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THE ROLE OF TOXIC CHEMICAL MODELS IN EVALUATING THE IMPACT OF CONTAMINANTS ON OUR WATER RESOURCES

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Abstract

Modelling offers a mechanism for optimizing the often competing demands of regulation, environmental protection, and efficacy and cost of control measures. However, the sophistication of current toxic chemical models does not allow the impacts of toxic contaminants on our water resources and human health to be evaluated and predicted with great confidence. There is still a great need for quantitative data in areas such as toxic chemical loads to aquatic systems and biological metabolization. Sediment transport processes are also poorly represented in the current toxic chemical models. A means of correlating the results of ecotoxicology analyses with model predicted biotic uptake levels must also be developed. The use of expert system/artificial intelligence frameworks has greatly expanded the flexibility and scope of model applications. Toxic chemical management for large drainage systems is now possible through the use of systems such as the RAISON model (Regional Analysis using Intelligent Systems on a Microcomputer).

RÉSUMÉ

La modélisation offre un mécanisme d'optimisation des demandes souvent conflictuelles en matière de réglementation, de protection de l'environnement et d'efficacité et de coût des mesures de contrôle. Cependant, la complexité des modèles actuels de produits chimiques toxiques ne nous permet pas d'évaluer et de prévoir avec une grande confiance les impacts des contaminants toxiques sur nos ressources en eau et sur la santé humaine. Les données quantitatives dans des domaines comme les charges en produits chimiques toxiques dans les systèmes aquatiques et la métabolisation biologique sont encore très insuffisantes. Les processus de transport des sédiments sont également mal représentés dans les modèles actuels de produits chimiques toxiques. Il faut également mettre au point un moyen de corréler les résultats des analyses d'écotoxicologie et les niveaux d'absorption biotique prévus par le modèle. Le recours à des systèmes experts/intelligence artificielle a considérablement augmenté la souplesse d'utilisation et le champ d'application des modèles. La gestion des produits chimiques toxiques dans les grands réseaux de drainage est maintenant possible grâce à l'utilisation de systèmes comme le modèle RAISON (Regional Analysis using Intelligent Systems on a Microcomputer) (analyse régionale sur micro-ordinateur à l'aide de systèmes intelligents).

Management Perspective

As increasing pressure is applied to enforce the guidelines presented in the new Canadian Environmental Protection Act and, in Ontario, the MISA program for assuring water quality downstream of contaminant sources, greater emphasis will also be placed on the development and application of toxic chemical water quality models. The models will be used to optimize the competing demands of regulation, environmental protection, and cost of proposed control measures. This presentation outlines the current state-of-the-art in toxic chemical modelling and the areas of weakness which will require future research and development. The current and future toxic chemical modelling research at NWRI to protect the river environment are outlined.

PERSPECTIVE-GESTION

Face aux pressions de plus en plus fortes en vue de l'application des directives présentées dans la nouvelle Loi canadienne sur la protection de l'environnement et, en Ontario, dans le programme MISA afin d'assurer la qualité de l'eau en aval des sources de contaminants, il faudra mettre encore plus l'accent sur la mise au point et l'application de modèles de qualité de l'eau en ce qui a trait aux produits chimiques toxiques. Ces modèles serviront à optimiser les demandes conflictuelles en matière de réglementation, de protection de l'environnement et de coût des mesures de contrôle proposées. Ce rapport fait le point des connaissances actuelles sur la modélisation des produits chimiques toxiques et souligne les domaines qui nécessiteront des travaux de recherche et développement. On y présente également les travaux de recherche actuels et futurs en matière de modélisation de produits chimiques toxiques réalisés à l'INRE en vue de protéger les milieux fluviaux.

Introduction

An ever widening range of toxic chemicals in waters, sediments and biota generates an equally if not greater uncertainty in human and aquatic health effects. Effective remedial action and management of these contaminants requires careful examination of the complex cause and effect mechanisms that ultimately determine chemical fate, longevity, and toxicity. Toxic chemical models are continually being developed and upgraded to optimize the often competing demands of regulation, environmental protection, and efficacy and cost of control measures. The predictive capability of a mathematical model makes it possible to develop a credible and defensible water quality management program. The extent of the use of models for water quality management in Canada is not well documented (Beanlands and Duinker, 1983) but it would appear that there is still very little use being made of models in this country for environmental impact assessments and to evaluate the cost and effectiveness of legislation and treatment methods. The lack of user-friendly and well documented models has possibly prevented a more wide-spread use of models by regulatory personnel. The development of knowledge-based expert systems should help to expand the use of models in the area of water quality management.

Areas of Application

1) Ranking

The world's chemical industry generates 200-1000 new synthetic chemicals each year for which the ecological effects that they will produce must be predicted. Many countries now have legislation that requires tests for ecological effects. The first legislation was the Toxic Substances Control Act (TSCA), which was enacted in the United States in 1976.

In Canada, the Canadian Environmental Protection Act (CEPA) was enacted in 1987, incorporating and building upon the Environmental Contaminants Act. These pieces of legislation as well as MISA, for example, which is the program for assuring water quality in Ontario, have put pressure on the scientific research community to develop and improve the procedures and expertise required to predict the effects of these chemicals on ecosystems.

When laboratory and field data are not available, chemicals can be ranked using relationships such as QSAR (Quantitative Structure-Activity Relations). This classification may be used to roughly predict the behaviour of the chemical in the environment by assuming that it will behave in a manner similar to the other chemicals in its class which have been studied in the laboratory and the field. Most QSAR analyses are performed using acute tests with aqueous exposure of a few days. Very few sublethal effects tests are carried out for different species over a complete life cycle. The number of scientists working in the field of QSARs is increasing but, at present, QSARs are primarily suited for comparison or ranking purposes rather than prediction. The use of the increasing number of QSARs can certainly help in preparing priority lists of chemicals.

Another ranking method (PUC,1986) combines fate and toxicity data into a standardized index with the range 0...1. A third ranking procedure (Halfon and Reggiani,1986) is based on the hypothesis that a set of numbers (attributes) is generally necessary to create a ranking file. In this method, instead of an index, a Hasse diagram is used to display the ranking results. However, such simple empirical models do not take into consideration the environmental processes which control the ultimate toxicity of these chemicals and are usually not reliable enough to be used in final hazard assessments.

2) Chemical Fate

The wide range of physical and chemical properties of toxic chemicals finding their way into the environment results in a correspondingly diverse number of pathways being followed. Determining the "fate" of toxic chemicals in aquatic systems involves an evaluation of the final distribution of the chemical in the system. The "fate" processes are the set of transformation and transport processes that govern the distribution and nature of chemicals into aquatic systems.

At the National Water Research Institute (NWRI) we have tried to integrate experimental and field study results with model formulation. Key processes of study include air-water interface dynamics of the transfer of volatile organics, fine-grained particle transport, sorption-desorption, hydrolysis, complexation and precipitation, photodegradation, biodegradation, sedimentation, burial, resuspension, and bioaccumulation.

The type of model employed will depend on the nature of the particular application and also on the amount and quality of input data available for running the model as well as measured data for model calibration and verification. In many cases, data are incomplete and the models can only be used to determine bounds on the expected behaviour of the chemical. However, these kinds of results provide an efficient means to direct further studies to obtain specific information for future modelling efforts and regulatory decisions.

3) Exposure Evaluation and Risk Assessment

Analyses required for ecological effects evaluation are often more multifarious than those for exposure assessment. In evaluating exposures, the spatial and temporal concentration of a toxicant is required. Daughter products can normally be treated conceptually as separate, but linked state variables. The dimensions of the problem are far greater for ecological

effects assessment. There are a wide variety of possible effects at different hierarchial levels. Possible areas of study may include lethality, nonlethal effects, direct effects on any number of possible species present, and any indirect effects brought about by alteration of interactions between biotic species. Consequently, a model for analysis of ecological effects should be capable of predicting responses at all of these levels. Using such results, decisions could be made for regulating a chemical. At this time, however, we are still lacking the knowledge required to produce a model with advanced resolution.

There are different levels of resolution which can be used, depending on the application:

1. -analysis of steady-state chemical activity of toxicant in selected populations
2. -analysis of time-dependent chemical activity of toxicants in biota and the resulting effects in selected populations or small sets of interacting populations
3. -analysis at the ecosystem level in which direct effects are considered in the context of ecosystem interactions as well as indirect effects resulting from ecosystem interactions in the presence of direct effects

Given that the temporal and spatial concentrations of a contaminant can be predicted for ecosystem compartments, the probability of exposure must be known in order to predict effects. This would require the use of a Monte Carlo technique, which by its nature would add significant computational time to ecosystem model execution. However, it is possible that, in practice, careful preselection of conditions and biotic systems can be carried out during model development so that the selective use of a limited number of scenarios can be used heuristically to reduce model complexity.

4) Evaluation of control measures

Waste load allocation models have been developed (majority of them in the U.S.) to help implement water quality criteria for toxic pollutants. These criteria consider both magnitude of a pollutant concentration and duration of exposure of organisms to that concentration. Steady-state models are widely used to develop waste load allocations for wastewater discharges; however, they cannot predict the variation over time of receiving water assimilative capacity or effluent quality and quantity. The impact of receiving water variability on the duration and frequency of criteria violations are often implicitly included by the design condition. Consequently, dynamic models are more appropriate since they explicitly predict the concentrations of a contaminant in the receiving water and the effluent variability. Prediction of complete probability distributions allow the risk inherent in alternative treatment strategies to be directly evaluated.

Current State-of-the-art of Toxic Chemical Models

There are a wide range of models available for toxic chemical evaluations. The prognostic models are normally used by professionals in government regulatory offices whereas the diagnostic models are used by applied researchers. These range from statistical (DYNTOX) to large deterministic models (EXAMS, TOXIWASP, WASP4), which are generalized models which try to include all key physical and chemical processes.

Of the many models in the literature, only a few have been used extensively in the public domain, due to the lack of the basic data required in applying the models or because the models have not been well documented or designed to be user friendly. Models are currently capable of predicting the fate of chemicals based on their physical and chemical properties. However, the capability to predict the effects of toxic chemicals is currently at a much less well developed level.

There are two major classes of models; a) empirical and b) deterministic. The major advances in risk analysis modelling have been the incorporation of deterministic algorithms that permit analyses based on chemical and environmental properties, with less reliance on empirical relationships of the behaviour of the chemical in various environmental systems. This approach is now taken in a number of models (EXAMS, WASP4, and QWASI, etc.) which incorporate both equilibrium and kinetic algorithms to represent processes that rely on measured or estimated values. In the steady-state mode, the evaluation of the general climate of chronic exposures to be expected can be evaluated. When models are run in the time-variable mode, the seasonal patterns of exposures and the frequency and severity of acute stress events on resident species and populations can be evaluated from the concentration time series output data. These models are very useful in indicating which processes are dominant and can be used to direct field and laboratory programs. The models also allow a systematic means of extrapolation of the results of laboratory tests to environmental systems.

In order to maintain consistent evaluations in water quality management of toxic chemicals a hierarchial evaluation scheme should be followed according to a basic protocol. The incorporation of the basic protocol and a hierarchy of assessment models into an expert system framework would appear to be the best available method of performing toxic chemical assessments. The expert system could contain libraries of essential information such as physical-chemical properties of toxic chemicals, expected ranges for model parameters, and standard application scenarios.

At the lowest level, the expert system may be used to increase the performance level of the model user by providing advice on procedures/inputs which require judgmental

expertise. The inputs that require advice are normally those that are estimated rather than measured. Inputs such as forcing functions are system specific and should be measured whenever possible. Calibrated coefficients and system definition inputs are key candidates for an expert system. The expert system model for toxic chemicals would include the following basic components:

1) Expert system shell (includes inference engine)

2) Data base (declarative)

3) Knowledge base (relational)

4) Process models or sub-models

5) Geographic information system

The main benefit of an expert system approach to environmental assessment modelling is the immediate availability of both physical and chemical behaviour data for the large number of possible chemical contaminants that could be released to the environment. The knowledge base would contain information that would allow values for the physical and chemical properties of chemicals as well as model coefficients, which are not in the data base, to be estimated. These values would then be available to be entered into the model, along with their associated uncertainty values. The expert or knowledge-based systems are designed to compile the experience of any number of experts in a given field into a series of rules, which are then used to draw inferences and, at a higher level, to suggest to the model user a course of action to deal with a given problem.

The control or inference structure of the expert system can be developed to specify how the data and knowledge can be manipulated to solve the problem. If the expert system is designed to utilize a large number of models or sub-models, the expert system could search

the knowledge base model library for models which best meet the objectives of the user. If no one model completely satisfies these objectives, the expert system could be developed to the level where it could construct a model from the available models, sub-models, and process algorithms contained in the model library.

At NWRI, Burlington, Ont., an expert system/intelligent interface has been developed and applied to the regional analysis of acid rain as well as chemical spill management. The expert system software is known as the RAISON Micro system. The RAISON (Regional Analysis by Intelligent Systems ON a microcomputer) system (Swayne and Fraser, 1986; Lam et al., 1988) is developed basically to meet the demand of environmental applications in which the knowledge base involves physical, chemical and biological disciplines and the data cover the air, soil and water regimes. RAISON is designed with five interlinked subsystems: map, database, inference rules, models and analysis. In RAISON, with all five components interlinked, the application from one problem to another can be achieved readily, with capability to link to other existing expert system shells.

An example of application is on acid rain problems. The problem arises from the emission of sulphur dioxide and nitrogen oxide from industrial and other sources. These chemicals are transported in the atmosphere over large distances and are deposited, both in the dry and wet forms, onto the land surfaces. Information from air, land and water has to be integrated and the predictions have to be made by selecting the most appropriate models according to a set of heuristic rules and the overlayed map system. For example, in one case, the knowledge rules are based on simple partition values of the acid neutralizing capacity (Lam et al., 1988). In another case, indepth rules are constructed for the incorporation of the influence of organic acidity produced in bogs and forests which can

interact with the inorganic acidity from acid rain. Figure 1 shows a possible tree structure relating the condition of dissolved organic carbon (DOC) to water movements, water temperature and forest coverage. These rules are based on knowledge provided by domain experts in this area of study. For relatively still water areas such as bogs and wetland, the production of DOC is known to be higher than streams or lakes with moving water. In general, warmer water temperature and greater abundance in coniferous trees are conducive to higher DOC. The results (Figure 1) as recommended by the expert system are based on the logical combination of these conditions. Based on the recommended classification, an appropriate organic acid submodel (Lam et al. 1988) can be selected to be used in conjunction with the inorganic acidity model (Lam et al., 1988). Similar design for other environmental problems can be based on the selection of models or model coefficients by integrating information from database, map and heuristic rules.

Current Areas of Weakness

1) There continues to be a problem of a limited amount of appropriate quantitative data that is required for calibration and validation of existing models.

2) The large number of possible metabolites which can be formed from a single parent compound in different biota makes predictions very difficult. This is not only true for different species but also for the same species at different times of the life cycle and season.

3) Many priority pollutants are preferentially associated with sediment. These sediment associated contaminants are ingested by benthic organisms and are subsequently biomagnified in the food web. It has been observed (Ongley et al., 1988) that there is little comparability between toxic response of whole water samples and suspended

sediments contained in the whole water samples. There was also a much greater toxic response and a greater number of priority chemicals associated with suspended river sediments than in water samples. It was also observed that priority chemicals can exist in water or on sediments, yet produce no toxic response in one or both of bioassay procedures (*Panagrellus redivivus* nematode assay and a nonstandard modification of the Ames bacterial test) used. Consequently, it is suggested that water alone is often insufficient to characterize toxic chemicals in aquatic systems or to use as the sole water quality criterion for water management.

4) Significant uncertainties exist in correlating the results of ecotoxicology analyses with model predicted biotic uptake levels. These exist for a number of reasons:

(a) Usually more than one compound is involved and there may be several degradation products or metabolites formed which have different biological effects.

(b) Several compounds may interact to produce a specific biological effect.

(c) The actual periods and concentrations of exposure are difficult to predict for mobile organisms

(d) Species, and different groups within species, react differently to the same exposure, for both genetic and environmental reasons

(e) Effects may be mediated not only by direct toxic effects on individuals, but also indirectly by altering the abiotic environment.

5) The use of toxic chemical models by management is limited by the user's lack of knowledge of the basic assumptions and understanding of the process algorithms used in the model. The user is also often unfamiliar with the acceptable ranges of values which can be used for the model parameters and coefficients. These problems can be overcome

by the model developer supplying a detailed user's manual, or perhaps, even more effectively, by the use of knowledge-based expert system models.

Conclusions

1) Current models are capable of predicting the relative amounts or concentrations of a chemical in an environmental compartment, the dominant chemical reactions, principal transport routes and overall persistence with reasonable accuracy.
2) The current models are not capable of predicting ecotoxicological effects with reasonable certainty.
3) It is questionable whether we will ever be able to predict with absolute certainty the ecotoxicological effects of chemicals
4) Knowledge-based expert systems should allow a larger percentage of the people working in the area of water quality management to use toxic chemical models more effectively
5) It is unlikely that even the most sophisticated artificial intelligence models will ever be capable of the high degree of integrative and interpretive analysis and insight of the human mind. The user of an expert system would still be required to be aware of the abstract and hypothetical nature of the environmental scenarios which are represented by the models. It would always be the responsibility of the human analyst to exercise control over the selection of scenarios and the interpretation of results.

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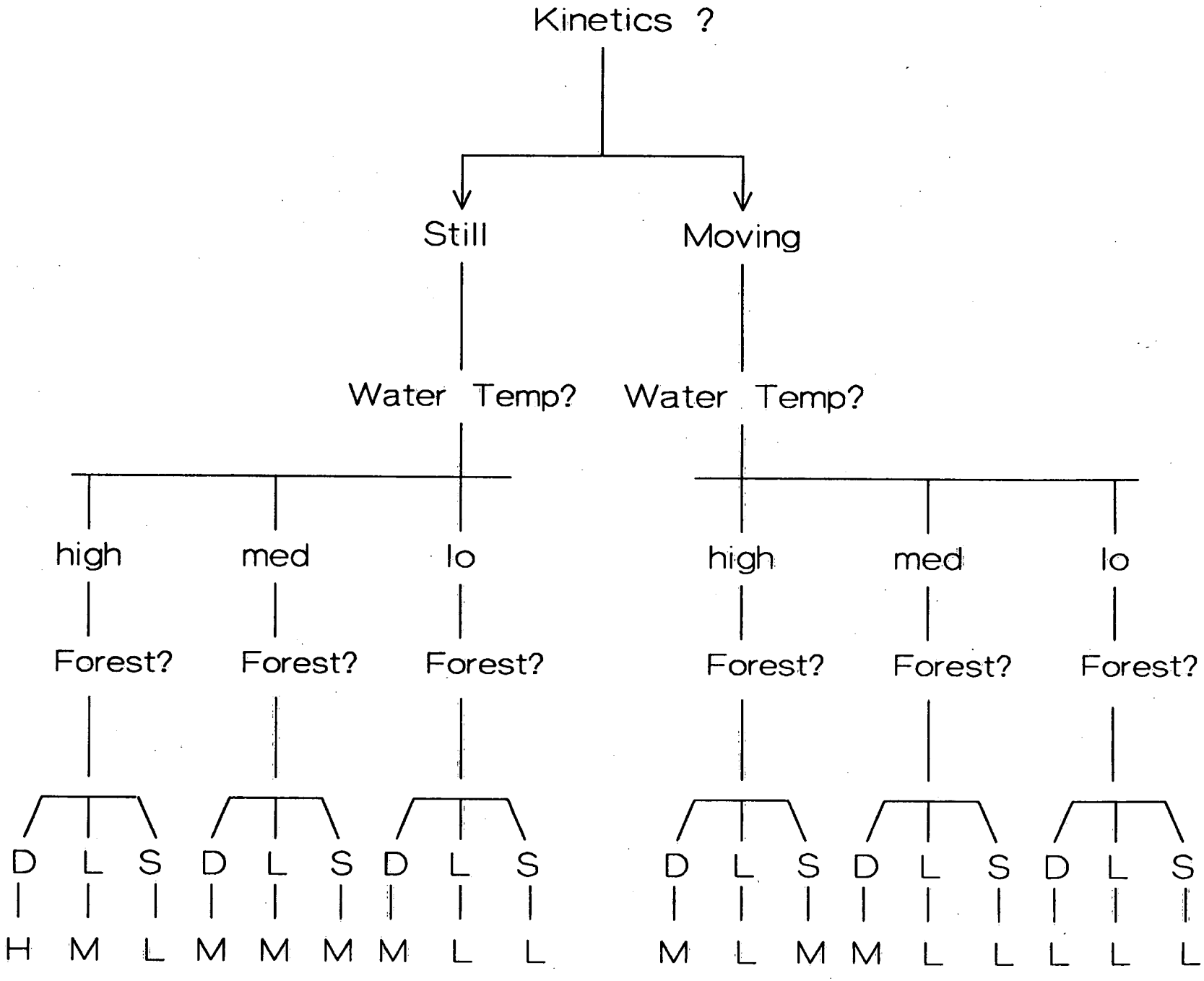
Figure 1. Example of tree structure used for relating DOC concentration to water flow, temperature and forest; where: H = high DOC, M = medium DOC, and L = low DOC; D = dense forest, L = light forest, and S = sparse forest.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