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Fitting CMLS Model to Brazilian Conditions: Results and Recommendations

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“Scientists conduct experiments to understand natural processes. From this understanding they create models that help to extend this knowledge to new areas and new conditions. Models are generally made for a specific purpose. They always involve simplifications. The model developer has a responsibility to enable the user to understand these simplifications. The model user must select a model which is consistent with the system of interest, the answers required, and the data available.”

David Nofziger

Preface

The use of mathematical models is an important component of environmental studies, and the need of having adequate models for tropical and subtropical environments, in contrast with temperate conditions, has often been pointed out. This technical report is a written compilation of annotations from an international workshop on adapting the model Chemical Movement in Layered Soils – CMLS, as a study-case, to Brazilian soil and weather conditions. Changes and additions to the model were discussed as well as the need for Brazilian data on soil properties and pesticide sorption and degradation. The discussion on these items was thought provoking and stimulating, and a consensus was reached in some cases to decide the approach to be taken for CMLS customization.

I am grateful to many people at Embrapa Environment, Embrapa Secretariat for International Cooperation, Embrapa Labex, Embrapa Information Technology, Inter-American Institute for Cooperation on Agriculture, and Herbicide in the Environment Committee of the Brazilian Weed Science Society for their diligence and efforts. I would like to extend my thanks to the participants for their valuable contributions, especially to Dr. Arthur Hornsby, University of Florida, Dr. David Nofziger, Oklahoma State University, and Dr. Rai Kookana, CSIRO, Australia.

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Contents

Fitting CMLS Model to Brazilian Conditions: Results and Recommendations

Claudio A. Spadotto

Introduction

There are two basic approaches in modeling hydrologic processes and solute transport in soil. The mechanistic modeling incorporates the most fundamental mechanisms and defines the change rate of water content and solute concentration. Research models are examples of mechanistic models that deal with knowledge seeking better understanding of processes, and provide insights to develop simplified, more practical models. They are useful to identify information gaps and areas of needed research, and researchers concepts may raise questions based on using research models. Research models can also be used in coordinating multidisciplinary work. Functional modeling incorporates simplified treatments of solute and water flow, defines changes in amounts of solute and water content, uses capacity factors and is oriented to management or decision-making. Decision-making models deal with information and are easy and economical to use. Models can be deterministic or stochastic. Deterministic models can simulate the system's response to a single set of assumed conditions, thus a given set of events leads to a uniquely definable outcome. Stochastic models are structured to account for the uncertainty and take into account the variability of both input conditions and model predictions (1, 2, 23).

There is an array of different pesticide models. For instance, the Chemicals, Runoff, and Erosion from Agricultural Management System - CREAMS (5, 6, 7, 8, 10) is a general, flexible model to evaluate relative Best Management

Practices (BMP) effects on water quality. It is continuous, field scale, daily time step, and physically based with some empirical relationships. The Groundwater Loading of Agricultural Management System - GLEAMS (11, 12, 13) evaluates effects of agricultural management on chemical movement within and through the root zone. It is continuous, field scale and daily time step model. The purpose of the Integrated Simulation Model for Non-point Source Pollution at Field Scale - OPUS (4, 21) is to study effects of weather and management inputs on water and pollutant movement in small watersheds. It is continuous, field scale and daily time step model with option for detailed storm event, and physically based with some empirical relationships. The Pesticide Root Zone Model - PRZM (14) is a dynamic model to simulate chemical movement in the vadose zone of soils. It is continuous, field scale and daily time step model, and provides information regarding pesticide transformations and movement needed to evaluating registration and use requirement. The Leaching Estimation and Chemistry Model - LEACHM (9) simulates chemical fate and transport in transient-flow field situations as well as in laboratory columns subject to steady-state or interrupted flow. It has a subroutine (LEACHP) that estimates pesticide transport. The Chemical Movement in Layered Soils Model - CMLS (15,16, 17) estimates the movement of organic chemicals in soils in response to downward movement of water, and also estimates the degradation of the chemical and the amount remaining in the soil profile.

CMLS Model – An Overview*

Developers:
D. L. Nofziger, Department of Agronomy, Oklahoma State Agricultural Experiment Station, Oklahoma State University, Stillwater/OK; and A. G. Hornsby, Dept. of Soil & Water Science, University of Florida, Gainesville/FL.

Description:
CMLS94 is an update to the original CMLS model (15, 17) written to serve as a management tool and a decision aid for the application of organic chemicals. CMLS can be used to estimate the movement of chemicals in soils in response to downward movement of water. The model also estimates the degradation of the chemical and the amount remaining in the soil profile. CMLS was specifically formulated for ease of use. All of the parameters required by the model are relatively easy to obtain. CMLS94 includes routines to estimate daily infiltration and evapotranspiration values from historical weather records.

A new feature of CMLS94 is the ability to assess uncertainty in leaching estimates due to unknown future weather at a site, spatial variability of soils, and uncertainty in chemical properties. This additional capability provides the decision-maker with insight into the range of leaching expected or the probability of leaching more than a specified amount of chemical past some critical depth. Various types of graphs and forms of tables are provided to view results. Extensive data entry and editing capabilities are also provided. The model is written for MS-DOS computers and is available on the Internet.

Water Quality Applications:
Examine the position and amount of pesticide in the vadose zone as a function of time for specific soils, application dates, application depths, weather and irrigation regimes, and other site-specific conditions. Obtain probability distributions for the amount of chemical leaching beyond a critical depth, the depth of chemical at a specific time, and the time required for a chemical to reach a specified depth. Compare the leaching potential of different pesticides for a specific soil-management system. Rank pesticide leaching for different pest management systems. Estimate the current depth of an applied pesticide to determine if an additional application is needed. Demonstrate the impact of specific soil properties, chemical properties, weather, and management

* From CMLS web site: http://soilphysiscs.okstate.edu/software

practices upon pesticide leaching.

Features:

CMLS94 is an interactive model in which the user defines the soil - chemical - management system using pull-down menus and interactive screens. Context sensitive help messages are available to aid the user. A batch version of the software is available for large studies and geographic information system (GIS) work.

The effect of unknown future weather at a site upon leaching estimates can be determined using a built-in Monte Carlo simulator and the Weather Generator - WGEN (20). Soil and chemical properties required in the model are easily obtained. A soil profile can be made up of up to 20 layers with different soil properties. Sorption coefficients and degradation rates of chemicals can change from layer to layer. Extensive database management capabilities are built into the software to enable the user to enter and reuse soil and chemical properties for their sites.

Sixteen types of graphs and numerous types of tables are provided so the user can easily examine the results of simulations. These include histograms and probability distributions for examining the range of behaviors resulting from uncertainties in future weather at the site as well as naturally variable soil and chemical properties.

Supplemental irrigation can be read from a file, applied on a periodic basis, or scheduled by depletion of water in the root zone. The impact of tillage upon leaching can be estimated by simulating transport using different curve numbers appropriate for each practice. Daily infiltration amounts can be provided by the user or estimated from daily weather records. Daily evapotranspiration can be read from user-provided input files or estimated from daily weather data using one of several built-in estimators.

Limitations:

The CMLS94 user's manual (16) describes in detail all the processes incorporated into the model and the assumptions made in it. In some applications the assumptions may be limitations, but in many cases they represent useful simplifications based on comparisons with research models.

CMLS94 does not attempt to estimate pesticide concentration profiles, but only the location of the center of mass and total amount of pesticide. It does not track the production, transport and fate of chemicals produced during degradation of the applied pesticide. Upward movement of pesticide in the profile is ignored. This may lead to overestimating leaching in very dry regions. The degradation rate is not adjusted for temporal changes in temperature or soil water content. CMLS94 does not attempt to estimate preferential pesticide movement through large soil pores and cracks.

Discussion Summary

Below is a summary of the discussion as well as a table of features and capabilities wanted in the revised version of CMLS for Brazil.

How does CMLS deal with compacted layers?

Concern was initially raised by Dr. Spadotto about the impact of restrictive layers in the soil upon CMLS estimates. Layers with lower conductivity will not alter the way CMLS handles water movement. It will continue to redistribute water very rapidly. If the layer is totally impermeable, the flow will be two or three-dimensional since the water will flow down to the impermeable layer and then move downhill along the top of the impermeable layer. No one-dimensional model will be able to accommodate these layers since flow is not one-dimensional. If the layer is a conductive layer but just lower in conductivity, water will move through the layer at a smaller rate, so the estimated chemical depth in CMLS will likely occur a few days after the date predicted by CMLS.

Dr. Hornsby stated that the presence of such a layer could limit root penetration and so would alter the depth of root zone entered into CMLS. Various individuals indicated that both fragipans and plow pans, or traffic pans are present in Brazil's soils. The issue of layered soils was not resolved, and the group asked Dr. Nofziger to investigate methods of incorporating these layers into the water balance component of the model or to demonstrate that it is not needed.

This discussion led to take into account runoff and infiltration estimates. Many participants are very concerned about dealing with runoff. Assuming that all of it enters the soil is not a satisfactory assumption for participants. One problem is that U.S. Soil Conservation Service (SCS) curve numbers are not known for soils in Brazil. After discussing this issue at some length, it was decided that there is a need to speak with hydrologists and soil scientist working on erosion to determine how rainfall is partitioned into runoff and infiltration. Dr. Nofziger offered to incorporate the Brazilian system of partitioning rainfall into infiltration and runoff into the Brazilian version of CMLS. If SCS curve number continues to be used, documentation for it should be incorporated into the model itself so the user can better define an appropriate parameter. Dr. Dornelas de Souza requested that tillage effects on infiltration be incorporated into the model. The problem pointed out is that no one can reliably state the impact of tillage and the duration of that impact.

How does CMLS deal with pH effects?

A point discussed was how to incorporate pH dependent sorption of ionizable compounds. As noted by Drs. Spadotto and Regitano, a function describing the dependence of sorption on pH is needed, since soil pH has a direct and indirect impact on sorption. Direct effect is exerted via changes that pH causes in the chemical characteristics of pesticides, such as the acidic compounds would dissociate as pH increases and vice-versa. The indirect effect is expected through the influence of pH on the soil properties, such as pH dependent charge and possibly physical changes in organic matter matrix affecting accessibility of compound to hydrophobic sites (22). Although the Brazilian soils have variable charge the net charge on this soils are negative, except some subsurface soils. Therefore it was concluded that the primary driver of sorption is via pH determined fraction of ionic versus neutral species.

It was recognized that pH of the soil is not considered in CMLS. The group agreed that pH and pK (ionization constant), and maybe ionic strength, must be incorporated into any model expecting to predict transport of ionizable pesticides. Dr. Nofziger stated that he fully expected to expand the databases for soils and chemicals to accommodate more properties. For example, he certainly expected to include soil pH by depth in the database. Dr. Nofziger asked how to use that information to improve our estimate of sorption coefficient (Kd) or organic carbon partition coefficient (Koc), and this stirred considerable discussion and thoughts. One approach is to list Koc values in the database for several pH values. If the pH of the soil matched one of these, that value would be used. If it did not, an equation would be used to obtain it.

How does CMLS deal with temperature effects?

The topic of the impact of temperature on transport and fate was introduced by presenting analysis of retardation factor (RF) and attenuation factor (AF) assuming steady water flow where degradation, volatilization, and sorption were considered functions of temperature, based on Paraiba and Spadotto (18). In this modified form of AF the effect of temperature on degradation, volatilization, and sorption were considered by taking a minimum AF approach, to represent worst-case scenario. While this demonstrated the effect on temperature on the above process, the only component that is amenable to inclusion in the currently model is the temperature effect on degradation. For sorption it is advisable to ignore the temperature effect. This is because firstly the impact is small, secondly the model based on activation energy does not suit the partitioning mechanism and thirdly the activation energy data would put intensive pressure on resources to generate data. The effect on volatilization can possibly be included in the model but it would have to assume that volatilization losses could only occur from within certain specified depth. No resolution was reached on this aspect.

How does CMLS deal with different rainfall regimes?

Considerable discussion revolved around high rainfall intensity and possible constraints to infiltration of water. Several conditions can contribute to runoff of fraction of water, and soil properties are only one of the factors. Under this circumstance, it was decided that the group need to explore the availability of infiltration rates for soils. It would be highly desirable to measure and use the actual infiltration rates in CMLS, as water movement is crucial component of pesticide leaching. The model output is expected to be highly dependent on this parameter.

Dr. Nofziger explained that daily rainfall amounts from the area of interest must be provided. The CMLS model reads this data and uses it for the simulation. Similarly, potential evapotranspiration data must be available or calculated using weather data. He encouraged the group to use historical weather from 20 – 25 years or more instead of the weather generator.

How does CMLS deal with degradation rate changes with depth?

The group was interested in incorporating the general decline in degradation rate with depth in a soil. This adjustment is in addition to the correction for temperature. The group acknowledged that the manner in which degradation rate varied with depth was not known quantitatively. It was suggested that a literature study should be made of this topic and that someone attempt to find a rule of thumb that could serve as an improvement over assuming that degradation rate is constant with depth. That rule could be used until such a time that a more quantitative method is available.

Some operational problems with CMLS94 were also pointed out by Drs. Pessoa, Dornelas, Spadotto and Paraíba, and those have been listed in the following table along with all of the items wanted in the revised version of CMLS based on the workshop.

Summary list of wanted capabilities for "CMLS-Brazil".

Capability	Related Work
Ability to adjust water movement for impeding layers of reduced hydraulic conductivity.	Decision about how to identify impeding layers without adding excessive data requirements. Formulation of finite time for redistribution based on the properties of the impeding layer.
Ability to partition rainfall into infiltration and runoff.	Ask hydrologists and soil scientists in Brazil how that is done. If a workable model is available, incorporate it into CMLS; if not, see if they can assist in assigning SCS curve numbers to soils.
Ability to adjust infiltration characteristics for tillage practices.	Research to characterize this impact of tillage and the way it changes with time, number of rainfall events, or cumulative rainfall.
Ability to adjust sorption and subsequent movement for changes in pH of soil.	Obtain pK for compound and one or more Koc values at known pH values (in appropriate proximity to pK). Test model for interpolating Koc at pH not in database. Add Koc interpolator to model.
Ability to adjust degradation rates for soil pH, depth in soil, and temperature.	Investigate manner in which degradation rate changes with pH; estimate degradation rate changes with soil depth; assess temperature predictor for different cover cropping conditions in Brazil.
Ability to model ionic pesticides.	Above work for pH dependence is the first step.
Ability to estimate volatilization and other dissipation of chemical before entering soil.	Formulate model for these losses based on literature studies.
Implement weather generator for Brazil's weather	Collection of historical weather data from many stations throughout Brazil. Examination of suitability of WGEN (and other current weather generators) to reproduce these weather distributions. Develop new weather generator if needed.
Ability to deal with volatilization below the soil surface.	Perform sensitivity analysis of losses in this manner for soils with high temperatures.

Summary list of wanted capabilities for "CMLS-Brazil" (continued).

Capability	Related Work
Provide information in program about SCS curve number and how to assign values to soils.*	Find reference material on curve number, translate it into understandable terms if needed, and insert it into software.
Ability to deal with particle densities substantially different from 2.65 Mg m^{-3}.*	Provide model user with ability to define appropriate particle density or make error checking only a warning.
Ability to accumulate mass of pesticide in soil when multiple applications of the same product are made.*	Currently requires user to add these values together outside of the program. Add additional output option to calculate this internally.
Support floating point numbers as temperatures and rainfall amounts.*	Question: Is this a limitation in data stored or simply in the way it is displayed?
Support for multiple values of chemical properties for the same chemical. Possibly associated with different soils, areas, or simply different samples.*	Currently requires user to make names unique. Databases need to be restructured to facilitate this in any other way.
Warning to user if the are about to exit a "window" without saving information entered.*	More sophisticated editor required.
If more than one application of a chemical is being made in one simulation and the user manually edits the Kd or half life values for one application, ask if they want to change those for all applications instead of requiring them to enter them for each one.*	More sophisticated editor required.
Ability to save screen images of graphs or to print graphs.*	Incorporate this technology.
Ability to print all of the input data used for a particular run, including edited data.*	Add this to output options.

* Originally presented by Pessoa et al. (19).

Recommendations

Based on the discussion, Dr. Kookana summarized the following recommendations for revision of CMLS for Brazil as a cooperative work.

- Prior to application of CMLS under Brazilian conditions some customization and modifications in CMLS model are desirable. These will involve the inclusion of pH effect on sorption of ionizable pesticides and the effect of temperature in degradation. An appropriate function to extrapolate pesticide sorption coefficient (Koc) to different pH conditions should be identified. Depth dependent rates of degradation are worth of inclusion in CMLS, especially when the depth based pesticide fate data are not readily available. The effect of temperature on sorption is not worth pursuing at this stage, given the uncertainty of other parameters and lack of local environmental fate data. Capability of CMLS to deal with the locally relevant infiltration rates in soils should be enhanced. In this respect an effort should be made to gather and review data on infiltration on soils of the target area.

- A literature review of overseas reports shows that from the standpoint of groundwater contamination, herbicides and soil applied pesticides are of a greater concern. Therefore, Brazilian researchers may wish to consider this during the selection of target pesticides for the current project.

- Pesticide fate data for the select group of pesticides and soils would need to be developed locally. In this process several groups could collaborate together but the protocols adopted should be carefully considered and need to be uniform across the group.

- The weather data would need to be gathered. This is a crucial set of information for CMLS application and there is an excellent opportunity to do so.

- The soil physics contribution to this project is crucial and efforts should be made to obtain greater input from this discipline into the current project.

- Obviously the transport of pesticides is governed to a large extent by water movement. Therefore, the water movement in the local soils needs to be adequately understood first, before dealing with chemical and biological factors affecting pesticide transport.
- Finally, there is high degree of similarity in soil and climatic conditions between Australia and Brazil. Therefore, it is of mutual benefit that the collaboration initiated through the present activity is further enhanced and efforts need to be made by both parties to foster an environment of active collaboration in the future.

A suggested standard protocol was presented by Dr. Hornsby and discussed for future collaboration among workshop participants to ensure compatible experimental methodology and results as follows. Future researches on pesticide fate in Brazilian soils should be a cooperative effort among workshop participants. During the conference and workshop the participants learned of each other's research and some expressed a desire to collaborate with one another. This is an opportunity to share expertise, ideas, and funding using common objectives and protocols. This will result in rich, compatible databases on pesticide environmental fate data that can be used for developing or adapting environmental fate models for use in Brazil or multiple objective decision support systems to assist farmer maintain their economic stability while simultaneously protect the environment. The following suggested protocol approach is offered as a possible starting point for a collaborative research effort:

1. Select a set of "benchmark chemicals" that are highly relevant to objectives of interested researchers.

2. Similarly select a set of "benchmark soils" to be used for collaborative pesticide fate studies. These soils should be representatives of areas of important crop production and/or environmental concerns.

3. Conduct all experiments with commonly agreed protocols, that is, for each determination set forth a protocol (procedure) agreed by all individual researchers. The following list of determinations could then be addressed: (a) sorption coefficients, (b) degradation rate, and (c) soil physical and chemical properties

4. Soil samples collected for these studies should be taken for each morphological horizon, or other depth intervals relevant to study needs and the site characterized with respect to soil map unit or soil type, depth intervals of horizons, position in the landscape, and global positioning system (GPS) coordinates of the soil sampling sites. Soil type should be verified by a soil scientist knowledgeable about soil classification. Analytical procedures of soil parameters will be those presented in Embrapa publication (3) or other procedures mutually agreed upon by the project participants. Physical characteristics measured should include as a minimum: bulk density, particle density, particle size distribution, saturated hydraulic conductivity, and water-release curves, and clay content and mineralogy. Chemical characteristics measured should include as a minimum: organic carbon content, soil pH and zero point of charge (ZPC) using standardized common methodologies. Sorption and degradation experiments should be conducted with soils where pH has been adjusted to the following range of pH values: 2.0, 3.0, 4.0, 5.0, 6.0, and 7.0. Sorption should be measured on soil with organic mater (OM) and with organic matter removed. Methodology for adjusting pH and OM removal should be a common protocol. Degradation studies should be conducted at a range of temperatures relevant to Brazilian soil and climatic conditions.

Conclusions

Several aspects were discussed at the workshop, including adequacy of data, how to include pH and temperature effects in CMLS. The different precipitation regimes in Brazilian conditions and soil compaction aspects were also considered. Results and recommendations from the workshop are not restricted to the CMLS model and include the following: recognition on the part of Brazilian scientist of the need to work together, share ideas and common interests, use common protocols for conducting pesticide environmental fate studies and the need for a model that is relevant to Brazilian soil properties. Dr. Nofziger plans to make changes to the existing version of CMLS to accommodate the need for a Brazilian version of the model.

Brazil has numerous scientists actively working in the pesticide fate and transport. No doubt more scientists in Brazil have data that is relevant to understanding and predicting pesticide movement in Brazilian soils. There is sufficient data available now to begin a major effort in modeling pesticides in Brazilian conditions. In the process of doing this modeling, knowledgeable scientists can synthesize current data, develop and test new components of the pesticide fate puzzle, assemble data and perform sensitivity and uncertainty analysis to guide more widespread data gathering, and highlight weaknesses in our current understanding and available data. It is not likely this effort will be achieved as a secondary or “add-on” responsibility of current scientists. Instead it needs to be their primary responsibility and focus.

Overall conclusion was that for several parameters the protocols adopted should be carefully considered and need to be uniform across the group. Embrapa Environment has clearly taken a lead role in establishing an active research project with an objective to minimize the adverse environmental impact of pesticides in Brazil. The research work being carried out in Embrapa and other research organizations and universities is very relevant and impressive. The spirit of cooperation and collaboration involving Embrapa and other organizations as well as the willingness of various groups to contribute to this area of work was impressive indeed. There is a wide range of highly developed skills existent within Embrapa and in other organizations that can be harnessed to develop effective management strategies to deal with the pesticide issues in Brazil, that will be useful in minimizing the adverse environmental impact of pesticides in Brazilian environment.

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