ENHANCED LEARNING EXPERIENCES THROUGH EFFECTIVE USE OF SIMULATION AND VISUALIZATION TECHNOLOGIES FOR DEMONSTRATION OF ENVIRONMENTAL SYSTEM MODELING

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Abstract

Learning experiences with simulation and visualization tools can greatly enhance a student's ability to seamlessly integrate mathematical modeling and attain a generalized understanding of environmental phenomenon. Environmental modeling relies heavily on system-based approaches to generalize environmental processes and make spatial and temporal predictions about the environmental fate and transport of anthropogenic pollutants. In the Fall 2013 semester, we have effectively used STELLA software for classroom simulations and visualizations to demonstrate the effectiveness of a system-based approach to model environmental processes. Various real-life examples were mathematically modeled and later simulated using the STELLA software. The STELLA software offers robust simulation and visualization compared to traditional EXCEL software. This study documents the effectiveness of STELLA software in modeling selected environmental processes such as transformation and deposition of sulfur dioxide, transformation and metabolites rate kinetics of atrazine. It includes an assessment of the practical applications of the STELLA environment through direct questions related to the design of stock and flow diagrams for the degradation of perchloroethylene and associated difference equations. The modeled environmental phenomenon was not only simulated using STELLA, but also tested through statistical methods such as chi-square and paired t-distribution tests to be certain the simulated model was valid at least at a 95% confidence level.

Introduction

Environmental system processes are difficult to understand, primarily due to the enormous complexity and interrelationships involved. This problem is further compounded by the fact that environmental processes often do not remain restricted to one environmental media. Environmental persistence and mobility of various organic pollutants in multi-media (surface water, air, soil, and groundwater) environments requires mathematical modeling to predict the fate and transport of pollutants as well as the net effect of discharging pollutants on nation's aquatic resources. Modeling of given environmental processes helps in predicting spatial and temporal distribution of pollutants across different media. Pure mathematical modeling can be difficult to understand if the developed model is not simulated and tested for different situations. Mathematical models without simulation may not be effective and may not provide an enhanced learning experience to undergraduate students.

The objective of using simulation and visualization tools in classroom demonstrations is to make the learning process more dynamic and effective. In the active learning process, the students are meaningfully engaged and, focused on the assigned tasks. This is particularly important given

modern communication tools such as iPhones, iPods, and personal laptops currently used by students. It has been reported that access to computing devices, particularly laptops, has shown to negatively affect several measures of learning including the understanding of course material and overall course performance (Fried, 2008). Furthermore, given the ready access to PowerPoint presentations posted through Blackboard, the proportion of students visibly engaged in taking notes is on the decline. Modeling environmental processes requires both attention and student engagement. While the implicit assumption is that the use of technology will achieve a deeper learning experience, there is no assurance that it will indeed enhance understanding. Very often technology coupled with additional stimuli is required (Goldstein et al., 2005). Nonetheless, simulation technologies such as STELLA software can be useful in stimulating and maintaining students' interests, particularly when analyzing the sensitivity or robustness of the developed model. The user friendly interface offers students ample opportunity to improve upon their model and simulate in real time.

The objective of this manuscript is to document the effective use of simulation technology for the demonstration of modeling environmental system processes. Visual demonstrations of complex mathematical models using STELLA software have been proved to be effective in engaging students and allowing them to be self-reliant in formulating advanced stock and flow diagrams, as well as accurately writing initial difference equations related to the model. Students enjoyed simulating various models such as depletion of a reservoir, determination of steady state and peak concentration, and transformation and mineralization of organic pollutants.

Environmental System Modeling Demonstration

Our Environmental System Modeling (ENVE 301) class is offered on a biennial basis. The catalog course description, "*Apply conceptual and numerical techniques to model environmental systems. Use differential equations to describe processes*" clearly indicates the mathematical approach to modeling. The description emphasizes using conceptual and numerical techniques for model development, but does not imply the tools to be employed for effective dissemination of the formulated models. Prerequisites require students to have prior knowledge of differential equations (Math 306) and an understanding of data analysis and synthesis covered in ENGR 112. The students are also expected to have background knowledge of principles of engineering II (ENGR 222) and fluid mechanics (ENVE 300). The course covers a wide range of topics relevant to the discipline of environmental engineering.

The system modeling course begins with an introduction to the rudimentary building blocks of the system approach. These basics consist of reservoirs, processes, converters, and interrelationships. The environmental system models were developed using these building blocks. For example, a simple first-order degradation model can be built by using a reservoir with initial pollutant concentration and the converters showing the rate at which the degradation process is operating. Given the reservoir initial conditions and rate constants, the model can then be simulated. Various types of models in environmental engineering were considered for classroom demonstration. The approach was to provide a thorough mathematical analysis of the model prior to its simulation and demonstration. The models ranged from simple traditional growth and decay models to the more complex models involving consecutive reactions. The lecture modules were geared toward theoretical and mathematical aspects, whereas the

laboratory section was intended for hands-on modeling, simulation, and demonstrations. Students were grouped in teams of three to four and assigned different initial values and rate constants for the model simulation. The simulated models were later tested for their statistical validity using chi-square, student t-test, and simple regression analysis.

Models considered for classroom simulation and demonstration

Model 1: Sulfur dioxide transformation and deposition model

The model was developed based on the data provided in the recommended text book, Dynamic Modeling of Environmental Systems by Michael Deaton and James Winebrake. In this model, major sources of sulfur dioxide in the environment were discussed in detail. Human health consequences due to elevated levels of sulfur-dioxide as well as relevant air pollution regulations were discussed. Particularly, the importance of National Ambient Air Quality Standards and real time monitoring of sulfur dioxide were discussed. Information was also provided regarding how real time monitoring helps in establishing air quality index and issuance of related health advisories.

A comprehensive understanding of the sources of sulfur dioxide (natural and anthropogenic) was provided to students prior to developing the model. Discussion on how elemental sulfur present in coal when burned, produces sulfur dioxide, and the subsequent transformation and deposition of sulfur dioxide, sulfur trioxide, sulfurous acid and sulfuric acid was also presented to the class. The sulfur dioxide model was discussed in two phases. The first phase of the model was discussed only with regard to the transformation of elemental sulfur into sulfur dioxide and sulfur trioxide. The later portion of the model was more comprehensive as it included both transformation and deposition model as well. Student understanding of sulfur model was tested through a direct question on the transformation model and at least 75 % of the students were able to develop the model correctly. Figure 1 shows the stock and flow diagram for the complete model that includes transformation of and deposition as well as simulation of the sulfur dioxide model.

Using the stock and flow diagram, the initial difference equation for the sulfur dioxide reservoir (SO_2) can be written as:

$$SO_2(t+\Delta t) = SO_2(t) + (input - output) * \Delta t$$

The analytical solution for the SO_2 reservoir then can be written as:

$$SO_2(t) = \frac{1}{k_1 + k_2}\left[input - (input - (k_1 + k_2)SO_{2o}) * e^{-(k_1+k_2)*t}\right]$$

Where, $(SO_2)_o$ is the initial concentration at time t =0; k_1 and k_2 are the transformation and sulfite deposition rates respectively.

Since part of SO_2 is being transformed into sulfur trioxide (SO_3) at the rate k_1. The transformed SO_3 further converts to sulfate at the rate of k_3. The sulfate is eventually deposits. The difference equation for the (SO_3) reservoir can be written as:

$$SO_3(t+\Delta t) = SO_3(t) + (input - output) * \Delta t$$

The analytical solution for the $SO_3(t)$ reservoir then can be written as:

$$SO_3(t) = \frac{k_1 * input}{(k_1+k_2)*k_3}\left[1 - \frac{k_3 * e^{-(k_1+k_2)*t} - (k_1+k_2)*e^{-k_3*t}}{k_3-(k_1+k_2)}\right] + \frac{k_1 * SO_{2_o}}{k_3-(k_1+k_2)}\left(e^{-(k_1+k_2)*t} - e^{-k_3*t}\right)$$

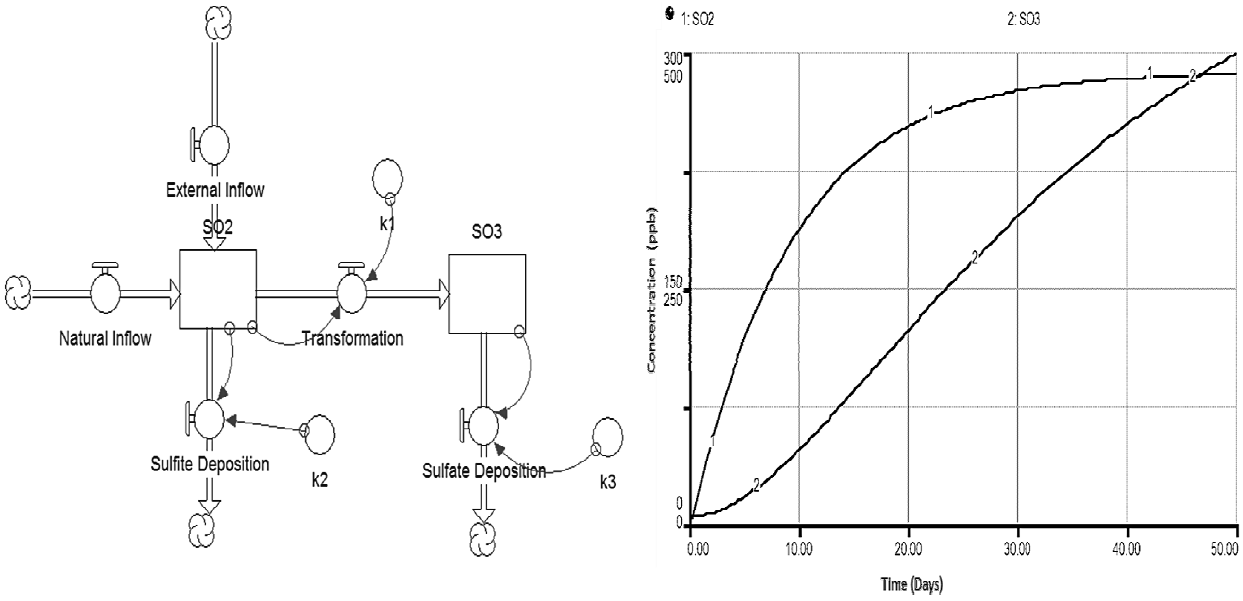

Figure 1. The stock and flow diagram for the sulfur dioxide transformation and deposition model followed by simulation using STELLA software

Model 2: Anaerobic degradation of atrazine

The idea for this model came from the paper, "Biodegradation of atrazine under denitrifying conditions" by Crawford et al. (1998). In this model, the authors discussed the anaerobic biodegradation of atrazine (A_T) by bacterial isolate M91-3 and subsequent metabolites hydroxyatrazine (HA_T) →ammonia (NH_3) and Carbon dioxide (CO_2) formation. Figure 2 shows the stock and flow diagram for the transformation and mineralization of atrazine followed by the simulation of the modeled results. The model was developed as a consecutive reaction model with hypothetical rate constants. Each group of students was assigned different initial concentrations of atrazine and transformation and mineralization rate constants. Using the stock and flow diagram, the initial difference equation for the anaerobic transformation of A_T can be written as:

$$A_T(t+\Delta t) = A_T + (input - output) * \Delta t$$

The analytical solution for the atrazine reservoir then can be written as:

$$A_T(t) = A_o * e^{-k*t_1}$$

Where, A_o is the initial A_T concentration at time t =0 and k_1 is the transformation rate.

The HA_T is further being mineralized to form ammonia at the rate k_2 to form NH_3 and CO_2. The difference equation for the HA_T reservoir can be written as:

$$HA_T(t+\Delta t) = HA_T + (input - output) * \Delta t$$

$$HA_T(t+\Delta t) = HA_T + (k_1 * A_T - k_2 * HA_T) * \Delta t$$

The analytical solution for the HA_T reservoir then can be written as:

$$HA_T = \frac{k_1 * A_o}{k_2 - k_1}\left[e^{-k_1*t} - e^{-k_2*t}\right]$$

The final analytical solution was simulated for the hypothetical intial values of A_T reservoir and accompanied transformation and mineralization rate constants. Figure 2 shows the stock and flow diagram and simulation of tranformation of A_T to HA_T and to NH_3 and CO_2 using STELLA software

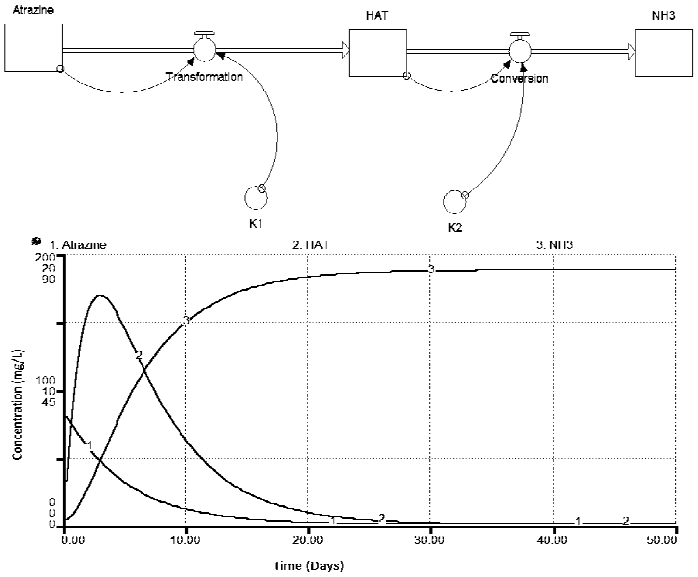

Figure 2. The stock and flow diagram for the anaerobic transformation and mineralization of atrazine model followed by simulation using STELLA software

Performance in Class

Students' understanding of the system modeling approach was tested through a direct test question related to formulating the stock and flow model of final degradation of

perchloroethylene (PCE) to vinyl chloride (VC). Background information on the occurrence, fate and transportation of PCE was provided to students in an earlier class (Groundwater Hydrology, ENVE 320) and as such, very little discussion on PCE occurrence was provided. The idea for this model came from the paper published by Kielhorn et al. (2000) where the authors have systemically shown the degradation pathways of PCE to vinyl chloride. The students were asked to formulate a STELLA model using stock and flow diagram showing the reservoirs for all the intermediates along with their respective degradation rate constants. Students were also asked to write the initial difference equation for the degradation of PCE. Almost all students were able to successfully draw the stock and flow diagram and also able to write the difference equation. Figure 3 shows the PCE degradation pathways and related stock and flow diagram. Their performance clearly reflects the fact that students are able to formulate a STELLA model and also able to write the difference equation. Since PCE degradation results into formation of several metabolites prior to its final mineralization to vinyl chloride, students were not asked to develop an analytical solution to this model. Analytical solution to this model is computationally intensive and given the duration of the examination, students may not be able to do it. Figure 4 shows the stock and flow diagram of the complete degradation of PCE and a simulation of the PCE degradation to vinyl chloride.

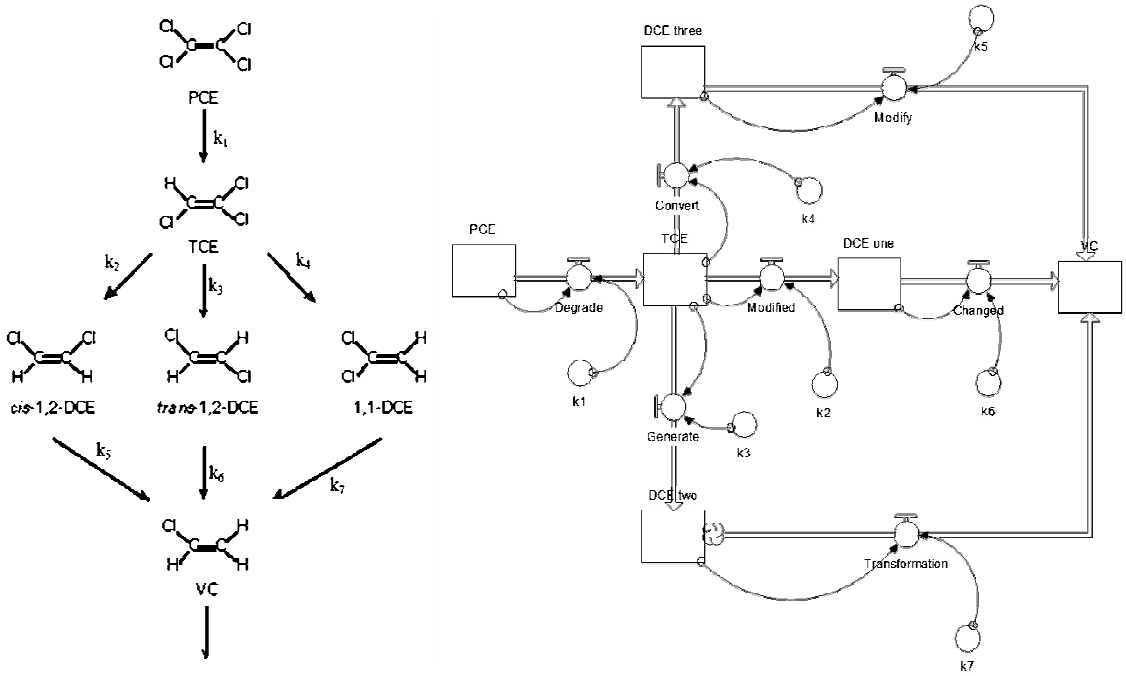

Figure 3. The degradation pathways of PCE and student developed stock and flow diagram for the complete degradation of PCE

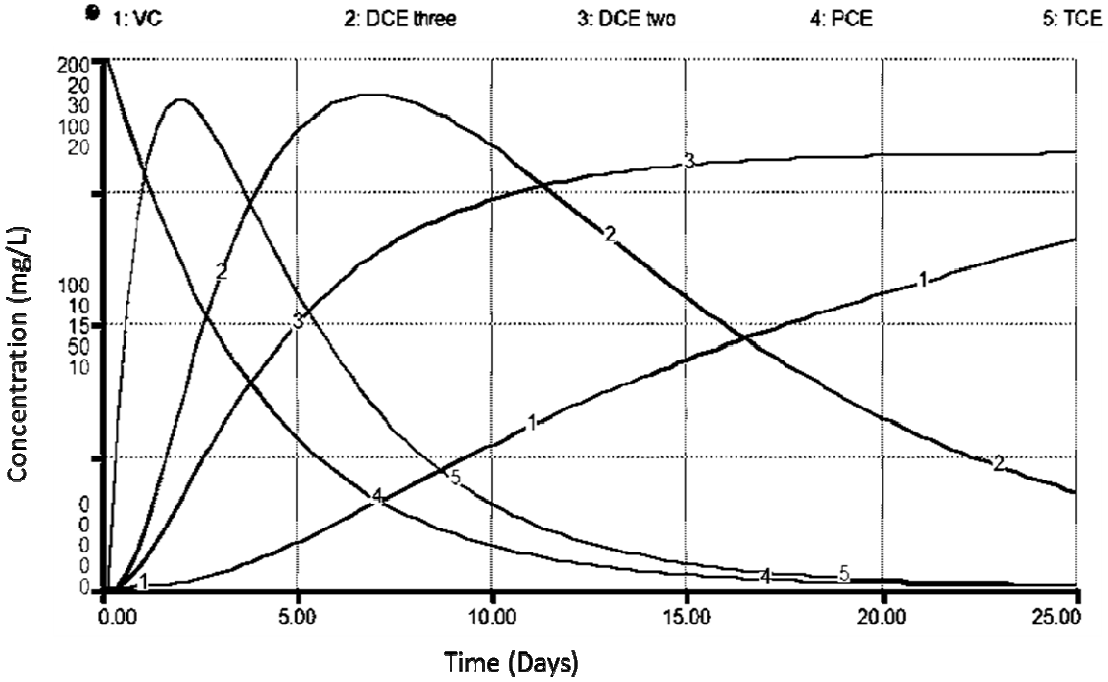

Figure 4. Simulation of the stock and flow diagram for the degradation pathways of PCE using STELLA software

Simulation and Visualization Technology

Models were simulated using the software package STELLA, developed by isee systems. The software is licensed; however, a practice demonstration version is free. For our class, we used STELLA v10.0.2, the latest version of the software. Model simulation and visualization was facilitated through the use of the STELLA software. STELLA is an icon-based model building and simulation tool which offers flexibility in terms of user input and immediate change in the system. It is a user-friendly software in terms of building the stock and flow diagram, and allows users to explore the model by changing parameters such as initial conditions, rate constants, and interdependence. The STELLA software, however, does not provide the mathematical solution of the stock and flow diagram. This is one of the biggest drawbacks of the STELLA software. Obviously, with more interrelationships and interdependence among system constituents, the model becomes computationally intensive. However, STELLA does not provide an analytical solution even to the simple models. At best, STELLA can be used to formulate the stock and flow diagram and model simulation but not for developing an analytical solution of the model.

Conclusion

The students clearly demonstrated an understanding of the STELLA environment by accurately drawing stock and flow diagram for the complex environmental system. Some further explored the modeling capacity of STELLA by simulating their own models. Although the students mastered the STELLA software, the lack of mathematical solutions for their models proved to be

a hindrance to their understanding. Furthermore, students with inadequate mathematical skills could not relate to the simulation of the STELLA models. Even with the prerequisite course, differential equation (MATH 306) which most of the students have completed in their junior year in college, students struggled in developing analytical solutions to the formulated model using STELLA software. Nonetheless, the simulation offered by STELLA was a good visual experience, and students can quickly see when the particular process has achieved a steady state or when the system is likely to run out of control. The utilities of STELLA software offer more freedom in terms of model behavior but a lack of mathematical derivation unfortunately dampens the understanding of complex models. Compared to STELLA, other mathematical modeling tools such as MATLAB offer much robust data analysis and exploration and allow the users to access large data files from external database; however, it requires specialized training in writing a MATLAB code and debugging the program (Pastorok et al., 2002). In addition to the complex mathematical code in MATLAB for an individual model, a modification or augmentation of the model warrants additional amendment to the written code. On the other hand, STELLA is more user-friendly because it is based on a graphical interface that makes it easy to add reservoirs, processes and interrelationships without the need to develop a complex code. In STELLA, the equations are automatically generated and any modifications thereof are automatically integrated in the equations. Both MATLAB and STELLA have their own pros and cons. The modeler has to make the choice based on the requirement of the model and the familiarity with the work environment in MATLAB and STELLA.

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