Computer Software Reviews

MacSimion. Version 1.0. Montech PTY LTD.: Monash University, Wellington Rd., Clayton, Victoria 3168, Australia. List price $399.00.

MacSimion is a program for the numerical simulation of the motion of charged particles in electric and magnetic fields. It is written in the C language for the MacIntosh family of computers. Two different versions are supplied on one diskette that is not copy protected. (Source code is not provided in the distribution package.) One version is for use with MacIntosh II computers, and the other is for use with MacIntosh SE and earlier MacIntosh machines. Implementation on a MacIntosh II with 16 color graphics is recommended.

Becoming facile with the use of MacSimion takes only a minimal amount of time—one or two hours. This ease of use is due to two factors. First, the program is very MacIntosh-like, making use of pull-down menus, icons, and the like. Thus, anyone familiar with operation of a MacIntosh should have little trouble adapting to MacSimion. Second, the operating manual is quite well organized and well written. It includes a tutorial section that steps one through the operation of the program, and it also includes a software reference section and a section that explains what calculations are actually being performed when the program is run.

MacSimion consists of three subprograms. The first is the "geometry" sub-program, which allows one to construct an arrangement of up to 127 distinct electrodes, each with its own electrical potential. This subprogram is interative and easy-to-use, resembling other MacIntosh graphics programs such as MacDraw.

The second, "refine" subprogram takes as input the electrode arrangement defined in the geometry subprogram, and by iterative application of Laplace's equation it solves for the electrical potential at all points in the two-dimensional array that represents the space in and about the electrodes. (Only two dimensions are needed because of the required symmetry in the electrode arrangement—see below.) On the MacIntosh II this refine procedure typically was completed very quickly (typically less than a minute). The result of the procedure is a contour map of the electrical potential in two-dimensional space. This contour map can be displayed directly on the MacIntosh monitor.

The "trajectory" part of the program takes as input the results of the refine procedure and, along with data specifying the initial conditions of an ion, calculates the trajectory of that ion in the vicinity of the electrodes. A choice of two algorithms for trajectory calculations is provided: (1) a "fast" algorithm, which uses linear field gradient interpolation and simple integration, and (2) an "accurate" algorithm based on the fourth-order Runge-Kutta technique which utilizes interpolation of the potential by means of a fitted fourth-order polynomial. Many other options are provided in trajectory mode, some for enhancing the speed or accuracy of the trajectory calculation (e.g. the option of fixed or variable time steps), others for modeling special physical situations (e.g. the fragmentation of an ion during its trajectory), and others for specifying the initial conditions of the ion. The output of the trajectory subprogram is an on-screen, real-time graphical representation of the trajectory, together with information pertaining to that trajectory (elapsed time, ion positions, ion energy, etc.). On a MacIntosh II, individual trajectories are calculated in times that are quite reasonable. On other MacIntosh machines trajectories may take about forty times longer than they do on the Mac II.

We found MacSimion to be a powerful easy-to-use program for the calculation of ion trajectories. Implemented on a Mac II the program allows one to modify electrode parameters and almost instantaneously see graphically the results of such modifications on electrical potentials and ion motion. One would expect the program to be very useful not only as a tool for the design of experimental apparatus but also as a pedagogical instrument. This having been said, it is also pertinent to outline some important limitations of the software package. First, the program allows only certain types of electrode arrangements to be constructed. In particular, only arrangements that have cylindrical symmetry or that extend infinitely in one direction are supported by the software. While the reasons for this limitation are clear, and while many electrode arrangements can be approximated within the confines of the limitation, one should be aware that is does exist. Second, the program can only handle temporally and spatially constant magnetic fields. Moreover, although ion trajectories are calculated in three dimensions, only two-dimensional trajectories are displayed. Third, the program can handle time-varying electrode potentials, but the time variations must be periodic and be either sinusoidal, square, or triangularly shaped waveforms. Fourth, the graphical output of trajectories, while providing very fast access to the calculated trajectory, also incurs some disadvantages. The screen resolution and size are such that convenient and accurate modeling of the electrodes is possible. However, viewing trajectories over distances much greater than the electrode system itself is difficult. This is unfortunate with respect to focusing systems which need to be characterized over the distance between lens and detector (e.g. a time of flight mass spectrometer system). Though this is an inconvenience, it is by no means fatal, as a good approximation of focusing behavior can be obtained over typical "geometry" dimensions, and far field behavior can be extrapolated in a straightforward manner. If one can tolerate these four principal limitations, the program's ease-of-use and speed make it quite attractive for ion trajectory calculations.

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Book Reviews*

Analytical Artifacts. GC, MS, HPLC, TLC and PC. Journal of Chromatography Library—Volume 44. By Brian S. Middleditch (University of Houston). Elsevier: Amsterdam and New York. 1989. xxiv + 1028 pp. $241.50. ISBN 0-444-87158-6.

This encyclopedic volume is a compilation of information on artifacts in the determination and identification of chemical substances. It includes generous doses of analytical folklore, arcana, gossip, and uncommon wisdom as well. The volume is thus invaluable to help the analytical chemist keep a watchful eye on artifacts of the analytical process ("artifact" wins handily over "artefact", according to the detailed statistics presented: 2447 to 648 overall, 556 to 123 in *Chemical Abstracts*, and 1048 to 437 in *Excerpta Medica*). Containing over 1100 entries from abietic acid to zinc dialkyl dithiophosphates and nearly 1000 complete literature citations, this is a labor of love (and determination) that few would be capable of undertaking and even fewer capable of completing. It is entirely a single-minded affair: there are no coauthors and no effusive/perfunctory acknowledgments to associates/graduate students. Rather there are cautionary notes under the entry "Literature Surveys" to never trust a librarian to do one's computer-assisted searches and to always follow up computerized searches with manual ones. Chemical Abstracts Service (CAS), recently chosen to devise a way to classify and modernize the retrieval of the holdings of the U.S. Patent and Trademarks Office, would be well advised to seek the services of the author to ensure that they are indeed doing a thorough job. The magnitude of this effort boggles the reviewer's mind; he can only offer his respectful tribute to the author and confess his total lack of jealousy of this achievement. Any criticism offered hereunder should thus be taken not as indices of diminution of the value or the scale of the undertaking, but as the duties of a critic.

The entries are in alphabetical order. The title for each entry contains the common name (not necessarily the CAS name), the molecular formula, and the mass spectroscopist's molecular weight (based on the most prevalent isotopic composition). The mass spectrum is then given (70 eV electron ionization throughout) in frames 200 amu wide. The chemical structure, CAS name and registry number, and the Merck Index reference number follows. Synonyms are given next. [Reader, are you informed enough to know what compound bears the synonyms (partial

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