)) , \tag{10}$$

here k_{13}^{-1} is the total amount of water during a year (= field capacity + precipitation surplus). Initial conditions for these equations are

$$(z_{l1}(0), \ldots, z_{l6}(0)) = (z_{l1}^{init}, \ldots, z_{l6}^{init}) . \tag{11}$$

Define z_{l1} as an amount of carbonates in the soil (meq/kg); z_{l2} is an amount of AL-(hydr)oxides in the soil (meq/kg). Carbonates and AL-oxides are materials which are washed out the soil slowly. There is no natural replacement of the substance. The next equations depend upon signs of values $z_{l2}(t-1)$ and $z_{l1}(t-1)$.

3.2 Carbonate system (Case 1 with $z_{l1}(t-1) > 0$)

Let x_{l10} be HCO_3 concentration. The value $x_{l10}(t)$ equals positive root in the interval $[0, 1.0]$ of the equation

$$x_{l10}^3(t) + x_{l10}^2(t)x_{l9}(t) - x_{l10}(t)c_1 - c_2 = 0 .$$ (12)

H^+ concentration $g_l(t)$ is calculated by Henry's Law

$$g_l(t) \stackrel{\text{def}}{=} c_1/x_{l10}(t) .$$ (13)

In the next step an Equilibrium Equation for $CaCO_3$ dissolution is used to obtain concentration of $Ca^{2+}(BC^{2+})$ ions

$$z_{l6}(t) = x_{l9}(t) + x_{l10}(t) - c_1/x_{l10}(t) .$$ (14)

here z_{l6} is base cations ($Mg^{2+} + Ca^{2+} = BC^{2+}$) concentration. The amount of carbonates remaining in the soil is calculated by mass balance:

$$z_{l1}(t) = \max\{0, z_{l1}(t-1) + k_5 - z_{l6}(t)/k_{13} + k_1 z_{l6}(t-1)\} ,$$ (15)

$$z_{l7}(t) = 0 ,$$ (16)

where

k_5 is base cations input to soil, it is equal to base cations deposition minus base cation uptake of plants.

3.3 Aluminum system (Case 2 with $z_{l2}(t-1) > 0$ and $z_{l1}(t-1) \leq 0$)

This is the case for noncarbonate soils or as soon as carbonates are exhausted but AL-hydroxides are still available . Initialize

$$z_{l7}(t-1) = z_{l7}^{init} ,$$ (17)

$$z_{l8}(t-1) = z_{l8}^{init} ,$$ (18)

$$z_{l9}(t-1) = z_{l9}^{init} .$$ (19)

Now we have to calculate the input of BC^{2+} to water contained in soil, where the net input $k_5 + k_2$ must be larger than some positive limit k_6. Using massbalance assumption, the available amount of BC^{2+} per period is

$$x_{l11}(t) = k_5 + k_2 + k_8 z_{l9}(t-1) + k_1 z_{l6}(t-1) ,$$ (20)

4

where k_2 is weathering rate.

Next the system of certain exchange and aluminum buffering must be solved as described in [5] equations (8), (19)-(25). Transforming these equations the problem is reduced to finding a root in the interval $[0, b_0]$ for x_{l12} (the constant b_0 is calculated following the Figure 14 in [5])

$$
\begin{cases}
h_{l1}(t) = 1 - x_{l12}(t) - k_7 x_{l12}^3(t) \ ; \\
h_{l2}(t) = \max\{0, x_{l11}(t)k_{13} - k_8 k_{13} h_{l1}(t)\} \ ; \\
h_{l3}(t) = k_9 x_{l12}(t)\sqrt{h_{l2}(t)/h_{l1}(t)} \ ; \\
k_{10}h_{l3}^4(t) + h_{l3}^2(t) + h_{l3}(t)(h_{l2}(t) - x_{l9}(t)) - c_1 = 0 \ ,
\end{cases}
\tag{21}
$$

x_{l12} is H^+ ions saturation in exchange complex. The system can now be solved for all ions: AL^{3+} ions in exchange complex

$$
z_{l8}(t) = k_7 x_{l12}^3(t) \ ;
\tag{22}
$$

BC^{2+} ions in exchange complex

$$
z_{l9}(t) = 1 - x_{l12}(t) - z_{l8}(t) \ ;
\tag{23}
$$

BC^{2+} concentration:

$$
z_{l6}(t) = x_{l11}(t)k_{13} - k_8 k_{13} z_{l9}(t)
\tag{24}
$$

H^+ concentration

$$
g_l(t) = k_9 x_{l12}(t)\sqrt{z_{l6}(t)/z_{l9}(t)} \ ;
\tag{25}
$$

AL^{3+} concentration

$$
z_{l7}(t) = k_{10}g_l^3(t) \ .
\tag{26}
$$

Remaining Al-hydroxid in soil calculated by mass balance:

$$
z_{l2}(t) = \max\{0, z_{l2}(t-1) + k_{11}k_2 - k_{13}^{-1}z_{l7}(t) + k_1 z_{l7}(t-1) - k_8(z_{l8}(t) - z_{l8}(t-1))\} . \tag{27}
$$

3.4 Noncarbonate soil without Al-hydroxid (Case 3 with $z_{l2}(t-1) \leq 0$)

For non carbonate soils with exhausted Al-hydroxid the equation describing solubility needs to be removed from the system. Solubility of Fe is not included in this model.

As in the previous case the BC^{2+} input is calculated

$$
x_{l14}(t) = k_{13}(k_5 + k_2 + k_8 z_{l9}(t-1) + k_1 z_{l6}(t-1)) \ .
\tag{28}
$$

In addition input of Al^{3+} is given by

$$
x_{l13}(t) = k_{13}(k_{11}k_2 + k_8 z_{l8}(t-1)) \ .
\tag{29}
$$

5

The system is solved for exchangeable BC^{2+}, z_{l9} by finding a root in the interval $[0, x_{l12}(t) \ / \ k_8 k_{13}]$

$$\begin{cases} h_{l4}(t) = \max\{0, x_{l14}(t) - k_8 k_{13} z_{l9}(t)\} \ ; \\ h_{l5}(t) = h_{l4}(t)/z_{l9}(t) \ ; \\ h_{l6}(t) = \sqrt{h_{l5}(t)} \ ; \\ h_{l7}(t) = x_{l13}(t)/(k_{12} h_{l6}(t) h_{l5}(t) + k_8 k_{13}) \ ; \\ h_{l8}(t) = x_{l13}(t) - k_8 k_{13} h_{l7}(t) \ ; \\ h_{l9}(t) = 1 - z_{l9}(t) - h_{l7}(t) \ ; \\ h_{l10}(t) = k_9 h_{l9}(t) h_{l6}(t) \ ; \\ h_{l10}(t)(h_{l10}(t) + h_{l8}(t) + h_{l4}(t) - x_{l9}(t)) - c_1 = 0 \ . \end{cases} \qquad (30)$$

For the other ions in the system we get:

BC^{2+} concentration

$$z_{l6}(t) = x_{l14}(t) - k_8 k_{13} z_{l9}(t) \ ; \qquad (31)$$

Al^{3+} ions in exchange complex

$$z_{l8}(t) = x_{l13}(t)/(k_{12}\sqrt{z_{l6}^3(t) z_{l9}^{-3}(t)} + k_8 k_{13}) \ ; \qquad (32)$$

Al^{3+} concentration

$$z_{l7}(t) = x_{l13}(t) - k_8 k_{13} z_{l8}(t) \ ; \qquad (33)$$

H^+ ions in exchange complex

$$x_{l12}(t) = 1 - z_{l8}(t) - z_{l9}(t) \ ; \qquad (34)$$

H^+ concentration

$$g_l(t) = k_9 x_{l12}(t)\sqrt{z_{l6}(t) z_{l9}^{-1}(t)} \ . \qquad (35)$$

4   Pollution Control and Cost Functions

There are basically four ways to reduce sulfur nitrogen emissions originating from energy combustion:

1. Energy conservation;

2. Fuel substitution;

3. Use of low sulfur fuels;

4. Desulfurization during or after fuel combustion.

For options 2 – 4 the model RAINS contains a formal procedure to estimate potential reductions and cost of their applications [2]. Costs of energy conservation strategies are not investigated within RAINS, because goals other than pollution control may motivate energy conservation policies. Therefore, energy pathways are simulation parameters for the model (see Chapter 3 and "use" Chapter of the book [9]).

We consider that energy pathway for each country could be received as a solution of some other optimization problem. Suppose that each year t, $1 \leq t \leq T$ country i spends amount u_{tij} of money for emission reduction of gas j. If we designate by r_i the interest rate coefficient for the country i then during the time t the country i will spend money

$$\sum_{\tau=1}^{t}(1+r_i)^{T-\tau}u_{\tau i_j}$$

for reduction of emission of gas j. We suppose that real valued function $\nu_{ij}(v)$ determines the dependence of emission of gas j from the money v spent for emission reduction of this gas. The function $\nu_{ij}(v)$ is a convex and monotonically decreasing one, it can be received as a solution of other optimization problems (see "use" chapter of the book [9]). The function $E_{ij}(t, u_{ij})$ in formula (1) can be defined as follows

$$E_{ij}(t, u_{ij}) = \nu_{ij}\left(\sum_{\tau=1}^{t}(1+r_i)^{T-\tau}u_{r_{ij}}\right), t = 1, \ldots, T; \tag{36}$$

$$u_{ij} = (u_{1_{ij}}, \ldots, u_{T_{ij}}).$$

Designate by $\phi(u)$ the total amount of money spent by all countries during the time T

$$\phi(u) = \sum_{i=1}^{I}\sum_{j=1}^{3}\sum_{t=1}^{T}(1+r_i)^{T-\tau}u_{tij}, \tag{37}$$

here and later we designate vector $\{u_{tij}\}$ by u.

The definition of ϕ takes into account interest rate coefficients r_i.

Further we are going to minimize the value $\phi(u)$ subject to environmental and financial constraints.

We describe two variants of the model: stochastic and deterministic.

4.1 Deterministic model

In this case we suppose that in equation (1) coefficients $\alpha_{ilj}(\omega) = \alpha_{ilj}$ are not random. It means that, instead of random values, some average values were taken. In the model there are two kinds of constraints: financial and environmental.

Financial constraints:

$$\sum_{i=1}^{I}\sum_{j=1}^{3}u_{tij} \leq \bar{u}_t, \quad t = 1, \ldots, T, \tag{38}$$

$$u \geq 0 \, , \tag{39}$$

i.e., all countries can not spend more than $\bar{u}_t$ amount of money during year t.

Environmental constraints

$$g_l(t) \leq g, \quad l = 1, \ldots, L; \quad t = 1, \ldots, T \, , \tag{40}$$

i.e., the pH value for each location point l should not be greater than some threshold g during the time T.

We use nonsmooth penalty functions to include inequality constraints (40) into the objective function. In any case, objective function will be nonsmooth since there is *max* operation in dynamic equations and function $g_l(t)$ is nonsmooth with respect to control vector u. The reduced problem is

$$f(u) = \phi(u) + K \sum_{\substack{l=1,L \\ t=1,T}} \max\{0, \; g_l(t) - g\} \quad \rightarrow \quad \min_{u \in R^{T \times I \times 3}} , \tag{41}$$

subject to constraints (38) and (39). Coefficient K can be interpreted as the price for the violation of constraints (40), i.e., this is some money for recreation of soil if it is acidified (or the cost of environmental damage). This objective function $f(u)$ consists of two parts: money for the emission reduction and penalties for environmental constraints violations.

4.2 Stochastic model

Since coefficients $\alpha_{ilj}(\omega)$ are random in equation (1) then pH values $g_l(t)$ also are random. In this case problem (41) can be modified as follows:

$$\bar{f}(u) = \phi(u) + KE \sum_{\substack{l=1,L \\ t=1,T}} \max\{0, \; g_l(t) - g\} \quad \rightarrow \quad \min_{u \in R^{T \times I \times 3}} , \tag{42}$$

subject to constraints (38) and (39).

The second term in the objective function can be interpreted as a mathematical expectation of losses from environmental constraints violations.

5   Solution Techniques

To solve problem (41) one can use some subgradient nonsmooth optimization method (see, for example [6], [10] and [12]). Standard algorithms for dynamical systems can be applied [1] to calculate subgradients of the objective function $f(u)$.

To solve the stochastic problem (42), scenario analysis technique [13] or quasigradient algorithms (see [4], [7], [8], [11] and others) could be used. Stochastic quasigradients can be calculated with the formulae described in the paper [1].

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