**Case Study 4**

**Ecological Level Management of lakes through pH control using deterministic optimal control methods**

**Dr. Urmila Diwekar1 and Dr. Yogendra Shastri2**

1 Viswamitra Research Institute, Chicago, IL

2 Indian Institute of Technology Bombay, Mumbai, India

**Background:**

Mercury can exists in the water bodies in various forms, the important forms being: elemental mercury (Hg), inorganic mercury (Hg(II)), organic methylmercury (CH3Hg) and complexes of these with dissolved organic carbon or suspended particulate matter. Of the various chemical forms of mercury, methylmercury (MeHg) is considered to be the most dangerous due to following reasons:

* All forms of mercury can be converted to methylmercury by natural processes in the environment.
* Methylmercury bioaccumulates and biomagnifies in aquatic food webs.
* Methylmercury is the most toxic form of mercury.

“Bioaccumulation” refers to the net uptake of a contaminant from the environment into biological tissue via all pathways. It includes accumulation that may occur by the direct contact of skin or gills with mercury-contaminated water as well as by the ingestion of mercury-contaminated food. “Biomagnification” refers to the increase in the chemical concentration of a contaminant in organisms at successively higher trophic levels of a food chain as a result of the ingestion of contaminated organisms at lower trophic levels. The concentration of methylmercury in large aquatic animals (such as predatory fishes) is many times more than its water column or sediment concentration owing to its high bioaccumulative potential. Generally, the methylmercury fraction in a water column is not more than 25% of the total mercury content. In lakes without point source discharges, this fraction is typically less than 10%. However, it has been observed that almost all of the mercury present in fish tissues is as methylmercury, confirming its preferential bioaccumulation.

The concentration of MeHg in water depends on the equilibrium between the methylation and demethylation reactions, which occur in water column as well as sediments. Studies have shown a strong correlation between acidic conditions, i.e. low pH values, and high mercury bioaccumulation in fish. This correlation could be due to the higher concentration of bioavailable methylmercury in the ecosystems caused by altered chemical partitioning of methylmercury across the sediment-water interface, increased input of methylmercury to lakes from the terrestrial ecosystems or precipitation, or increased in-lake production of methylmercury. Even though the individual contribution of these factors is not precisely known, the overall strong correlation between pH and mercury bioaccumulation suggests a possible option of lake liming to reduce mercury bioaccumulation.

Liming is the addition of a base, such as limestone, to the water body to neutralize acid waters and soils, and buffer them from rapid fluctuations in pH. The base treatment increases the supply of basic cations, thereby improving water quality and fostering the presence of a broader array of organisms than found in acidic waters. The possible liming agents include: limestone minerals such as calcite (CaCO3) and dolomite (CaMg(CO3)2), hydrated lime (Ca(OH)2) and soda ash (Na2CO3).

Although lake liming has been relatively successful in Scandinavian countries, there are various issues related to liming that need further in-depth research. These are:

1. Liming accuracy: Presently, most liming decisions (liming dosage) are based on rule of thumb. The amount of lime to be added is decided using parameters such a lake volume, current lake pH, targeted pH and water salinity. These are mostly static decisions and do not account for the dynamic nature of the natural system (lake). It is obvious that such heuristics based decisions do not lead to accurate liming results.
2. Cost of liming: Liming entails considerable costs. Hence, it is essential that the liming operation is optimized to reduce expenses. Even though the liming technique is the major factor deciding the expenses, efficient implementation of the selected technique can reduce expenses.
3. Presence of uncertainty: Liming operation has to deal with the presence of various kinds of uncertainties, such as the lack of information on the exact pH of the lake, seasonal variations in lake pH, and the topological effects of liming. Moreover, the spatial and temporal effects of liming on lake biota are subjective.One needs to incorporate these uncertainties in the analysis to make liming implementable.

**Problem statement**

To make liming more accurate, an effective approach is to use time dependent liming where liming decisions (amount of lime to be added) change with time based on the current lake conditions. The reliability of liming can further be improved if these dynamic liming decisions are based on a systematic approach rather than heuristics. Such an approach is expected to simultaneously achieve cost effectiveness. In this case study, the goal is to use optimal control theory, an extension of the theory of optimization to dynamic systems, to determine the best liming policy to meet the lake pH targets.

**Specific activities for optimal control model formulation**

1. Identify and code the lake liming model
2. Identify the control variables in the model
3. Formulate the optimal control problem, including the objective
4. Identify a solution method to solve the problem numerically
5. Program the optimal control problem and solution method in a software (FORTRAN/MATLAB)
6. Exercise: Solve the model and analyse the results

**Connection to Case Study 2 and 3**

In case study 2 and 3, we discussed the economically efficient management of mercury pollution in a watershed using pollutant trading. However, some mercury will always be released in the watershed. Moreover, mercury from air will eventually be added to various water bodies due to dry and wet deposition. Therefore, the management of mercury at the lake/river scale will also be necessary.

**Identification of the lake liming model**

The basic lake liming model used here has been adapted from literature. It is a mixed model consisting of both statistical regression and dynamic interactions. An empirical model is used to predict the initial pH (mean annual pH). The model also includes a regression that predicts the natural pH. In addition to these empirical sub-models, the lake liming model consists of dynamic (time dependent) interactions. It is a compartmental model with three different compartments, namely, water, active sediment and passive sediment. Accordingly, the three model variables are:

1. Lime in water (
2. Lime in active sediment (
3. Lime in passive sediment (

Four continuous flows of lime connect the three compartments:

1. Sedimentation to active sediments
2. Internal loading from active sediments to water
3. Outflow from the lake water
4. Transport from active to passive sediments.

In addition, two flows give the inflow of lime from the liming, one to the lake water and one directly to the active sediments. The model is easy to handle since all input data can be obtained from maps and no field measurements are necessary.

The necessary input parameters in the equation are:

1. Lime distribution coefficient (*Dc*)
2. Internal loading rate (*ILR*)
3. Dynamic ratio (*Dr*)
4. Lake water retention time (*Rt*)
5. Sedimentation rate (*Sr*)
6. Active sediment age (*ASA*).

These parameters are dependent on other basic lake chemical and physical properties such as lake area, lake mean depth, lake maximum depth, lake color, lake total phosphorous concentration, drainage area and mean annual precipitation. The governing ordinary differential equations of the model are:

The lake pH needs to be connected to the lake liming model variables mentioned here. This is done by using the following equation which correlates lake pH with the lime in lake variable ().

The fourth equation needs to be converted into an ODE, and can be written as follows:

Here, the model assumes, for the sake of modelling, that the base value of lake pH is also due to the addition of lime. is the lime required to reach the base lake pH value assuming that the total lake pH is only due to lime addition. Therefore, any improvement in the lake pH can be achieved by additional lime addition (), which is then translated into the corresponding change in the lake pH. The model reported here has been developed using several assumptions which the students should read from the original paper by Shastri and Diwekar (2008).

In this model, is the total lime input to the lake, which is the control variable. is the tuning parameter of the model that is used for better linear approximation of the nonlinear pH relationship with respect to lime addition. The linear approximation is acceptable in the pH range of 4-10. Therefore, if the lake is highly acidic with the pH being lower than 4, then the complete nonlinear model needs to be used.

**Objective function formulation**

The formulation of the objective function is the next step. Here, the objective is to achieve a target pH of the lake and maintain that pH at the target level during the simulation horizon. Therefore, the objective function considers the value of pH during the whole simulation horizon. Let *T* represent the total simulation horizon. Then the objective function of the optimal control problem will be:

where, is the target pH of the lake.

This objective function does not consider the cost of liming. However, in reality, the cost of liming will play an important role in deciding the liming policy. If an accurate pH control costs a lot, it might be better to allow minor errors in pH control if that leads to significant cost savings. Therefore, the objective function can be modified to include the cost of liming. Here, the cost of liming is given as:

Therefore, the objective function can be modified as follows:

Here, and are the weights given to the respective components of the objective function.

**Optimal control problem formulation**

We will use the maximum principle to formulate the optimal control problem. The theory of optimal control problem formulation has been explained in the introduction section. The lake liming model presented earlier is the model of interest. The state variables of interest are - .

**Model application data:**

The proposed model of lake liming to control the lake pH can be applied to a hypothetical lake with the following parameters:

Initial lake pH = 6.15

Lake area = 1.26 km2

Lake mean depth = 8.5 m

Lake maximum depth = 26.2 m

Drainage area = 51.5 km2

Mean annual precipitation = 602 mm/year

Active sediment age (*ASA*) = 519.6 weeks

Internal loading rate (*ILR*) = 0.001 (1/month)

Lime distribution coefficient (*Dc*) = 0.5

Settling velocity = 0.074 meter/week

Additive constant = 2.375

*k* = 0.62

=5000

=3000

The other parameters are computed using these basic parameters as per the following relationships:

Lake volume = Lake area \* Lake mean depth

Water discharge = 0.01\*DrainageArea\*Precipitation/600

Lake water retention time in week (*Rt*) = Lake volume/(Water discharge\*60\*60\*24\*365/7)

Sedimentation rate per week (*Sr*) = Settling velocity/Lake mean depth

Dynamic ratio (*Dr*) = Lake area0.5/Lake mean depth

Simulation time horizon = 100 weeks

Simulation time step = 1 week

Upper limit on lime addition = 100 Mg/week

**References for further reading**

1. Håkanson, L., 2003a. Consequences and correctives related to lake acidification, liming and mercury in fish—a case-study for lake Huljesjon, Sweden, using the LakeWeb-model. Environ. Model. Assess. 8, 275–283.
2. Håkanson, L., 2003b. A general management model to optimize lake liming operations. Lakes Reserv.: Res. Manage. 8, 105–140.
3. Henrikson, L., Brodin, Y., 1995. Liming of Acidified Surface Waters. Springer, Berlin.
4. Håkanson, L., Boulion, V., 2002. The Lake Foodweb. Backhuys Publishers, Leiden.
5. Ottosson, F., Håkanson, L., 1997. Presentation and analysis of a model simulating the pH response of lake liming. Ecol. Model. 105, 89–111.
6. Riely, P., Rockland, D., 1988. Evaluation of liming operations though benefit-cost analysis. Water Air Soil Poll. 41, 293–328.
7. Sorensen, J., Glass, G., Schmidt, K., Huber, J., Rapp, G., 1990. Airborne mercury deposition and watershed characteristics in relation to mercury concentrations in water, sediments, plankton and fish of eighty northern minnesota lakes. Environ. Sci. Technol. 24, 1716–1727
8. Bertilsson, L., Neujahr, H., 1971. Methylation of mercury compounds by methylcobalamin. Biochemistry 10 (14).
9. Clair, T., Hindar, A., 2005. Liming for the mitigation of acid rain effects in freshwaters: a review of recent results. Environ. Rev. 13 (3), 91–128.
10. Donnelly, A., Jennings, E., Allott, N., 2003. A review of liming options for afforested catchments in Ireland. In: Biology and Environment: Proceedings of the Royal Irish Academy, vol. 103B, pp. 91–105.
11. Erikkson, A., 1998. Are the effects of acidification postponed and aggravated by lake liming? A laboratory study on a re-acidification of the limed Lake Gårdsjön, SW Sweden. Technical report, Department of Physical Geography, Göteborg.
12. Hindar, A., Kroglund, F., Lyderson, E., Skiple, A., Høgberget, R., 1996. Liming of wetlands in the acidified Lake Røynelandsvatn catchment in southern Norway: effects on stream water chemistry. Can. J. Fish. Aquat. Sci. 53, 985–993.
13. Nagase, H., Ose, Y., Sato, T., Ishikawa, T., 1982. Methylation of mercury by humic substances in an aquatic environment. Sci. Tot. Environ. 32, 147–156.