TECHSIGHTING
SOFTWARE

A Frozen Database

Maintaining a well-organized laboratory freezer or other storage compartment is not a trivial task. Freezerworks 5 is a relational database that simplifies the task of managing the contents of a lab's freezers. Its users begin by entering into the program the number of shelves, racks per shelf, boxes per rack, and tubes per box in their freezer. Next, they set up an image of the actual freezer in Freezerworks with the "Add New Freezer" command from the pull-down menu. After definition and setup of a "virtual" freezer, users can enter samples in the database manually one at a time (the method of choice for most users) or automate the process with a routine that allows fast entry of multiple samples with either the keyboard or a bar code reader. Aside from an entry in the "Sample" field, each sample can have "Notes," "Transactions," and "Audit Trail" fields associated with it, enhancing the searching capabilities of Freezerworks. A powerful function of this program is its ability to use the "Next Assignable Position" (NAP) command, which allows the program to automatically assign positions as new samples are entered.

Freezerworks 5
Dataworks Development Inc.
Mountlake Terrace, WA.
$995
425-741-1411
www.dwdev.com

The ability to specify exceptions in the design of a new virtual freezer allows the user to handle freezers with irregular features. As with any database, the search engine is the key to its quality. With its extensive search capabilities, Freezerworks rates high in this category. The simplest way to search the database is by "Sample ID" or "Sample Date." However, more comprehensive searches can use any number of data fields. The operators AND, OR, EXCEPT, LESS THAN, and GREATER THAN can be used under this option to perform multicriteria searches. Nested searches can be performed so that carrying out a second search narrows the results of the first search. The program can also generate a wide range of reports.

Although Freezerworks looks identical when run with both the Windows and the Macintosh systems, the Macintosh interface needs improvement. For example, there are no keyboard equivalents for menu choices, and the "OK" buttons in the various dialog boxes are not highlighted to indicate that pressing the return key would select this option. Regardless, Freezerworks succeeds in bringing to the laboratory a powerful database that can effectively keep track of those messy freezers. No laboratory should be without such a program.

—YIANNIS A. IOANNOU

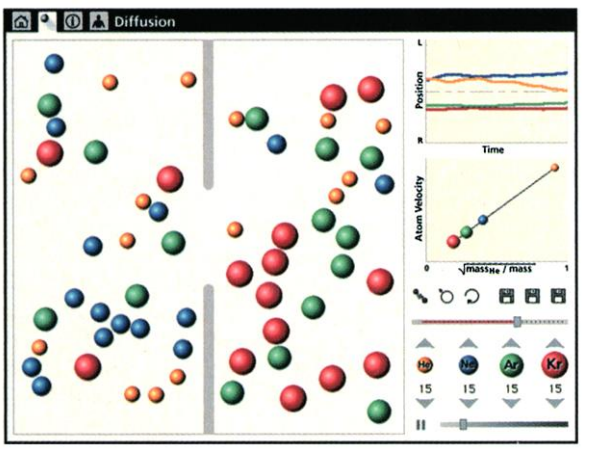
Department of Human Genetics, Box 1498, East Building, Room 14-70A, The Mount Sinai School of Medicine, New York, NY 10029, USA. E-mail: ioanny01@doc.mssm.edu

TECHSIGHTING
SOFTWARE

Seeing the Physics of Chemistry

Stark Design's 3-D Molecular Dynamics (3DMD) program uses state-of-the-art interactive visualization software to simulate atomic motion. Although the target audience is the typical college undergraduate student, the software is also useful for advanced physical chemistry and graduate students.

The four main modules of the program are Introductory Topics, Gas Behavior, Condensed Phases, and Advanced Topics, which covers most of the basic chemical principles. These include Dalton's law of partial pressure, diffusion, Maxwell-Boltzmann speed distribution, pressure/temperature and pressure/volume relationships, LeChâtelier's principle, collision frequency, mean free path, pressure fluctuations, and the time average of kinetic energy.



Animated gases. 3DMD illustration of the process of diffusion.

To view one of the concepts, a student picks a module and specific experiment from the home screen. For example, to study diffusion, the Gas Behavior module is chosen and diffusion is selected from the list of choices. A box appears that is divided into two compartments by a barrier (see figure). The opening between the chambers can be resized as desired. Next, the user selects atoms (helium, krypton, argon, and neon are the only choices) and introduces a specified number of each type into the system. The size of each atom is a function of its Van der Waals radius. By adjusting the temperature and time periods per screen update (with sliding switches), the atomic motion may be increased or slowed. This allows one to view the effect each parameter has on ultimately reaching equilibrium across the opening. In the Condensed Phases module, molecules actually "form" and "degrade" as the temperature changes. These processes may be hastened, or retarded, by the inclusion or exclusion of user-specified interatomic forces. While all this is happening, users can switch between two views—atoms as spheres or the classical view of atoms as circles with attached vectors.

3-D Molecular Dynamics version 2.5
Stark Design, Inc.
Morristown, NJ.
$180
877-384-8021
www.starkdesign.com

In addition to the molecular animations, two graphs are also visible for the diffusion module. The topmost graph displays the average position of an ensemble of atoms in the box in real time, and the bottom graph describes the relation between the atomic velocity and the square root of the ratio of the mass of a helium atom to the mass of any of the other three. The clever use of visualizations, combined with relevant graph plots, is a feature of all of the modules. Unfortunately, in the present version only Macintosh users can print screen views.

A short, clearly written manual describing each module accompanies the CD-ROM. The manual is largely free of mathematics, except as necessary to support the program's atomic illustration functions. 3-D Molecular Dynamics succeeds in teaching basic physical-chemical principles with clever visualizations. The addition of other atoms and even small molecules would be a welcome addition to future editions.

The program comes in both Macintosh and Windows formats.

—JOHN WASS

Immunochemistry R&D Group, Abbott Laboratories, Abbott Park, IL 60064–6199, USA. E-mail: john.wass@add.ssw.abbott.com