

Microcomputer Programs for Chemical Engineers

Edited by
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PREFACE

Microcomputers offer easier/better access to computing power than do mainframe units. They are "friendlier" than scientific calculators, too. But they are not going to replace either—that's expecting too much. In 1978, CHEMICAL ENGINEERING introduced its first book of calculator programs for chemical engineers. But, just as the scientific calculators replaced slide rules for engineering computation, they were destined to be virtually replaced in just a few years by microcomputers.

Now, CHEMICAL ENGINEERING is proud to present its first volume of microcomputer-program listings for chemical engineers. But, not only are program listing offered here. In addition this book provides an introduction to microcomputers, and articles on how to develop technical software, the use of spreadsheet software to solve engineering problems, and applications of microcomputers for process design, energy management, simulation and process-systems engineering.

The BASIC microcomputer programs presented here are interactive and easy to use. They are intended as a single-source library of programs, specifically designed to solve chemical engineering problems, and are based on material carefully selected from the pages of CHEMICAL ENGINEERING. The contents of the programs listed cover the full range of chemical engineering principles from engineering mathematics to physical-properties correlation to design-oriented programs for solving fluid flow, heat transfer, mass transfer, and engineering-economics problems.

The programs are written for the Apple II microcomputer, but are easily adaptable for use on other popular personal computers. See the next section for further details on program listings.

PROGRAM LISTING NOTES

The BASIC programs in this book are written for the Apple II microcomputers. But owners of other microcomputers should not despair—the programs are easily adaptable. In fact, the only variations in BASIC dialect are for display commands, such as those to clear the screen (“HOME” for the Apple, but “CLS” for the IBM PC), or to move the cursor vertically (for instance, “VTAB 4” moves the cursor down four lines on the Apple II microcomputers). Accordingly, users of other microcomputers should change programs listings for these commands.

The programs are interactive and easy to use. For each program, the user is given instructions via the program menu, and at that point told which data should be entered and how to proceed from there to the solution. In many cases, a variety of engineering units can be used.

The program listings are in BASIC, and the programming logic should be understandable to most readers. For those more proficient in programming, the listings can easily be modified for customizing to the individual problem.

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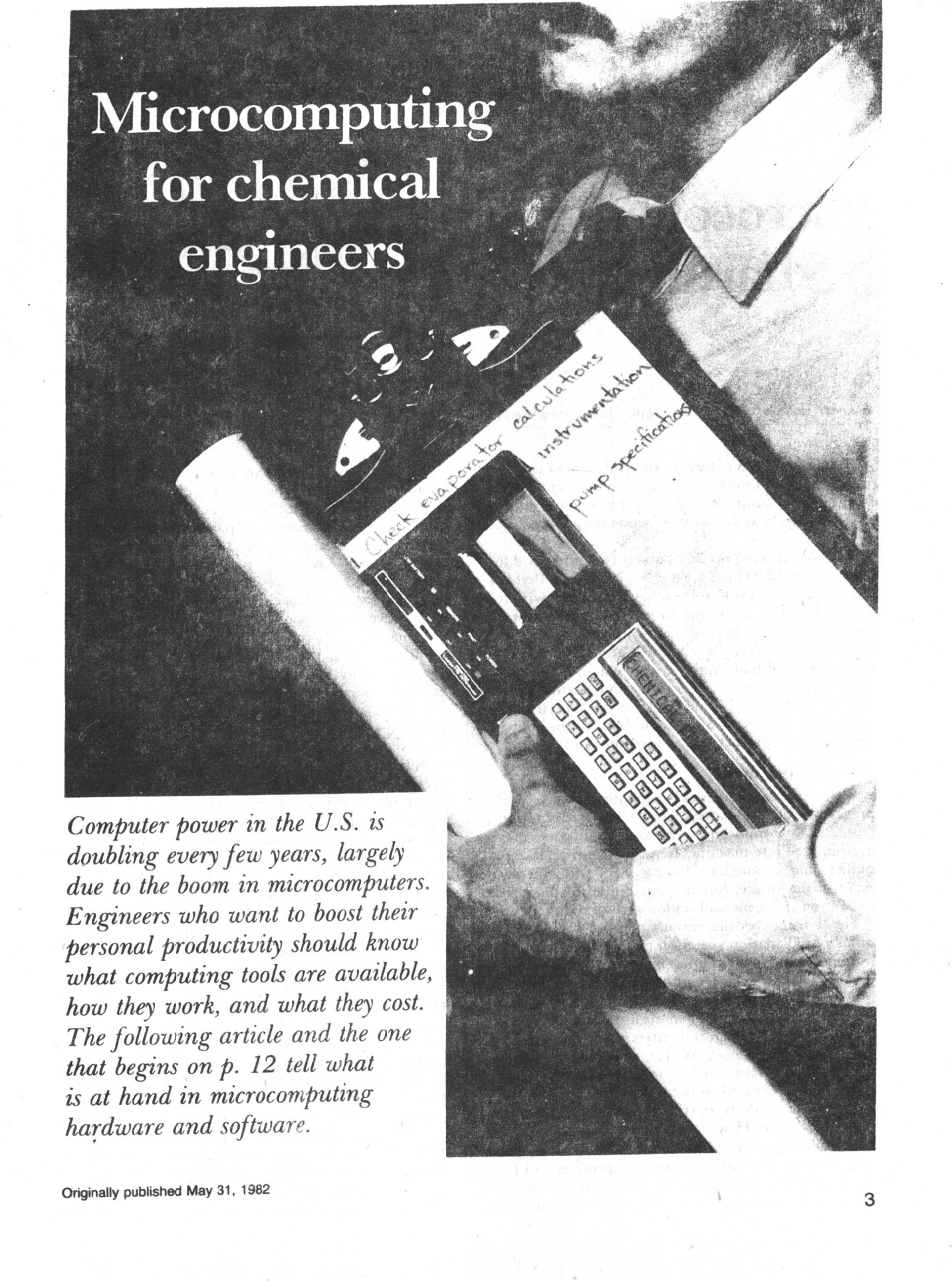
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Section I

Introduction

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Microcomputer data-acquisition
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BASIC, FORTRAN and Pascal
Microcomputer systems for process design
Computer horizons in process-systems engineering—Part I
Computer horizons in process-systems engineering—Part II
Microcomputers in energy management—I
Microcomputers in energy management—II

Microcomputing for chemical engineers



Computer power in the U.S. is doubling every few years, largely due to the boom in microcomputers. Engineers who want to boost their personal productivity should know what computing tools are available, how they work, and what they cost. The following article and the one that begins on p. 12 tell what is at hand in microcomputing hardware and software.

Originally published May 31, 1982

Microcomputing hardware

Stewart Goldfarb and Steve Griffin, Dow Corning Corp.

□ Today's microcomputer is powerful enough to solve real engineering problems, yet inexpensive enough that every engineer could have one. Such technology means improved productivity for those who take advantage of it.

However, making decisions about computers is difficult because the technology is changing so fast. Perhaps the best approach is to solve today's problems with today's computing tools, and to leave tomorrow's problems for the tools that will be available then.

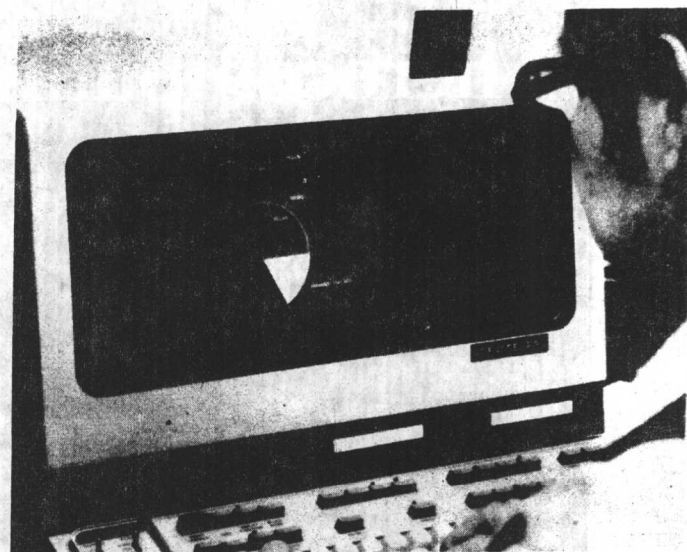
This article focuses on handheld and desktop microcomputers, which an engineer can own and use professionally because they are powerful and relatively inexpensive. But first a brief look at the spectrum of computers is in order. Since some of the terms may be unfamiliar, a glossary is provided on p. 11.

Micro, mini, maxi

Engineers use a variety of computers in their work: programmable calculators, handheld and desktop microcomputers, minicomputers and mainframe microcomputers. These machines frequently overlap in capabilities, and distinctions among them will blur even more in the future, but the capabilities of those that remain on the scene will undoubtedly expand greatly.

Fig. 1 compares the various types of computers in terms of calculation speed—number of floating-point (decimal, as opposed to integer) multiplications per second. Not shown is the variation in data storage and handling capability, which is at least as important as sheer number-crunching in many applications. On such a scale, "business" microcomputers would outshine "scientific" ones, by design. We can now describe each of the computer types briefly, focusing on differences in their capabilities and costs.

Programmable calculators, such as the Texas Instruments TI-59 and the Hewlett-Packard HP-41 series, are widely used by chemical engineers in design and operations because they are compact, inexpensive, and handle engineering math well. Though limited in the past by their modest memory and few non-math functions,

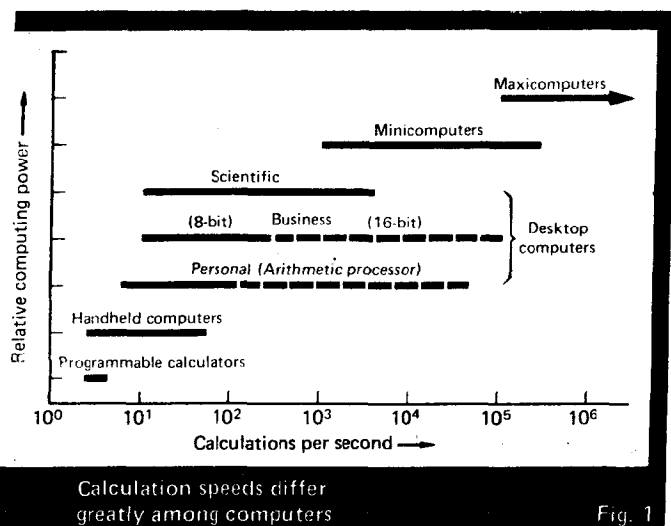


programmable calculators are now becoming more versatile. For example: The HP-41C calculator can be augmented by: a link for communicating with compatible instruments; a memory-expanding module or cassette recorder; a card or bar-code reader; and a printer/plotter. Retail prices for programmable calculators range from \$50 to about \$500.

Handheld microcomputers are about the same size as calculators, yet offer alphanumeric display (24 characters), a miniature typewriter keyboard, and the high-level BASIC language. With BASIC, programs are easier to develop, debug and transfer to other computers than are calculator programs. Table I shows a simple heat-transfer calculation in BASIC and in a calculator language. Early models (such as the Radio Shack TRS-80 PC-1 shown on the cover) are roughly comparable with calculators in speed and storage capability, and cost about \$200–250. But recent improvements offer greater speed, plus useful accessories such as color printing.

Desktop computers are called by several names. Here we will separate them into three types: personal computers for general math and data manipulation; business microcomputers, with greater storage, manipulation and display capability; and scientific computers, with powerful calculation, graphics and data-acquisition. Desktop computers range from about \$300 to over \$3,000, depending on the type of microprocessor, storage capacity, and built-in accessories. A complete system, however, can run from \$1,000 to \$20,000 or more, depending on the types of peripheral devices (for storage, printing, etc.) attached to the computer.

Minicomputers are bigger and faster than desktop computers, which allows them to do any calculation a chemical engineer might need except for simulations of complex processes. The difference between minicomputers and microcomputers is somewhat hazy, in that today's microcomputers are as powerful as some of yesterday's minis. In fact, Hewlett-Packard and Digital Equipment now sell their bottom-of-the-line minicomputers as desktop computers. Minis are still the workhorses of industrial applications, however, because they



can handle several users and they calculate faster. For example: A minicomputer might do a tray-by-tray distillation calculation in several minutes, while with a microcomputer such a nested iterative calculation could take hours. Costs for minicomputer systems range from about \$20,000 to \$250,000.

Maxicomputers are the most powerful computers built today: the fastest number-crunchers, with the greatest memory and peripheral-device capability, and able to handle the most users. Compared with the business microcomputer, the maxi has up to 256 times as much memory, and performs calculations 1,000 times as fast. But it is also 100 to 1,000 times as expensive, with costs

ranging between \$250,000 and \$10 million. Note that a maxi is not necessarily any less "personal" than a desktop computer, since current designs allow each user to think he or she has the whole computer alone. But in practice, the user will usually be aware of other users slowing down the computer's response.

Though chemical engineers employ all these computing machines, for the rest of this article we will look only at handheld and desktop microcomputers. These can handle many engineering problems that do not require lengthy iterations, and are so priced that an engineer can expect to obtain one for personal use.

Handheld microcomputers

At the heart of a handheld computer is a microprocessor. Earlier models, such as the Radio Shack TRS-80 PC-1, and the similar Casio and Sharp computers, use microprocessors that handle relatively small amounts of information (4 bits) at a time. They therefore run programs about as fast as programmable calculators do. Recent models, such as the TRS-80 PC-2 or Sharp PC-1500, use an 8-bit microprocessor. This means that they perform calculations nearly as fast as desktop computers, and much faster than calculators.

The ability to run programs in the BASIC language is an important advantage of the handheld computer, because BASIC is relatively easy to write and can be transferred to other computers. There are differences, however, in the versions of BASIC used by the various computer manufacturers. Therefore, some modification of programs may be needed. Transferring to other microcomputers is generally not a problem, since the handheld-computer version of BASIC is derived from Microsoft BASIC, a *de facto* standard for micros. But extra effort is needed when transferring to computers that use a different version of the language.

In a recent article,* an engineer compares the TRS-80 PC-1 computer with the HP-67 programmable calculator. For his circuit calculation, the program for the handheld computer took one-fourth as long to write, had better prompting features, was easier to follow and more easily modified. The author was pleased that the display on the handheld computer is not used for computation, because this allows him to interrupt easily. But he preferred the calculator's magnetic-strip storage to the computer's cassette recorder.

The early handheld computers now cost about \$200, and the newer models are about \$250. Peripherals for printing and program storage are generally comparable to those available for programmable calculators, with a few exceptions. For example, Panasonic provides add-on modules to expand its HHC computer into a desktop computer (the whole unit fits into a briefcase), and Radio Shack's new TRS-80 PC-2 offers a color printer/plotter. Table II summarizes features and prices for a few of the available handheld computers.

Desktop computers

Desktop computers are becoming a familiar sight in the chemical process industries, finding uses as word processors, terminals for communicating with other

High-level language vs. programmable-calculator language

Table I

Equations for heat-exchange calculation:

$$\Delta T = (T_1 - T_2 - T_3 + T_4) / \ln((T_1 - T_2) / (T_3 - T_4))$$

$$Q = UA\Delta T$$

Programmed in BASIC:

```
60 T(5) = (T(1) - T(2) - T(3) + T(4)) / LOG (T(1) - T(2))
    / (T(3) - T(4))
70 Q = U * A * T(5)
```

Programmed in calculator language

```
RCL    06    )
01     RCL    )
-      05    =
RCL    -      STO
02     RCL    05
=      06    x
STO    ÷      RCL
05     (      07
RCL    LN    x
03     (      RCL
-      RCL    08
RCL    05    =
04     ÷      STO
=      RCL    00
STO    06
```

*Lewart, Cass R., Pocket Computer Solves for LC Resonance Using BASIC, *Electronics*, June 16, 1981.

computers, data-acquisition systems, and computational tools. Manufacturers tend to use the term "personal computer" for many desktop computers, resulting in some confusion about capabilities and applications. Here we will be more specific, defining three categories of desktop computers:

- Personal microcomputers, inexpensive enough for home and hobby applications.
- Business microcomputers, dedicated to professionals for their day-to-day office work.
- Scientific desktop computers, for high-powered calculation and laboratory work.

All desktop computer systems include a typewriter keyboard, some type of multiline display such as a cathode-ray tube (CRT) or television set, and a means of saving and loading data and programs. We will now look at each of the three types of systems in more detail.

Personal microcomputers

Personal microcomputers most familiar to engineers are models such as the Radio Shack TRS-80 Model-III, Commodore PET, and Atari 400. Such a computer can be used for job-skill improvement (learning about programming), recreational uses such as games, educating children, and a variety of hobby applications such as keeping track of personal records.

Such computers are "personal" because they are so inexpensive: A system with a few needed peripherals often costs \$1,000 or less. Table III lists several computers that might be used in such systems.

Those willing to spend more can get a more powerful processor and greater memory in a computer such as an Apple II, HP-85 or IBM Personal Computer. With a few peripherals, a system based on such a computer might cost \$1,500–2,500, and would offer the hobbyist enough power for most home or recreational applications. However, such computers can also form the heart of a business microcomputer system—what differs is the amount of storage and the type and quality of peripheral devices. Such computers are also listed in Table III.

Handheld computers offer calculator-like portability

Table II

Maker	Model	List price	Memory	Remarks
Panasonic	HHC	\$500	2K-4K	Includes printer. Wide range of peripherals available.
Radio Shack	TRS-80 PC-2	\$280	2.6K	New model. Original TRS-80 PC-1 is the same as the Sharp below.
Sharp	PC-1211	\$230	1.9K	Comparable in speed to programmable calculators.
Casio	FX-702P	\$200	1.7K	

Business microcomputers

The distinction between personal and business microcomputers is not perfectly clear, because most of the differences are those of degree. The business microcomputer system has more memory, more mass storage, a larger display, and greater communication capability than the personal microcomputer system, because the computer itself may be somewhat different and because the system includes more peripheral devices of greater quality and capability.

To highlight the differences between the computers themselves and between the types of systems, let us look at the six basic hardware areas: computers, terminals, mass-storage devices, printers, plotters and communication devices. The computer itself typically accounts for only 20% of the cost in a business microcomputer system, so the peripherals deserve as much attention.

Computers: The heart of the computer is the microprocessor, an integrated silicon chip that performs the arithmetic and logic operations needed for all computer tasks. Table IV lists some of the microprocessors used in today's microcomputers.

Personal microcomputers vary in capability and cost

Table III

Maker	Model	List price	Memory	Remarks
Apple Computer	Apple II	\$1,300	16K	Expandable, includes BASIC and graphics, most supported in hardware and software
Atari	400	\$330	16K	Includes BASIC and graphics, cassette games
	800	\$1,100	16K	Expandable, includes BASIC, sound and graphics
Commodore Business Machines	VIC-20	\$300	5K	Expandable, includes graphics
	PET 4000	\$1,000	16K	Expandable, includes BASIC, graphics and display
	CBM	\$1,500	32K	Includes BASIC, graphics and display
International Business Machines	IBM Personal Computer	\$1,750	48K	Latest technology, very little software yet
Radio Shack	TRS-80 Model-III	\$1,000	16K	Expandable, includes BASIC, graphics and display
	TRS-80 Color Computer	\$400	4K	Principally for graphics, expandable
Texas Instruments	TI-99/4A	\$525	16K	Expandable, includes graphics and sound

The relative computing power of a microprocessor is proportional to the number of bits it can handle in a single step. Today, the 8-bit microprocessor dominates the desktop-computer field, but by the end of 1982 the 16-bit processor, comparable to a minicomputer, will take over. In the future, the 32-bit processor will bring another leap in performance.

An important consideration in choosing among computers is the potential for expansion. This depends on the design of the particular computer: In some, the microprocessor and other components are on a single circuit board, and cannot be altered or expanded. Other computers (such as the Apple II or the TRS-80 Model-II) provide a means for attaching other printed-circuit boards with added memory, language capability, and communication features. These systems can be upgraded as technology improves, which protects one's investment.

Terminals: The terminal links the user with the computer and other elements of the computer system. It consists of a keyboard and a CRT display, which may be included with the computer in a single unit in some cases (like the TRS-80 Model-III). Desirable features for the keyboard are non-glare sculptured keys, positive feedback when a character is entered, user-defined function keys, and ability to detach the keyboard from the computer for convenient use. The CRT display should have a non-glare screen, sharp and clear characters, and no less than 24 lines of 80 characters each. Other desirable features are reverse video, highlighting, cursor addressing and editing commands. A typical stand-alone terminal costs between \$700 and \$2,400.

Mass storage is used instead of random-access memory (RAM) to hold programs and data permanently. While personal applications may use cassette tapes, business applications usually demand the much faster disk drives. These can be either floppy disks (flexible plastic disks covered with magnetic media inside a protective

cardboard cover) or rigid Winchester-type disks. Floppy disks are inexpensive (\$3-8), can store from 70K to 1.25M bytes or more, and require a simpler drive than do Winchesters. But Winchesters can access data faster, meaning that the computer spends less time looking for information. Winchester-type disks can hold from 5M to 26M or more bytes of data.

Table V lists more information about disk drives. Note that performance specifications for the drives do not indicate system performance, because the actual speed of access depends on the computer and software and how they work together.

Printers come in two basic types: dot-matrix and impact. Dot-matrix printers use a column of wires in a print head to produce a matrix of dots on the paper as the print head moves across the carriage. The matrix density determines the sharpness of the characters and the cost of the printer: A 5x7 matrix is the least expensive, and least sharp, while a 9x24 matrix approaches letter quality. Dot-matrix printers can be purchased with various options, such as graphics, business-forms control, programmable character sets, and variable print density. Recent models that provide multicolor graphics and printing can be substituted for plotters, but to date there is little software to take advantage of such features.

Impact printers provide letter-quality printing, using either a flat wheel (e.g., Daisy Wheel) or a thimble (e.g., Spinwriter) as a printing head. Such printers are usually used with word-processing software to produce reports and memos. Dot-matrix printers are generally faster, and are therefore used for applications where print quality is less critical and speed is important. Table VI summarizes the various types of printers.

Plotters provide hard copies of video-graphics displays, generated by special software. Software is a key concern here, because a computer's ability to generate graphic displays and use a plotter depends on how it is programmed. A video-graphics software package should at least emulate a Tektronix 4010 graphics terminal, since it can then be used with a wide range of large-computer graphics packages such as SAS, Tell-A-Graph, and DISSPLA. One widely used emulation is the TEKSIM program for the Apple II, which costs about \$475 and works with the Tell-A-Graph or DISSPLA software package. Hewlett-Packard and Tektronix plotters are supported by all three of the mentioned packages.

The plotter itself typically produces either an 8½ x 11-in. or 11 x 17-in. plot, and costs about \$1,000-2,000 for the smaller and \$2,000-6,000 for the larger format. Features available include intelligence, automatic pen selection, communications buffers and paper feed.

Communication links provide access to other computers and information systems. Many computers include a cassette and printer interface, but serious users generally add on another type of link. The most widely used communications interface is the RS232C serial interface, which enables the computer to communicate over telephone lines (via a modem), and links the computer with compatible peripheral devices such as printers, plotters and analog-to-digital data-acquisition systems for instrument applications.

Microprocessors used in desktop microcomputers

Table IV

Type	Model	Original maker	Remarks
8-bit	8080	Intel	CP/M compatible
	6800	Motorola	
	6502	Mostek	Apple II, Atari, PET
	Z80	Zilog	CP/M
	8085	Intel	CP/M
	6809	Motorola	TRS-80 Color Computer
	8088	Intel	IBM Personal Computer
16-bit	9900	Texas Instruments	TI-99/4A
	8086	Intel	IBM Display Writer
	Z8000	Zilog	
	68000	Motorola	HP-9826
	99000	Texas Instruments	
32-bit	iAPX 432	Intel	Special, new

Modems are telecommunication links, accessible through an RS232C or other interface. Their cost depends on their speed: A 300-baud (30 character per second) modem costs less than \$250, while a 1,200-baud modem costs about \$1,000. Of course, the faster modems cut down the time wasted transferring data or programs. Besides speed, other desirable modem features are: direct connection, to avoid the noise problems caused by acoustic couplings, and originate-and-answer capability, to allow communication between microcomputer systems.

Communication can get very complex, since greater speed and access to certain devices require more than a single modem and RS232C. The IBM Personal Computer offers software (BISYNC, for about \$900) that allows it to communicate with IBM 360/370 and Series 30XX processors directly through a synchronous modem. With this capability, the Personal Computer can be added to existing IBM networks. Likewise, Radio Shack has expanded its TRS-80 Model II to be compatible with BISYNC, and has announced plans for compatibility with the ARC network from Datapoint.

Another desirable feature in business microcomputers for engineering applications is a floating-point arithmetic processor, which plugs into a compatible computer. This executes floating-point calculations 10-100 times faster than floating-point software packages. There are several such processors available, but it is difficult to use them because software for standard microcomputers is not designed to take advantage of them. New computers such as the IBM Personal Computer do offer such processors, and programming languages that use them are expected soon. With this innovation, iterative calculations that are too lengthy for today's microcomputers will become practical.

Using a business microcomputer system

Fig. 2 illustrates a typical business microcomputer system for an engineering office. Besides the microcomputer and key peripherals already discussed, the system shown includes a graphics plotter, and software to perform many basic tasks. Some of the programs that have been written for such a system (which includes a TRS-80 Model II microcomputer) at Dow Corning are:

- Preliminary design and cost-estimating for a distillation column and auxiliary equipment.
- Manpower planning, based on capital-spending data.
- Physical properties.
- Plotting and curve-fitting, used with a Houston Instruments intelligent plotter.
- Thermosiphon reboiler evaluation.
- Flash calculation.

The distillation-column program uses the Underwood-Fenske method, and will estimate 40 different cases in 15 minutes to find the minimum-cost design. Written in FORTRAN, the program is compiled so as to run faster.

A computer system that will perform all the functions needed in an engineering office will cost anywhere from \$10,000-15,000; the one in Fig. 2 adds up to \$11,000. A typical system may include a computer with a Z-80 microprocessor, currently the most popular for business

Disk drives add mass-storage capability

Table V

Type	Storage, bytes	Access time, milliseconds	Transfer speed, bits/s (baud)	Cost
5¼-in. floppy-disk	70K	250	125K	\$400
	140K	250	250K	\$600
	300K	200	250K	\$750
	930K	180	250K	\$1,000
8-in. floppy-disk	250K	70-200	250K	\$750
	500K	70-200	500K	\$950
	1,000K	70-200	500K	\$1,250
Winchester hard-disk	5M-26M	25-150	≈5M	\$3,000-8,000

applications, which can handle a memory block of up to 64K bytes. Two double-density 8-in. floppy disks will store at least 1M bytes of information. The letter-quality printer is needed for word processing, especially in offices that produce many reports and proposals. If communication with another computer is important, a modem will be required. A plotter is handy for preparing charts and graphs.

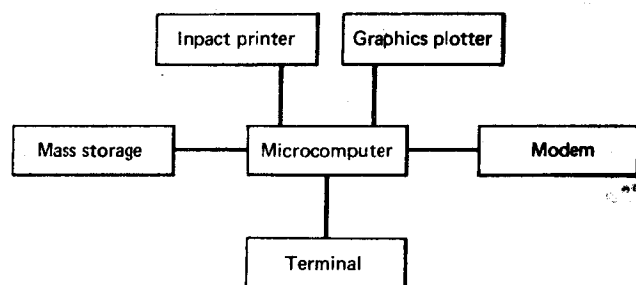
Since software constitutes a major cost, let us look briefly at the program packages included in the Fig. 2 system. There is a tremendous variety of software available for microcomputers, so these are, of course, just a few of the many options:

Electronic spreadsheets ease the analysis and presentation of numerical data and text, for applications such as financial statements, statistics and cash-flow projections. The T/Maker II package listed in Fig. 2 runs on the CP/M operating system, a *de facto* standard for microcomputers with the Intel 8080 or 8085 and Zilog Z-80 microprocessors. Other packages are VisiCalc and CalcStar. Note that CP/M capability itself is not always included in a microcomputer, but must be

Dot-matrix and impact printers for microcomputers

Table VI

	Dot-matrix printers		
	8½-in. carriage	14-in. carriage	Impact printers
Characters per line	80-132	132-220	132-158
Character type	5 x 7 matrix	5 x 7 to 24 x 9 matrix	Impact
Speed, characters per second	30-120	80-220	26-75
Cost range	\$400-1,000	\$1,000-2,500	\$1,700-5,000
Remarks	For light to medium duty in hobby or office applications.	For heavy-duty business printing. May include color graphics and/or word-processing features.	For word processing. May have graphics.



Hardware		Software	
Microcomputer	\$2,000	T/Maker II	\$275
Disk storage	1,500	WordStar	450
Printer	2,000	SpellGuard	300
Modem	300	BSTMS	200
Plotter	1,300	Milestone	300
Terminal	825	BASIC compiler	350
Total \$7,925		FORTTRAN compiler	500
		FPL	700
		Total \$3,075	

The microcomputer is about 20% of the cost in an engineering office computer system.

Fig. 2

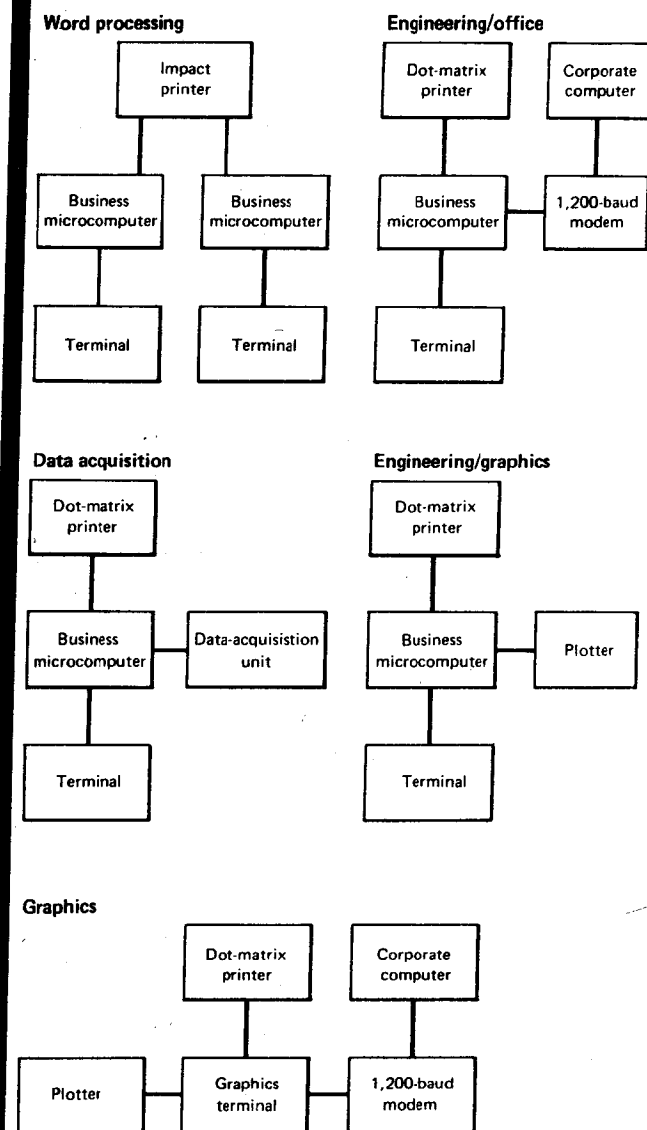
bought. Among current microcomputers, the Xerox 820 is supplied with CP/M, and the IBM Personal Computer emulates CP/M.

High-level languages needed for scientific programming (BASIC, FORTRAN, APL, etc.) are implemented either as interpreters or compilers. A BASIC interpreter is included with many microcomputers. On an 8-bit microcomputer, this runs programs about 10 times as fast as a calculator does—rather slow because the interpreter translates and executes the program line by line. Compiling a program (translating the entire high-level-language program into rapidly-executed machine code) before execution will speed up the calculation considerably. For example: A compiled FORTRAN program runs on a microcomputer about 100 times as fast as a calculator program. But using a compiler has its costs: investment in a compiler software package; delay in running a program while it is being compiled; less-direct contact between the user and the program. Overall, compiled high-level language pays off when a lengthy program is to be repeated a number of times.

Word-processing systems for business microcomputers compete favorably with stand-alone word processors. In Fig. 2, a word-processing program (WordStar 3.0) is combined with a dictionary program (SpellGuard) to produce error-free reports.

Special-purpose software is available for a variety of business and scientific applications, but engineering software must generally be developed by the user. The system in Fig. 2 includes: BSTMS, a package that enables the microcomputer to communicate with other computers; Milestone, for project scheduling and critical-path analysis; and FPL, for financial planning and analysis.

Two goals in putting together a microcomputer system are speed and integration. For engineering purposes, desktop microcomputers are acceptable for simple iterative calculations; but, even with a compiled



Research desktop computer systems at Hemlock Semiconductor

Fig. 3

high-level language, such a small computer has only one-thousandth the speed of a maxicomputer. Therefore, complex nested calculations, such as steady-state nonideal distillation-column designs, are simply not to be done on microcomputers. One will wait hours for answers to such problems.

Even more important is making sure that the computer system will work as expected when all of the cables are plugged in and the power is turned on. The term "integrated system" describes the desired situation where hardware and software are compatible in design and capacity, and will work together as an efficient package. Since an engineer is primarily concerned with solving engineering problems, and not with checking specifications for computers, it is recommended that a system be purchased from a local vendor who knows