Kirk-Othmer Encyclopedia of Chemical Technology.

COMPUTER-AIDED DESIGN AND MANUFACTURING (CAD/CAM)

Computer technology (qv) has made extraordinary advances in the past two decades (1). The electronic numerical integrator and computer (ENIAC) was the first electronic computer developed for the army during World War II. ENIAC was designed to analyze artillery and bombing trajectories. It was 30 m long and 3 m high, had 18,000 vacuum tubes and contained spaghetti-like wires. ENIAC could generate enough heat to raise the room temperature to 49°C. In 1959, to eliminate wires and for miniaturization, Texas Instruments and Fairchild Semiconductors co-invented the integrated circuit in the form of small wafers called microchips. In the early 1970s Intel introduced the microprocessor, a computer on a chip the size of a thumbtack, which was capable of performing arithmetic and logical functions. Today the speed of computers has reached the rate of 100–250 million floating-point operations per second (flops), and many source-code languages have also evolved, notably FORTRAN, C, PASCAL, and BASIC. QuickBASIC, introduced by the Microsoft Corporation, is both structured and easy to use.

With the aid of computers, design processes can be expedited and implemented with greater accuracy. Computers can simulate the shape of an object, make changes, and display a three-dimensional perspective of the object on a terminal monitor. Numerous computer-aided design (CAD) software packages are commercially available. In automating chemical processes and computations, companies must decide whether to use commercial software packages or to develop in-house CAD software. For drafting needs in engineering designs, AutoCAD and VersaCAD are among the most notable commercial CAD software packages. Other software packages meet computational, word-processing, tabulation, graphing, and other needs. This article discusses many of the underlying principles that have been employed in developing popular software packages.

Except for the physical processes, such as cutting, forging, and mixing, used to manufacture items, the commonly discussed topics in computer-aided manufacturing (CAM), such as material planning, process and procedure designs, numerical control, and scheduling, might also be considered CAD because design is involved (1–3). Computer-integrated manufacturing systems (CIMS) programs have played an important role in the development of CAM activities. Flexible manufacturing systems (FMS) refers to a more recent concept of adapting basic manufacturing modules to meet a particular manufacturing need. For companies that wish to remain competitive in the international marketplace, these modern technologies in computer automation are becoming almost indispensible.

Solid modeling now plays an important role in CAD/CAM. It allows a design item to be simulated on a display monitor, making possible a trial assembly of various design parts before they are actually fabricated.

1. Computer Application in Chemical Technology

The *Software Directory*, published by the American Institute of Chemical Engineers as a supplement to the journal *Chemical Engineering Progress*, shows the scope of computer utilization in chemical technology. Selection and evaluation of available software packages have been discussed (4). The topics covered in the second annual directory (Oct. 1990) include:

Absorption
Air pollution
Automatic control
Biochemical engineering
CAD/CAM
Costing investment analysis
Data acquisition
Database management
Data conversion
Development tools
Dispersion models
Distillation
Drafting
Electrical engineering
Equipment design
Expert systems
Extraction
Failure analysis
Flow analysis
Safety
Flow-sheet simulations
Fluid dynamics
Graphics
Industrial solid waste
Inventory
Maintenance
Management scheduling
Material safety data sheets
Mathematics
Network optimization
Particle dynamics
Petroleum production
Physical and chemical properties
Process control
Process economics
Process measurement
Programming and software
Project and production
Reaction kinetics
Reactor design
Regulations

Reliability
Risk analysis
Software utilities
Statistics
System analysis
Thermodynamics
Waste management

Steady-state chemical process simulation has been reviewed (5). Uses of computers manufactured by Apple, Control Data, Gould, Telex, Lear-Siegler, MINC, ICS, IMLAC, Vector General, IBM, Megtek, and Pet for applications in process design, kinetics, heat transfer, thermodynamics, and mass transfer have been reported (6), based on two surveys conducted by CACHE (Computer Aids for Chemical Engineering) Corporation. A survey on PC-based flow-sheet software (7) compared six process engineering packages; two versions of ASPEN; CHEMCAD; DESIN 2000; HYSIM; and PROCESS.

Supercomputers, such as the CRAY X-MP, CRAY Y-MP, and CRAY-2, are partially available and used for flow-sheet and optimization studies (7–10). Optimization modules using linear and nonlinear programming (LINPRO and UNLP1, based on a revised simplex, and Davidson-Fletcher-Powell and Broyden methods, respectively) are available in MicroMENTOR (11).

Networking provides easy access to software worldwide. NSFNet (National Science Foundation network), Ethernet (Xerox Corp.), ProNet (Proteon, Inc.), and DECnet (Digital Equipment Corp.) are among the most notable networks (12).

2. CAD Software Packages for Chemical Processing

Many commercially available software packages, such as AutoCAD and VersaCAD, can be used to draw chemical processes in block-diagram representation. Figure 1 illustrates typical screen displays of some in-house programs. To manipulate block diagrams, numerous automated procedures are also available. Various pointer devices (mouse, light pen, joystick, and others) are used for interactive selection of particular blocks or branches for simplification and derivation of the system's transfer function. The fundamental steps that need to be taken in such manipulations, using a program called IMPROVISA, have been explained (13).

The number of more elaborate software packages specially designed for chemical processing is rapidly increasing. Examples follow.

ADVENT, developed by Union Carbide Corp., is capable of minimizing the energy and capital requirements of process synthesis.

FLOWTRAN was made available in 1974 by Monsanto Co. for steady-state simulation of chemical processes based on sequential modular technology. It requires specification of feed streams and topology of the system. In 1987, an optimization enhancement was added.

GPSS/PC, developed by Minuteman Software (Stow, Mass.) for IBM-compatible personal computers, is based on the popular discrete simulation language GPSS (general purpose simulation system). Reference 14 provides more details.

MicroMENTOR is an educational package for solving distillation problems and includes MCCABE, PONCH, and BATCH for the MaCabe-Thiele, Ponchon-Savarit, and Batch binary distillations (11). The commercially available distillation software packages have been surveyed (15). For reactive distillation, ASPEN software (16) is well-known and widely adopted.

SimuSolv was developed by The Dow Chemical Company for simulating physical systems and optimizing their performances. It has been applied to processing engineering, pharmacology, chemical kinetics, toxicology,

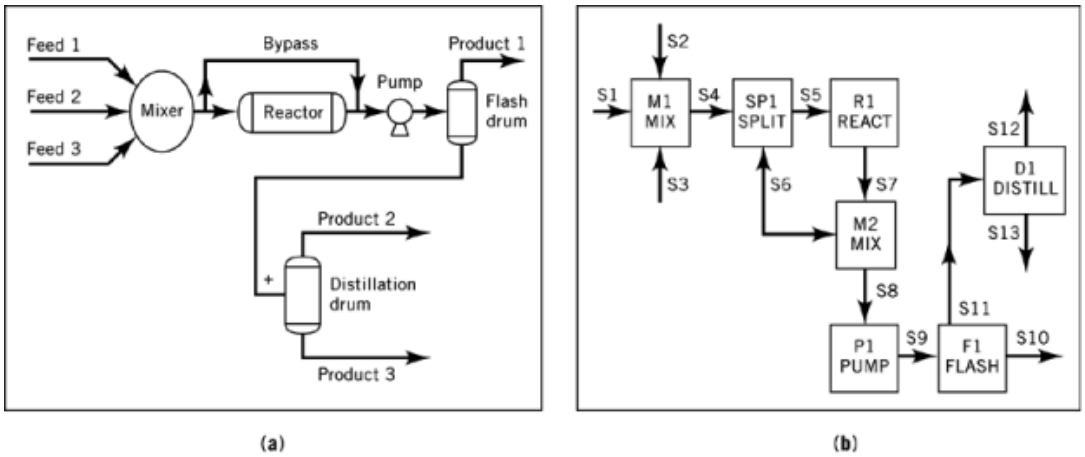

Fig. 1. Block diagrams of chemical processes.

environmental sciences, and agriculture. It uses DACSL (Dow advanced continuous simulation language) and applies the maximum likelihood method for optimizing the model parameters (9).

TUTSIM (Twente University of Technology Simulation program) is designed for computer modeling of dynamic systems (17). It has SUM, GAIn, MULtiply, DIVide, INTegrate, Laplace functions, logic blocks, Z-transform blocks, and other property blocks. With a schematic design tool software OrCAD/SDT III, which contains 600 library parts and over 40 integrated-circuit libraries, the TUTSIM block diagrams can be created by partitioning into small and connected, but more manageable, segments. TUT'S BLOCKS is a regular publication that promotes the use of TUTSIM.

Many developers of software for finite-element analysis (18) provide drafting of pipelines and associated flow analysis. These companies include Algor, McAuto, MacNeal-Schwindler, and FlowDesign. In software, in-house developed pipe fittings are modularized and isometric views of the piping systems with three-dimensional detailing are now commonplace.

Many more special-purpose software packages have been developed, particularly in teaching and research institutions. SMCM is software designed at the University of California in Los Angeles for partitioning of pollutants (19). Monte Carlo and molecular dynamic techniques have been adapted in a molecular simulation model at Cornell University for presenting a detailed atomistic description of the material under study (20). Novo-Nordisk A/S, a Danish biotechnology company, and Silicon Graphics, Inc. have also applied similar techniques for new drug development.

3. Computer Graphics in Instruction

The use of graphic displays as an essential element of computer-based instructional systems has been exploited in a number of ways. Molecular modeling and visualization techniques have supplemented the traditional set of stick models in courses on organic and inorganic chemistry, and animation of molecular motion and of the progress or mechanism of chemical reactions has been a useful classroom tool.

Some practical experiences in using graphic presentation of process simulation results to teach process analysis and dynamics have been described (21). Interactive graphic displays have been included in teaching chemical reaction engineering, process control, and staged operations (22). The development of computer graphics in the PLATO system at the University of Illinois has had a significant impact on the use of computers

in the chemistry and chemical engineering curricula. Experiments such as distillation are modeled by allowing the user to assemble the apparatus from pieces shown on the screen, charge the distilling flask, boil off the contents while accumulating a T–x curve, and even experience an explosion if the receiver overflows. A number of groups have explored the use of PLATO for instruction in chemical engineering (23–25).

The ubiquitousness of the personal computer and the increasing power of the program packages available for it have shifted the emphasis away from large, mainframe-based systems like PLATO. Instead, graphics are included in utility programs such as equation solvers, spreadsheet processors, and word processors.

4. Computer Graphics and Chemical Structural Analysis

CAD/CAM techniques have provided the framework for using the computer as a tool in the drawing and analysis of chemical structures and, more recently, in the use of chemical structures to design reaction pathways and new products. The essential elements in these applications of CAD/CAM are that the possible structures are relatively deterministic and that allowable changes in structure through reaction are governed by thermodynamic, stoichiometric, and steric constraints.

4.1. Two-Dimensional Representation of Chemical Structures

The IUPAC standardization of organic nomenclature allows automatic translation of a chemical's name into its chemical structure, or, conversely, the naming of a compound based on its structure. The chemical formula for a compound can be translated into its structure once a set of semantic rules for representation are established (26). The semantic rules and their application have been described (27, 28). The inverse problem, generating correct names from chemical structures, has been addressed (28) and explored for the specific case of naming condensed benzenoid hydrocarbons (29, 30).

An important approach to the graphic representation of molecules is the use of a connection table. A connection table is a data base that stores the available bond types and hybridizations for individual atoms. Using the chemical formula and the connection table, molecular structures may be generated through interactive graphics in a menu-driven environment (31–33) or by using a linear input of code words (34, 35). The connection table approach may be carried to the next step, computer-aided molecular design (CAMD) (36).

A difficulty arises in representing chemical structures in print or on a CRT (cathode-ray tube) because chemical structures are three-dimensional and the representations are two-dimensional. One approach to overcoming this problem has been the use of the linear notation developed by Wiswesser (37) to represent three-dimensional structures two-dimensionally. An implementation of this method for computer applications has been proposed (38). The CHEM program for phototypesetting (39) is an example. The widespread availability of text editors for electronic publishing has led to a number of commercial programs for drawing chemical structures (40, 41). These programs may be stand-alone, or they may create files that can be integrated directly with text files.

The Chemical Abstracts Service has institutionalized the use of graphic representations for identification of and retrieval of information about chemical compounds through their Graphical Data Structure (GDS) and connection table (CT). Two information packages, Messenger and STN Express, are the basis for this on-line retrieval system (42).

4.2. Three-Dimensional Modeling of Chemical Structures

The two-dimensional representations of chemical structures are necessary to depict chemical species, but have limited utility in providing true understanding of the effects of the three-dimensional molecule on properties

and reactive behavior. To better describe chemical behavior, molecular modeling tools that reflect the spatial nature of a given compound are required.

Early efforts to develop molecular models emphasized ways of representing three-dimensional aspects in two-dimensional projections. Some of the problems addressed were the folding of macromolecules (43, 44) and two-dimensional projections with hidden surfaces (45, 46). The state of the art in the early 1970s has been reviewed (47).

A number of groups developed approaches to molecular modeling, including a graphic system (48–50), the MAGIC system (51), the DRACO program (52), and the GRAMPS/GRANNY system (53). One relatively early program explicitly designed for producing three-dimensional structural representations was CDRAFT (54). This program provides an array of structures that can be assembled using a template and a set of special symbols.

The three-dimensional models used in modern organic chemistry have their origins in Newman projections (55, 56). The projections may be depicted using a stick-and-ball representation known as ORTREP (57) or a perspective-shading approach (also known as space filling) used in the SPACEFIL program (58). Ways to incorporate both stick and ball and perspective shading into molecular representations have been suggested (59). The SPACEFIL program has been modified to incorporate color graphics (60), and most of the currently available molecular modeling programs use the combined depictions.

A unique application of molecular modeling techniques has been the recreation of the Brookhaven Protein Data Bank (PDB) in the form of computer-generated molecular models (61). Many other programs use the space-filling approach (62–64). Interactive programs for macromolecular modeling include the GRAMPS/GRANNY system (53) and CHOODRAW (65).

Three-dimensional representations of complex molecules have opened the way for a number of applications. For example, structural models of opened double-stranded DNA have been used to study interactions of DNA with various intercalating drugs (66). Enzyme-inhibitor complexes have been studied using the models (67) and a movie illustrating the actions of zinc protease thermolysin that was made using the GRAMPS system (68). Graphic conformational analysis has been extended to peptide systems using the PepCAD system (69) to determine the minimum conformational energy for *N*-formyl-*N*′-methylalanineamide.

SPACEFIL has been used to study polymer dynamics caused by Brownian motion (60). In another computer animation study, a modified ORTREPII program was used to model normal molecular vibrations (70). An energy optimization technique was coupled with graphic molecular representations to produce animations demonstrating the behavior of a system as it approaches configurational equilibrium (71). In a similar animation study, the dynamic behavior of nonadiabatic transitions in the lithium–hydrogen system was modeled (72).

5. Molecular Modeling for Reaction Path Synthesis and Molecular Design

Applications of CAD/CAM to drawing and modeling chemical structures are essentially passive; that is, although the user decides which compound to draw, strict rules govern what that compound will look like. A reasonable goal for the application of molecular modeling capabilities is the ability to design chemical syntheses based on the structure of a desired product, a set of potential reaction pathways, perhaps defined on the basis of a connection table and a Gibbs energy minimization routine (see Molecular modeling).

Emulation of the reasoning path of a chemist in developing molecular structures was the basis for the program CONGEN (73). The reasoning was guided by a set of constraints applied to the evolving structure. However, determination of a structure on the computer must be guided by more than a comprehensive set of rules. For example, spectroscopic information must be considered (74, 75).

Techniques for the synthesis of reaction paths on the basis of enumeration of all possible reactions are fairly well developed. The SYNCHEM2 system conducts a backward search of possible reaction paths from

a desired product (76). Because the procedure is limited by the rapid growth of combinatorial problems, a heuristic approach for choosing desirable paths was developed. This enumeration approach was first suggested in 1969 (77).

An alternative approach (78, 79) is based on a set of possible reaction schemes that are used to generate potential new pathways. Under both approaches, the problem, in part, is how to evaluate the utility of a particular scheme. A computer-assisted approach to predicting potentially useful reactions has been developed (80). The union of existing capabilities in modeling chemical structures with selecting reaction pathways has not yet taken place.

An area that has used chemical structures for predictive purposes quite successfully is the estimation of thermophysical properties of compounds. There has been an extensive compilation of estimation methods (81), and prediction of physical properties has been automated using these techniques (82). More recently, the use of group contribution techniques to design new molecules that have specified properties has been described (83). This approach to compound design is being used to develop replacement materials for chlorofluorocarbons.

6. Pattern Recognition and Interactive Graphics Applications

The graphics capabilities of the CAD/CAM environment offer a number of opportunities for data manipulation, pattern recognition, and image creation. The direct application of computer graphics to the automation of graphic solution techniques, such as a McCabe-Thiele binary distillation method, or to the preparation of data plots are obvious examples. Graphic simulation has been applied to the optimization of chemical process systems as a technique for energy analysis (84).

The interactive features of the modern computer allow the use of graphic methods to be further expanded. An early effort to couple data fitting with interactive computing was the VIPER program (85). In the VIPER system the user changes parameters within a curve-fitting routine with a light pen, after viewing the results from the previous fit. A somewhat similar approach was suggested for analyzing results from a shock-tube experiment by selecting candidate kinetic models, viewing the results, and then modifying the model until satisfactory results are obtained (86). The capability of interactively selecting multiple fitting models for a set of data is now commonly available in a number of spreadsheet programs, such as Lotus 1-2-3 and Quattro-Pro. The use of Lotus 1-2-3 in multivariant kinetic analyses has been described (87).

The graphic operating framework has been effective as a basis for image processing applications. Early work (88) using digitized images of bubbles in a gas–liquid reactor demonstrated the utility of interactive image processing in research. Examples of similar studies include drop-size studies in sprays (89) and mixing studies (90).

The use of graphic simulators for flow visualization has grown from relatively simple models, such as the generation of natural convection streak lines (91), to sophisticated commercial programs for the analysis of complex flow regimes. Examples include the simulation of plastic injection molding by Graftek, Inc., and the flow simulator FLOW3D developed by the HTFS consortium. Perhaps the ultimate graphic simulation is the visual depiction of process equipment as it is being designed, using a program such as the Intergraph, Inc., Design-Review system.

7. CAD/CAM Applications in Process Flow-Sheet Development

The use of the computer in the design of chemical processes requires a framework for depiction and computation completely different from that of traditional CAD/CAM applications. For this reason, most practitioners use computer-aided process design to designate those approaches that are used to model the performance of individual unit operations, to compute heat and material balances, and to perform thermodynamic and transport

analyses. Typical process simulators have, at their core, techniques for the management of massive arrays of data, computational engines to solve sparse matrices, and unit-operation-specific computational subroutines.

The more traditional CAD/CAM approaches do, however, have a significant place in chemical process design. The creation and optimization/modification of a process flow diagram lends itself to the CAD/CAM framework. Early work (92) was restricted to the synthesis of piping networks as components of the process flow sheet. A system specifically designed for the creation of process flow diagrams using an experimental program, PFDII, has been described (93, 94). PFDII was based on an adaptation of Rubin's graph reduction and embedding procedure to construct and automatically modify the process flow sheets. In a somewhat different approach (95) a relational database was employed to store and retrieve the symbols for creating the diagram, and interactive methods allowed the user to both create and update the flow diagram.

The introduction of menu- and icon-driven interactive programs has permitted improvements in computer–user interfacing. Two programs, PFG for process flow sheets and PIG for piping and instrumentation diagrams, use icon and menu input (96). ChemShare has offered a version of the DesignII program that interfaces directly with Microsoft Windows, providing a traditional process design simulator with the capability of drawing process flow schematics.

One opportunity for the use of CAD/CAM solids visualization techniques is in the three-dimensional depiction of chemical process equipment as a possible replacement for the process models that are now commonly used as guides for construction piping and equipment layout. An interactive program (97) for this purpose uses a number of primatives generated from polyhedrons to create shape clusters that can be used to represent the three-dimensional shapes of processing equipment. An equipment visualization capability is incorporated in the Intergraph, Inc., DesignReview software.

Most of the recent flow-sheet drawing applications involve interfacing with process design simulators so that a flow sheet entered into the simulator may also be depicted by associated graphics software. One example of add-on software is a program called GRAF that accepts input files from the ASPEN simulator to create a process flow diagram (98). Some commercially available packages that include graphics as integral parts of the program are ChemcadII from COADE, ASPEN PLUS with ModelManager, and ProSim. The ChemShare Design PFD system is an example of a process flow-sheet program designed to operate in association with a comprehensive process simulator.

A future goal for the integration of graphics and process design simulators is to be able to use an interactive graphics program to prepare the input to the process simulator. This capability would allow true on-line process modification, flow-sheet optimization, and process optimization, and is likely to be one of the key developments in this field in the 1990s (99).

8. Graphics Applications in Process Optimization and Control

The capabilities for computer-aided process design and for utilization of CAD/CAM techniques in association with design have progressed further than similar applications in the design of process control systems. Direct application of graphic techniques to the design of process control systems has been limited to certain approaches, for example, one in which graphic display of the frequency response of feedback controllers is used as part of an interactive design method for feedback control systems (100). The CHESOPS program (101) took a similar approach to operability analysis of a process. The basis for performance calculations with the CHESOPS system was a conventional process simulator, which was run for a number of cases to simulate dynamic behavior. The graphics consisted of a series of two-dimensional plots that explored the feasible operating region for the plant. The optimization of a semibatch free-radical polymerization using interactive CAD tools (102) also used graphic display of computed results as an aid to interactive analysis.

The goal of integrating automated process optimization with automated design of process control and instrumentation diagrams will likely be more difficult to attain than the integration of graphic input for

process simulation programs. The computational engines for optimization are under development at this time, as are effective dynamic simulators.

There are, however, two areas in which graphic methods have had a significant effect on both process design and process control. The synthesis of heat-exchange networks is an exercise in examination of multiple combinations of hot and cold streams transferring heat across heat-exchanger nodes. The network synthesis methods (103) are intrinsically graphic in approach. An interactive software package, RESHEX (104, 105) has been developed to implement this approach. The HEXTRAN program by Simulation Sciences, Inc., is another example of the automation of heat-exchanger network design.

The second area, the implementation of a modern process monitoring and control system, is the most dramatic current application of CAD/CAM technology to the chemical process industry. The state of the art is the use of computer graphics to display the process flow diagram for sections of the process, current operating conditions, and controller-set points. The process operator can interact directly with the control algorithms through the keyboard or with a light pen to change the set points. The controllers may consist of conventional feedback or feed-forward loops that are coupled directly with the process; alternatively, they may be devoted simulators that make decisions based on computed projected performance.

The process monitors and controllers typically also have the capability for data logging, analysis, and display. This capability has made on-line control of pilot plants, as well as commercial-scale processes, desirable. Pilot-plant applications for on-line control have been described (106), and the use of such systems for both monitoring and process diagnosis has been discussed (107). A number of commercially available process control programs that run on microprocessors have been reviewed (108). Virtually all of them incorporate graphic display as an integral part of the interactive capability of the program.

9. Essential Elements for Developing In-house, Special-Purpose CAD Software

Any program developed in-house must be easy to use, or user-friendly. If the program has various options for input, analysis, computation, and output, then it must provide the user with a fast way to select them. To meet this need, the system is likely to be menu-driven. The peripheral interactive devices such as mice, joysticks, light pens, graphic tablets, and templates are helpful and often used to expedite the selection process.

10. User-Created Cursors of Various Shapes and Sizes

When a microcomputer system is powered on, the connected display monitor shows a flashing (underline), a filled rectangular block, or another predesignated shape. Such prompting signs are cursors that alert the user to enter character or characters via the keyboard as part of a program or as a command. Figure 2 provides an example of two types of cursors used in the AutoCAD software. The left panel shows a filled bar cursor appearing as the background for the word “DRAW,” which can be moved up and down by pressing the respective arrow keys on the keyboard; the right panel shows two hairline cursors, one horizontal and one vertical, which are moved using a mouse.

Cursors of different shapes and sizes can be designed easily by the microcomputer user through simple programming, such as using the BASIC commands GET and PUT. The movement of the user-created cursor is controlled through the use of the INKEY$ function and by testing the ASCII codes of the keyboard keys.

Two unfilled rectangular bar cursors of the same size and shape are used in Figure 3. The top bar cursor allows a particular menu to be selected by pressing the left or right arrow keys, and the lower bar cursor allows one of the items listed under the chosen menu to be selected by pressing the up or down arrow keys. A mouse can also be used to control the selection.

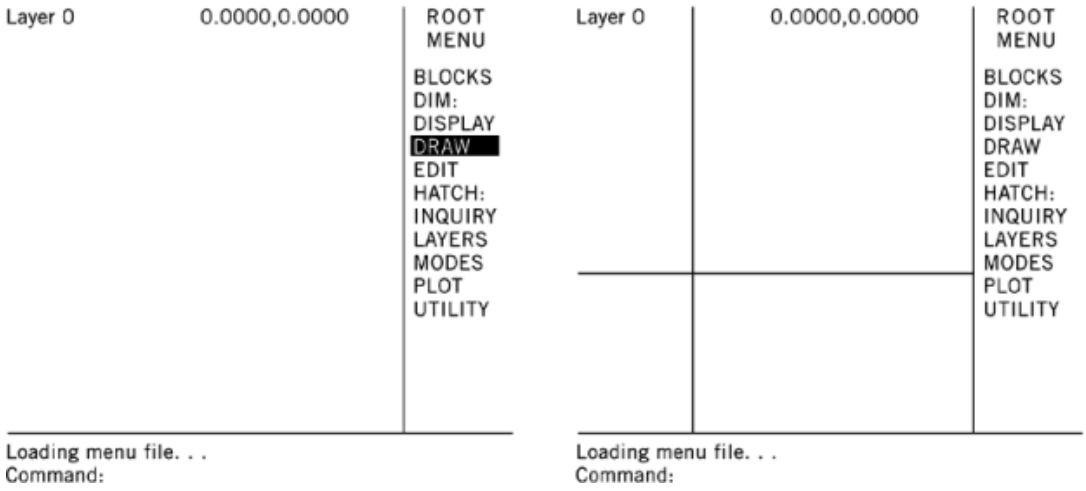

Fig. 2. Rectangular cursor (highlighted) in the left panel and horizontal and vertical hairline cursors in the right panel.(Courtesy of Autodesk.)

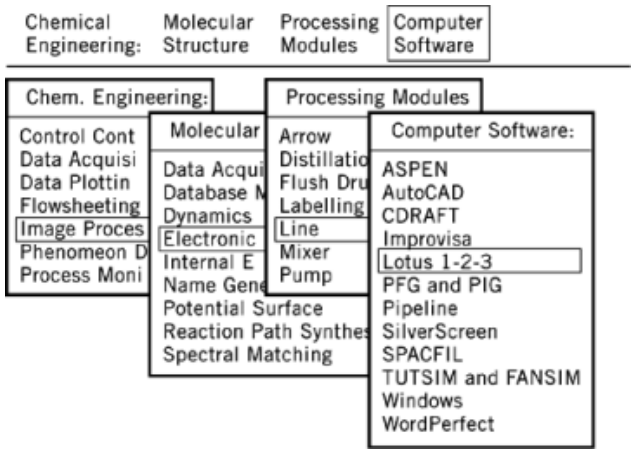

Fig. 3. Nested menus.

11. Menu, Tablet, Template, and Spreadsheet

Menu design is an essential element in microcomputer software development. Figure 2 shows a menu, "ROOT MENU." Figure 3 is presented to show all available menus. When there are more menus and the total width exceeds 80 columns, scrolling must be effected (109, 110). If the top bar cursor is moved to the first column, Menu 1, only the contents of Menu 1 will be displayed.

A tablet is a device for placing selectable menus or modules on a separate, peripheral plate. It is helpful for a user of CAD software to have all the modules available displayed on the screen for selection. The only drawback in such an arrangement is that it takes away a portion of the screen space and therefore less space is available for the actual CAD activities. Selection of an item from a tablet can be made with a mouse or light pen (Fig. 4).

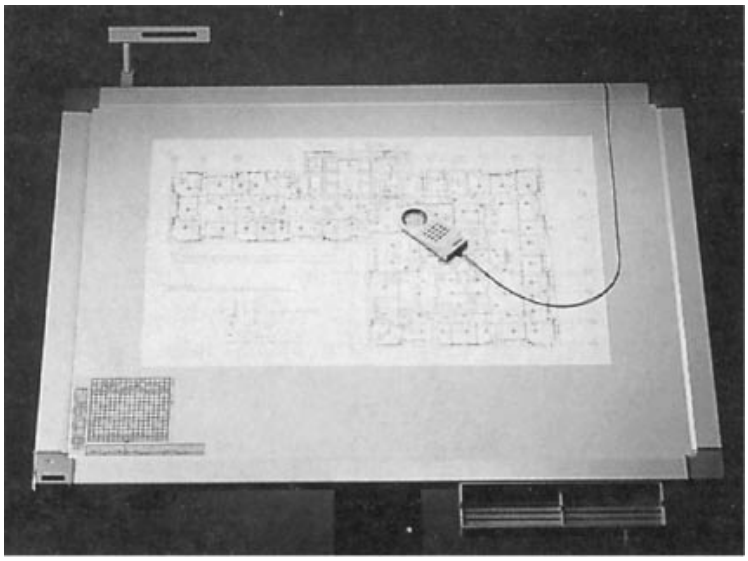

Fig. 4. Selection from a tablet with a light pen. Courtesy of CalComp Inc.

A template can be designed to be mounted or pasted on a keyboard for quick reference. It shows which function keys, in conjunction with the Shift, Alt, and Ctrl keys, have been assigned for implementing special tasks. A well-known example is the WordPerfect template shown in the left panel of Figure 5. A template is usually designed in conjunction with the function keys available on the keyboard. Template.Fon is a program developed to interactively use the display screen to design templates (1). In the right panel of Figure 5, specially designed fonts stored as disk files are drawn at desired locations to indicate the assignments of the 40 function keys for displaying, in this case, elements involved in chemical technology.

A spreadsheet is another essential element in developing CAD software. LOTUS 1-2-3 is well-known among the numerous commercially available spreadsheet software packages. Spreadsheet software is used to design tabulated forms for storing and editing data, for listing programs in matrix form, and for easily combining various elements in a matrix to print or to generate new rows and columns. Quick recall and access to a data set or program and the ability to combine it with other data sets or programs are the principal goals of designing spreadsheets. A spreadsheet can be used for drawing flow sheets and for optimizing chemical processes (111).

12. Modular Approach and Three-Dimensional Solid Modeling

Commonly used entities such as the pipe fittings shown in Figure 6 are increasingly being created and stored as graphic files for quick retrieval. In the construction of three-dimensional piping systems, they can be retrieved, rescaled, and positioned by use of a pointing device for connecting to the other pipe elements. Once a three-dimensional pipeline system has been constructed, it can be displayed on the screen using multiple views. Figure 7 is a four-way, split-screen display showing the front, top, isometric, and right-side views of an incomplete pipeline system. Detailing of a three-dimensional structure can be carried out in a multidimensional way, as illustrated in Figure 8. SilverScreen, developed by the Schroff Development Corp., is an example of commercially available software that is capable of implementing the latest trends in computer-aided drafting. It provides the capability for detailed annotation on the front, top, and right plane of a three-dimensional solid

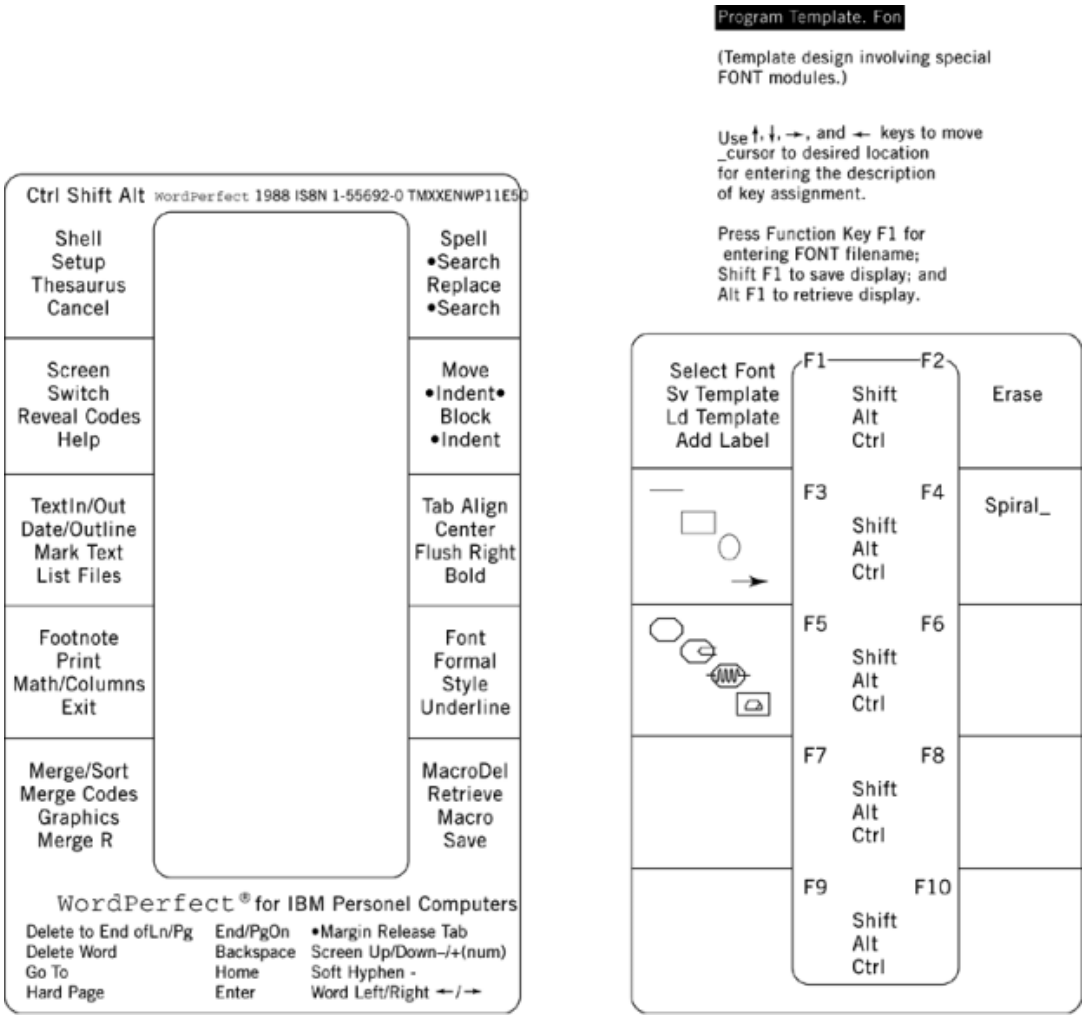

Fig. 5. CAD template. Left panel, courtesy of WordPerfect Corporation.

model, as shown in Figure 8. It is menu-driven and divides the screen, as shown in Figure 9, into a menu area (upper left corner), a status area (lower left corner), and a graphic area (the remaining portion on the right). SilverScreen enables the graphic area to be split up to eight ways for displaying a three-dimensional object. A pointing device such as a mouse or the arrow keys on the keyboard can be used to select an option from the menu list, and the Del (delete) and Ins (insert) keys on the keyboard can be pressed to adjust the increment being used for the movement of the screen cursor. The three-dimensional coordinates of the current position of the screen cursor (+, box, or trid) and the increment of its movement on the screen are all displayed in the status area. In Figure 9, the Menu Area shows a variety of the capabilities of SilverScreen. For example, the Language option enables computer programs written in BASIC and C to be implemented in conjunction with the SilverScreen commands. The I/O option enables the drafting or solid model files created by SilverScreen to be stored in a variety of formats compatible with other CAD/CAM software packages. The Window option enables a three-dimensional solid to be viewed using up to eight windows. The Presentation option enables

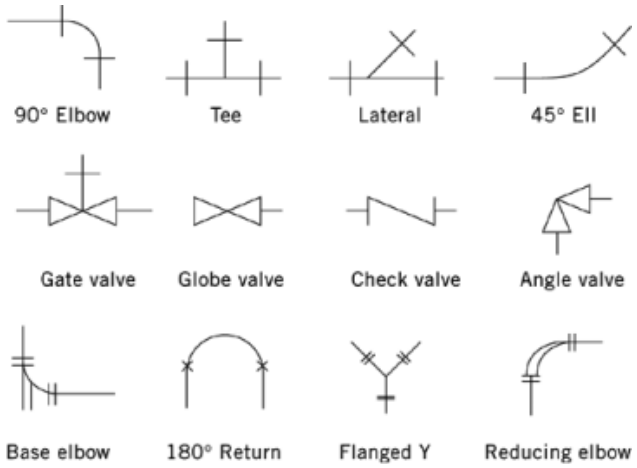

Fig. 6. Pipe fitting elements.

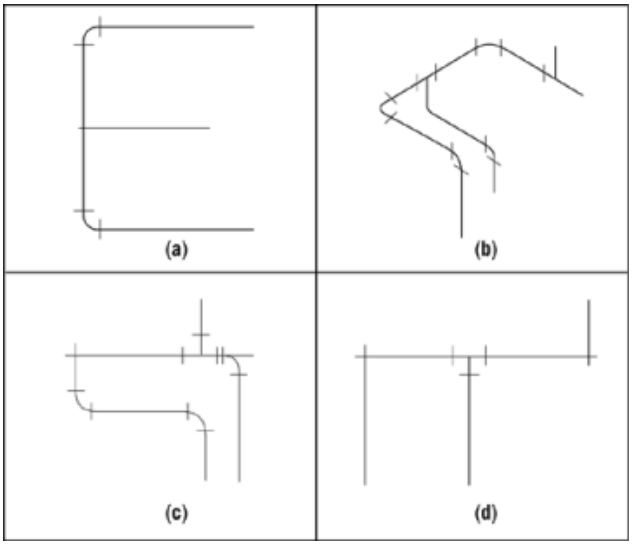

Fig. 7. Split screen viewing of designed parts. (**a**), Top view; (**b**), isometric view; (**c**), front view; (**d**), right-side view.

a three-dimensional object to be displayed with the hidden lines removed and shaded with different grays or rendered in color.

13. Other Capabilities

The creation and analysis of process flow sheets has become much easier because of the availability of automated systems to draw and revise them. The goal of the use of the flow sheet as the input for process simulation and for process control is likely to be achieved reasonably soon. The use of interactive graphic displays for process monitoring and control is pervasive today.

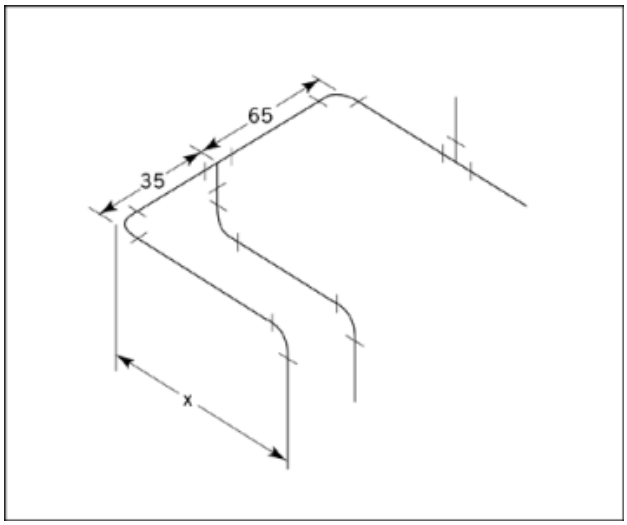

Fig. 8. Three-dimensional solid model.

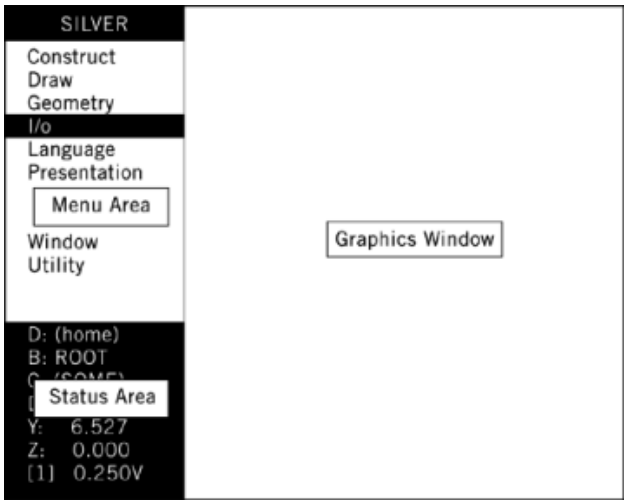

Fig. 9. Computer-aided drafting.

It is likely that there will always be a distinction between the way CAD/CAM is used in mechanical design and the way it is used in the chemical process industry. Most of the computations required in mechanical design involve systems of linear or linearizable equations, usually describing forces and positions. The calculations required to model molecular motion or to describe the sequence of unit operations in a process flow sheet are often highly nonlinear and involve systems of mixed forms of equations. Since the natures of the computational problems are quite different, it is most likely that graphic techniques will continue to be used more to display results than to create them.

Computer graphics will continue to provide an effective tool for drawing chemical structures. Great improvement in software packages can also be expected. As illustrated in Figure 10, SilverScreen can list the

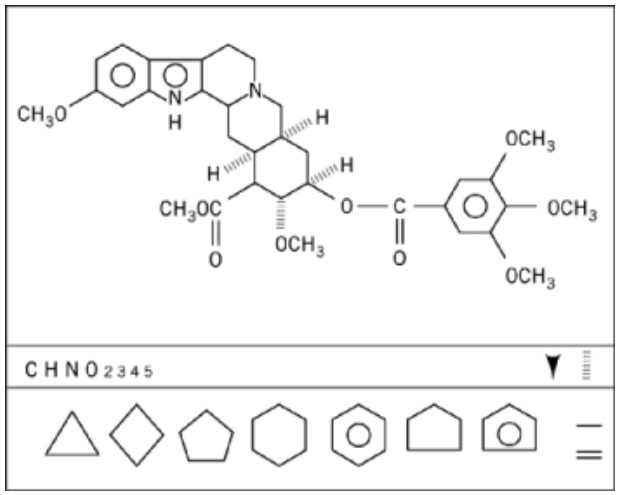

Fig. 10. Drawing chemical structures.

needed modules (benzene, ring, bond, CH_3, and N) at the bottom of the screen, and select for copying, rotate if necessary, and then place them at desired locations, all interactively.

The use of color graphics is also an effective means for displaying chemical structures. This method is far better than typesetting the three-dimensional architecture of complex multimolecule assembly (112). For developing in-house CAD software programs, the three-dimensional, solid-modeling capabilities of SilverScreen can also be utilized either in monochrome or color for construction of such structures (113).

CAD/CAM capabilities have had a subtle, but significant impact on chemical technology. Molecular modeling (qv) capabilities have led to the ability to describe chemical behavior and are showing promise in the design of new molecules. Pattern recognition techniques are being used to automate the analysis of chromatograms and spectral information.

It may be said that chemistry is about shapes, how things look, how things fit together, and how shapes change (114). For exploring noninteger dimensionality, fractals have emerged as a mathematical language. Unquestionably, CAD/CAM applications will be further expanded in already established areas and will be intensively explored in many new fronts.

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