Modelmaker 3.0 for Windows

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Introduction. ModelMaker 3.0 from Cherwell Scientific Inc. is an advanced mechanistic modeling program that runs on the Microsoft Windows operating systems. Although highly sophisticated in its design and use, it is user friendly and will be especially useful to the programming or mathematically challenged. Even those well initiated within the field of mathematical model development will find this software useful and cost effective from a development time perspective. ModelMaker allows the user to develop models in a visualized flow-diagram form, optimize the model, and view its results with a minimal amount of programming effort. It is designed for the development of simulation models that can be applied to a wide array of applications in the physical sciences. Some of these applications are environmental modeling, pharmacology, and process engineering.

System Requirements. The minimum recommended system requirements for running ModelMaker 3.0 are as follows: an IBM compatible PC with math coprocessor running Microsoft Windows 3.1, Windows 95, or Windows NT operating system and 4 MB of RAM. Eight MB of hard disk space are required as is a mouse or other pointing device.

The evaluation of ModelMaker 3.0 reported here is based on installation and use of a 133 MHZ Gateway PC running the Microsoft Windows 95 operating system with 24 Mb of RAM and approximately 150 Mb of free hard disk space.

Documentation and Support. A printed user's manual consisting of 362 pp was included with the software. Additional documentation and information including a frequently asked questions (FAQ) list is available from the Cherwell website at http://www.cherwell.com. The user's manual is extensive, well written, and helpful. It includes easy to follow step-by-step instructions for building simple simulation models, and the software contains a tutorial folder that can be used in conjunction with the manual. The tutorial contains several examples of simulation models that are relevant to chemistry, physics, engineering, biology, and even the social sciences.

The author sought support electronically from Cherwell on 2 occasions during the course of the review. The replies were rapid, concise, and helpful. Support is available through electronic mail, telephone, or fax. There is also an electronic mail internet list server for ModelMaker where users can share experiences, ideas, and questions.

Software Use and Performance. The heart of ModelMaker is its ability to develop complex mathematical relationships in a simple visualized format. As an example of ModelMaker's capabilities we have considered the environmental fate of a pollutant discharged from a hypothetical manufacturing facility into a nearby holding pond. Such mass-transfer models are quite common in engineering and environmental research.[1,2]

Figure 1 depicts a standard view of a model system created with ModelMaker. The compartmental boxes are dragged onto the worksheet and sized using a mousepad. Descriptive phrases for each compartment and initial starting conditions for the model are input into dialog boxes that are opened by double-clicking on the object with the mouse. Colorized text and images (bitmap) can be inserted to the diagram to create a more aesthetically pleasing look to the model. In this example a pollutant is discharged from a manufacturing facility into a nearby holding pond. Once into the pond, the pollutant may adsorb into the surrounding soil and sediment, volatilize to the atmosphere, bioconcentrate into fish and wildlife, or immediately begin to degrade by microbial means (biodegradation) or chemical means (hydrolysis). In fact, all of these processes occur to some extent, and we have emulated this with ModelMaker. The arrows in Figure 1 represent the flow of pollutant into or out of a compartmental box and the rate constants are identified as k1−k8. The set of differential equations which describes the concentration change of the pollutant in each of the compartments are given by

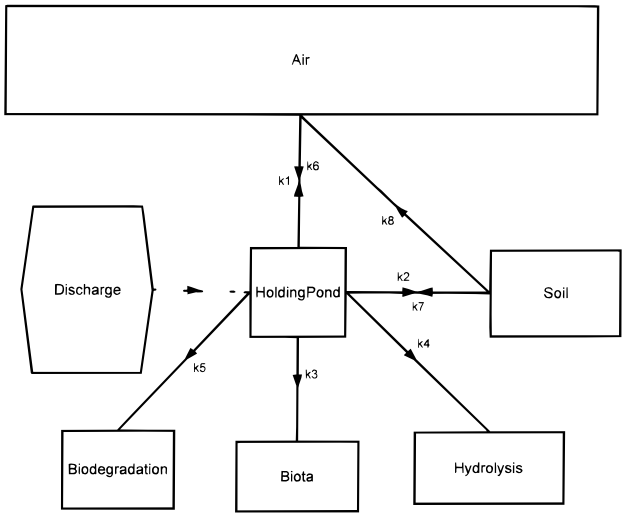

Figure 1. Discharge of a pollutant and its environment fate.

$$\frac{\mathrm{dHP}}{\mathrm{d}t} = \text{discharged} - (k_1\mathrm{HP} + k_2\mathrm{HP} + k_3\mathrm{HP} + k_4\mathrm{HP} + k_5\mathrm{HP}) + k_6\mathrm{Air} + k_7\mathrm{Soil} \quad (1)$$

$$\frac{\mathrm{dAir}}{\mathrm{d}t} = k_1\mathrm{HP} + k_8\mathrm{Soil} - k_6\mathrm{Air} \quad (2)$$

$$\frac{\mathrm{dSoil}}{\mathrm{d}t} = k_2\mathrm{HP} - k_8\mathrm{Soil} - k_7\mathrm{Soil} \quad (3)$$

$$\frac{\mathrm{dBiota}}{\mathrm{d}t} = k_3\mathrm{HP} \quad (4)$$

$$\frac{\mathrm{dHydrolysis}}{\mathrm{d}t} = k_4\mathrm{HP} \quad (5)$$

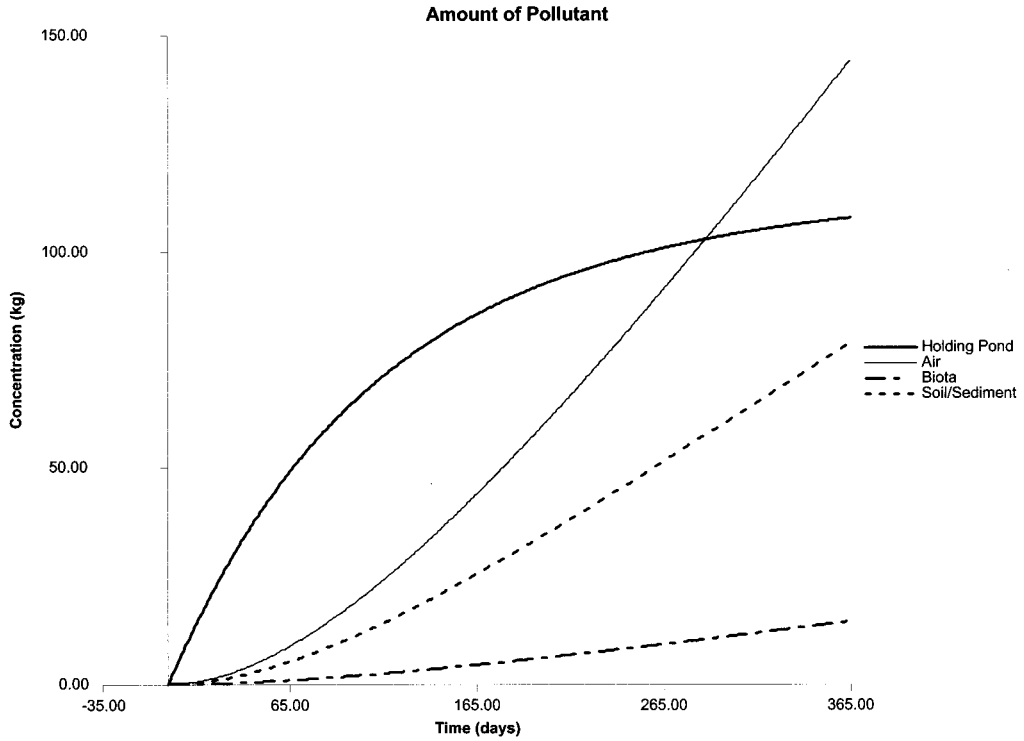

Figure 2.

$$\frac{\text{dBiodegradation}}{\text{d}t} = k_3\text{HP} \qquad (6)$$

where Discharged is the rate at which the pollutant is released to the holding pond, HP, Air, Soil, Biota, Hydrolysis, and Biodegradation represent the concentration of the chemical in each of the compartments, and k_x represents the rate constant for the flow of pollutant into or out of a compartment. The user does not need to input these equations, rather ModelMaker constructs them based upon the relationships shown in Figure 1. The user only inputs starting values for the initial rate constants and the amount of pollutant being discharged with respect to time from the manufacturing facility. ModelMaker does the rest.

Figure 2 shows the graphical output for the concentration of pollutant in the holding pond, biotic phase, air, and soil after the model has been run. This figure is typical of the graphical output capabilities of ModelMaker and can be customized by the user. The output can also be viewed as a table rather than graphically if the user so prefers. The model was run over 365 output steps (the default value is 100) in order to follow the concentration of the pollutant over 1 calender year. The actual amount of time it took to solve the equations and run this model on a desktop computer (133 MHZ, 24 Mb RAM) employing the Windows 95 operating system was slightly more than 1 s. The results of this example are completely dependent upon the values of the rate constants provided by the user. (The above example is for a hypothetical chemical, and the rate constants as well as the discharge were pure conjecture by the author.) It is emphasized that although ModelMaker is useful in developing models, the accuracy and reliability of such a model is only as good as the assumptions or data originally used to compose it.

More complex systems with hierarchical relationships are easily handled by the program through the use of submodels. Like the original example, submodels are developed in diagram form and can be linked to other submodels.

A single parameter can be systematically changed over a defined range of values as a model is repeatedly run in order to determine how sensitive other model components are to this change. The software also allows the user to preserve the values of model components from previous runs and use these values as the starting point for multistep runs. This option is particularly useful for periodic systems and stochastic models which can be generated by the user.

Although mathematical software packages can be used to generate simulation models, most lack the simple format and intuitive nature of developing the model in a visualized environment. No programming expertise is required in ModelMaker; however, it should be mentioned that experience in the C or C++ language will allow the user to take full advantage of the software's capabilities. There are instances where conditional events may need to be initiated, and this can be accomplished within the framework of the program with a few lines of simple code.

Once a model has been developed, configured, and run, optimization of selected parameters to find the best fit between the model and experimental data can be performed. The optimization methods available are the Marquardt and Simplex methods, and the convergence criteria are adjustable.

Differential equations are solved by the fourth order Runge−Kutta method by default, although the Euler, Mid-Point, and Bulirsch−Stoer methods are also available. Only initial value boundary problems are solved by ModelMaker; dual value boundary problems are not treated by the software. ModelMaker can only treat first order differential equations directly. Higher order differential equations can however be solved by linking a series of first order equations together. This process is somewhat cumbersome for certain applications but is sufficient to solve second order equations that might be encountered in vibrational motion or wave phenomenon.

Distribution. ModelMaker 3.0 is produced and distributed by Cherwell Scientific Publishing, Inc., 744 San Antonio

Road, Suite 27 Palo Alto, CA 94303. Tel: 415-852-0720. The software is reasonably priced at $699 (U.S.).

Conclusions. Most researchers will admire the ease in which mathematical relationships are developed and solved within the framework of ModelMaker. This reduces the need to develop models from scratch and write complex code in a high level programming language. This reduction in development time renders ModelMaker a cost effective tool for scientists interested in developing simulation models in the physical sciences or engineering fields. Moreover, this program runs efficiently on desktop computers using the Windows operating system thus reducing hardware costs. Like all modeling projects, the results are only as good as the model developed by the user, and this program will not correct for poor assumptions or unreliable data input into the original system.

REFERENCES AND NOTES

(1) Mackay D.; Patterson S. *Environ. Sci. Technol.* **1981**, *15*, 1006−1014.
(2) Geankoplis C. J. Mass Transport Phenomena; Holt, Rhinehart and Winston Inc.: New York, NY, 1972.

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