

Engineering & Science

California Institute of Technology | October 1980



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ALUMNI FLIGHTS ABROAD

1980-1981

This program of tours, originally planned for alumni of Harvard, Yale, Princeton, and M.I.T., is now open to alumni of California Institute of Technology as well as certain other distinguished colleges and universities. Begun in 1965 and now in its sixteenth year, it is designed for educated and intelligent travelers and planned for persons who might normally prefer to travel independently, visiting distant lands and regions where it is advantageous to travel as a group.

The program offers a wide choice of journeys to some of the most interesting and unusual parts of the world, including Japan and the Far East; Central Asia, from the Khyber Pass to the Taj Mahal and the Himalayas of Nepal; the surprising world of South India; the islands of the East, from Java and Sumatra to Borneo and Ceylon; the treasures of ancient Egypt, the world of antiquity in Greece and Asia Minor; East Africa and Islands of the Seychelles; New Guinea; the South Pacific; the Galapagos and South America; and more.

REALMS OF ANTIQUITY: A newly-expanded program of itineraries, ranging from 15 to 35 days, offers an even wider range of the archaeological treasures of classical antiquity in Greece, Asia Minor and the Aegean, as well as the ancient Greek cities on the island of Sicily, the ruins of Carthage and Roman cities of North Africa, and a comprehensive and authoritative survey of the civilization of ancient Egypt, along the Nile Valley from Cairo and Meidum as far as Abu Simbel near the border of the Sudan. This is one of the most complete and far-ranging programs ever offered to the civilizations and cities of the ancient world, including sites such as Aphrodisias, Didyma, Aspendos, Miletus and the Hittite citadel of Hattusas, as well as Athens, Troy, Mycenae, Pergamum, Crete and a host of other cities and islands of classical antiquity. The programs in Egypt offer an unusually comprehensive and perceptive view of the civilization of ancient Egypt and the antiquities of the Nile Valley, and include as well a visit to the collection of Egyptian antiquities in the British Museum in London, with the Rosetta Stone.

SOUTH AMERICA and THE GALAPAGOS: A choice of itineraries of from 12 to 29 days, including a cruise among the islands of the Galapagos, the jungle of the Amazon, the Nazca Lines and the desert of southern Peru, the ancient civilizations of the Andes from Machu Picchu to Tiwanaco near Lake Titicaca, the great colonial cities of the conquistadores, the futuristic city of Brasilia, Iguassu Falls, the snow-capped peaks of the Andes and other sights of unusual interest.

EAST AFRICA—KENYA, TANZANIA AND THE SEYCHELLES: A distinctive program of 5 outstanding safaris, ranging in length from 16 to 32 days, to the great wilderness areas of Kenya and Tanzania and to the beautiful islands of the Seychelles. The safari programs are carefully planned and comprehensive and are led by experts on East African wildlife, offering an exceptional opportunity to see and photograph the wildlife of Africa.

THE SOUTH PACIFIC and NEW GUINEA: A primitive and beautiful land unfolds in the 22-day **EXPEDITION TO NEW GUINEA**, a rare glimpse into a vanishing world of Stone Age tribes and customs. Includes the famous Highlands of New Guinea, with Sing Sing and tribal cultures and customs, and an exploration of the remote tribal villages of the Sepik and Karawari Rivers and the vast Sepik Plain, as well as the North Coast at Madang and Wewak and the beautiful volcanic island of New Britain with the Baining Fire Dancers. To the south, the island continent of Australia and the islands of New Zealand are covered by the **SOUTH PACIFIC**, 28 days, unfolding a world of Maori villages, boiling geysers, fiords and snow-capped mountains, ski plane flights over glacier snows, jet boat rides, sheep ranches, penguins, the Australian "outback," historic convict settlements from the days of Charles Dickens, and the Great Barrier Reef. Optional visits can also be made to other islands of the southern Pacific, such as Fiji and Tahiti.

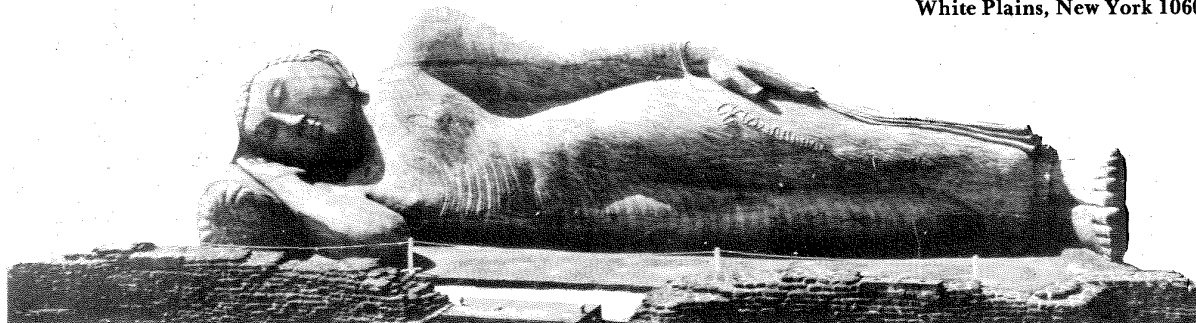
CENTRAL ASIA and THE HIMALAYAS: An expanded program of three itineraries, from 24 to 29 days, explores north and central India and the romantic world of the Moghul Empire, the interesting and surprising world of south India, the remote mountain kingdom of Nepal, and the untamed Northwest Frontier at Peshawar and the Punjab in Pakistan. Includes the Khyber Pass, towering Moghul forts, intricately sculptured temples, lavish palaces, historic gardens, the teeming banks of the Ganges, holy cities and picturesque villages, and the splendor of the Taj Mahal, as well as tropical lagoons and canals, ancient Portuguese churches, the snow-capped peaks of the Himalayas along the roof of the world, and hotels which once were palaces of maharajas.

THE FAR EAST: Itineraries which offer a penetrating insight into the lands and islands of the East. **THE ORIENT**, 30 days, surveys the treasures of ancient and modern Japan, with Kyoto, Nara, Ise-Shima, Kamakura, Nikko, the Fuji-Hakone National Park, and Tokyo. Also included are the important cities of Southeast Asia, from Singapore and Hong Kong to the temples of Bangkok and the island of Bali. A different and unusual perspective is offered in **BEYOND THE JAVA SEA**, 34 days, a journey through the tropics of the Far East from Manila and the island fortress of Corregidor to headhunter villages in the jungle of Borneo, the ancient civilizations of Ceylon, Batak tribal villages in Sumatra, the tropical island of Penang, and ancient temples in Java and Bali.

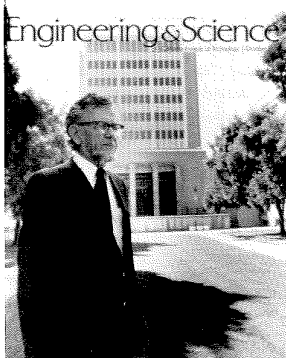
Prices range from \$2,350 to \$4,500 from U.S. points of departure. Air travel is on regularly scheduled flights of major airlines, utilizing reduced fares which save up to \$600.00 and more over normal fares. Fully descriptive brochures are available, giving itineraries in detail and listing departure dates, hotels, individual tour rates and other information. For full details contact:

ALUMNI FLIGHTS ABROAD

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In This Issue



Chemical Change

On the cover — John D. Roberts, Institute Professor of Chemistry, stands on some of his own divisional turf — the grassy area between Gates and Crellin Laboratories of Chemistry. It's a place of quiet beauty on the campus in spite of the architectural variations between new and old in the background, where 1967 Millikan Library looms over 1927 Gates Annex.

Quiet has never been the name of the Roberts game, however, and last January he enlarged his sphere of influence and doubled his activity — moving into the administrative offices on the third floor of Millikan and becoming vice president, provost, and dean of the faculty. "JDR" on page 10 tells a bit about how he got where he is and something of what he's doing now that he's there.

Getting It Together

Obviously, all members of the Caltech faculty know what the scientific method is and scrupulously adhere to it in their research. Or do they? Since that question can't be answered without agreement on what constitutes the scientific method, last May the Caltech Y sponsored an airing of the subject on its Evening Spotlight Series. David and Judith Goodstein, a practicing scientist and a historian of science, were invited to lead the discussion. "The Scientific Method" on page 23 presents their shared conclusion that the subject isn't as simple as it may sound.

The Goodsteins have been sharing not only conclusions but also lives ever since



Judith and David Goodstein

they met when they both attended Brooklyn College. Their PhDs come from the University of Washington, and their professional careers have been spent at Caltech, where they settled down in 1968 — except for the summers they spend in Italy where David is visiting scientist at Frascati National Laboratory and Judith does research on Italian science between the two World Wars.

Back at the Institute, David is beginning his second year as chairman of the faculty. He is also professor of physics and applied physics and is doing distinguished research into the physics of matter, particularly helium. He has, in fact, written a book on the subject that was published in 1975. He is known about campus as a dynamic lecturer and teacher and has recently helped redesign the required freshman course in physics.

Institute archivist Judith Goodstein has spent the last several years assembling a lot of historical material about Caltech and filing it away in the basement of Millikan Library, but she's about to make a change. Last spring she received a grant from the Haynes Foundation that will enable her to spend the next couple of years pulling materials out of those — and other — files to use as resources for the book she will be writing on the history of the California Institute of Technology.

STAFF: Editor — Jacquelyn Bonner

Staff Writer — Jane Dietrich

Photographer — Chris Tschoegl

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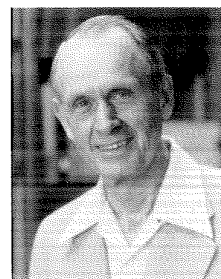
Engine-uity

Francis Clauser's interest in the emissions of combustion engines is actually more related to his background in aeronautics than it might seem. Some of the phenomena that account for the gasoline engine's pollution problems involve fluid mechanics, one of his main areas of research in aeronautical engineering.

And Clauser is also a traveling man. He and his wife, Catharine, have toured by car around several continents and even driven to Timbuktu. Although automobile emissions were not a problem on that trip across the Sahara, Clauser's basic familiarity with engines proved handy — just as it has off other beaten tracks all over the world.

In between trips Clauser has carved out an impressive career — with Caltech at both ends. He received his BS, MS, and PhD degrees here in the 1930s and, after leading a design research section at Douglas Aircraft, founding the department of aeronautics at Johns Hopkins, and becoming vice chancellor at UC Santa Cruz, returned to Caltech in 1969 to head the Division of Engineering and Applied Science. He is now Clark Blanchard Millikan Professor of Engineering — Emeritus as of this year.

His article, "Future Prospects for Low-Pollution Combustion Engines," finished just before the Clausers took off for China, appears on page 15.



Francis Clauser

Engineering & Science

October 1980/Volume XLIV/Number 1

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Carver Mead and other Caltech computer scientists pioneer new methods of coping with the complexity of tomorrow’s silicon chips.

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John D. Roberts was visible on campus even before he added the administrative jobs of vice president, provost, and dean of the faculty to his academic position as Institute professor of chemistry.

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by Francis H. Clauser

The research of a Caltech engineer shows that the fundamental limits of the combustion engine allow much lower emissions of pollutants than have so far been achieved. In fact, automobile exhaust cleaner by several powers of ten is possible.

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by David and Judith Goodstein

A physicist and a historian of science discuss the development of the scientific method and how — and whether — practicing scientists really use it.

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Signs of Life: Heinz Lowenstam continues to find biologically produced minerals in seemingly hostile environments.

Catalyst Converter: Fred Anson and his colleagues are testing complex molecules fashioned to act as improved catalysts in fuel cells.

Trevor Byer's software takes a hard look at telephone traffic.

As a result, calls flow more smoothly through the nationwide network.

Shortly after Trevor Byer came to Bell Labs in 1976, we asked him to join a design team tackling a big job. Their task: find a way to determine the accuracy, completeness and timeliness of the hundreds of millions of traffic measurements collected weekly in the Bell System. The job was important because engineers and managers at each Bell telephone company use the measurements to assure that enough equipment and circuits are available to meet customer demands.

The solution that Trevor Byer's team came up with was the Centralized System for Analysis and Reporting, or CSAR. Trevor focused on determining how

much information telephone company managers needed, and how that information could best be reported to them. His responsibilities ranged from software design and systems engineering to field testing of reports and training of CSAR users. With a BS and MS in Electrical Engineering from the University of Illinois, Trevor was prepared for the job.

Here's how CSAR works. Once a week all the Bell telephone companies transmit performance data from their computers to a central computer in Piscataway, N. J. Overnight, CSAR analyzes the information, organizes it for use in many ways, including management reports designed by Trevor, and stores it for retrieval the next day.

From their own computer

terminals, CSAR users in the telephone companies request a variety of reports: from summaries of switching system performance for an entire company to detailed performance of individual switching systems. The reports can be displayed graphically to summarize performance trends over weeks, months, or longer.

CSAR is one of more than a hundred computer-based systems used by the Bell System to provide better network performance and better service to customers.

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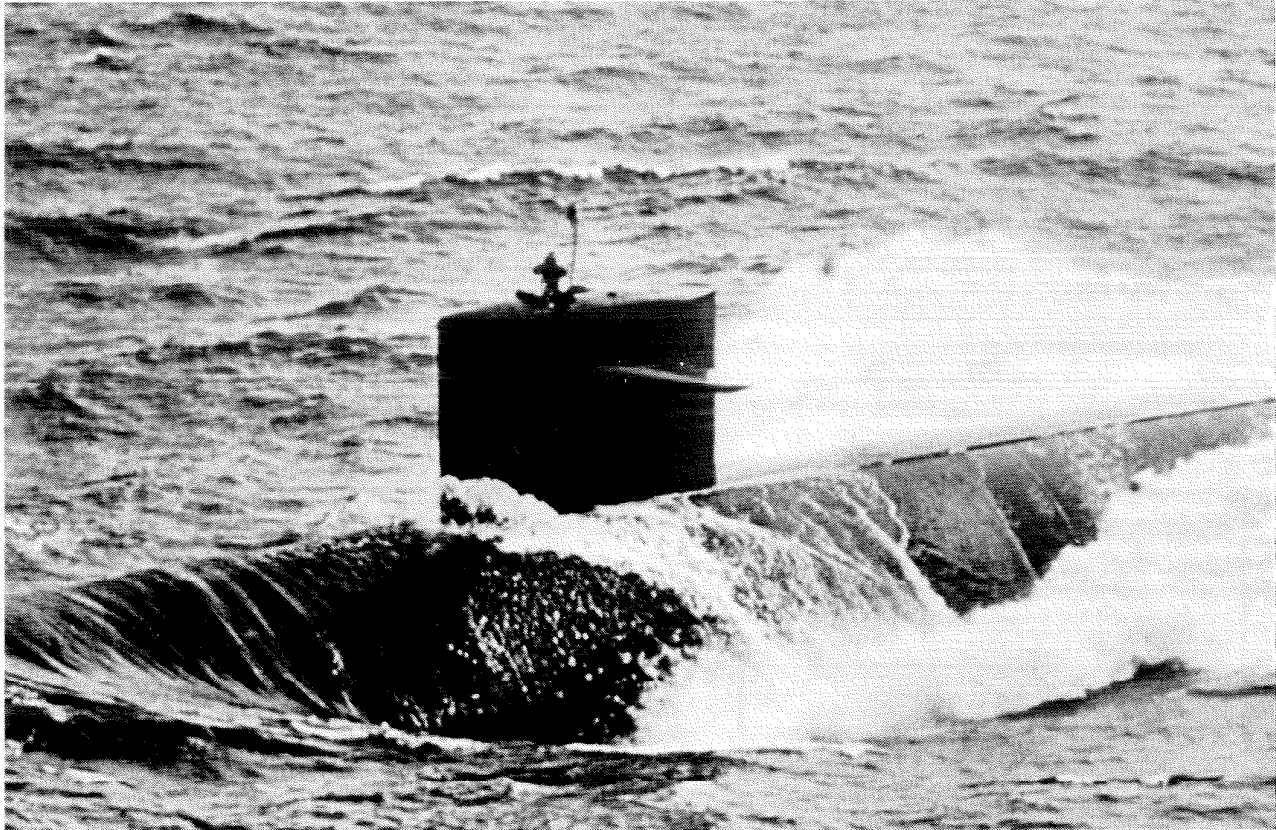
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Very Large Scale Integration

Designing "Street Maps" of North America

Theoretically, a million transistors (the equivalent of the entire works of a good-sized computer) can be put on a silicon chip one-tenth the size of a postage stamp. In fact, the technology for manufacturing transistors small enough for such Very Large Scale Integration (VLSI) actually already exists. One of its pioneers and most creative developers is Caltech's Carver Mead, the Gordon and Betty Moore Professor of Computer Science.

VLSI is the result of the marriage of the computer and semiconductor technologies, both of which have experienced phenomenally rapid evolution in the last three decades. Computer technology developed out of the pioneering work of John Von Neumann and others in the late 1940s. The semiconductor industry was born at about the same time with the invention, or discovery, of the transistor — a small low-power amplifier — by Walter Brattain, John Bardeen, and William Shockley. It soon became clear that transistors could replace the comparatively cumbersome tubes, resistors, and wires, and do everything a vacuum circuit could do in a computer — store one bit of information or combine two bits to make a logic function. And they could do it using a fraction of the space and energy, which also translated into a fraction of the cost.

In 1960 the microelectronic revolution got going in earnest with the birth of the integrated circuit, so called because silicon, a conductor of electricity that was one of the components of the first transistors, integrates the circuit itself with the technology that makes the transistor. Since conducting layers on the surface of the silicon can be used to interconnect transistors, the silicon can act as its own circuit board.

The first integrated circuit had 12 transistors and did just one of the elementary computing functions. Ten years later circuits had been so scaled down that silicon chips with a thousand transistors were being manufactured. Today several hundred thousand transistors can be put on a chip one-quarter inch on a side — about the size of a thumbtack.

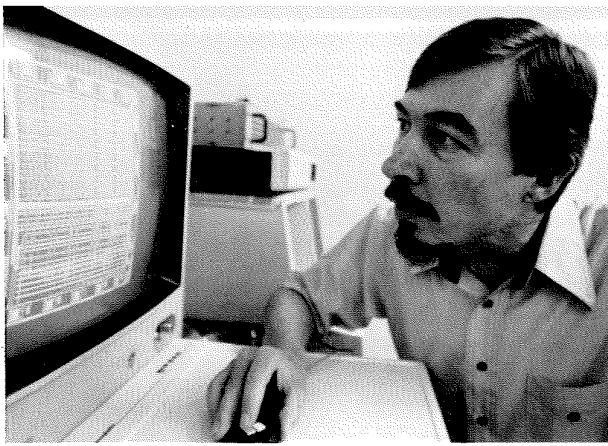
The process of photolithography makes it possible to manufacture integrated circuits. The integrated circuit is built up layer by layer — transistors, wiring, and contacts — into what is almost a three-dimensional architecture. Circuit designers (who work on a larger scale) create masks for each layer. An oxidized silicon wafer, which can contain many chips at one time in a four-inch-diameter

space, is coated with a thin film of photoresist (a light-sensitive material). With the mask laid over it, the photoresist is exposed to ultraviolet radiation, which makes it resistant to a solvent, thus leaving the pattern of the mask etched into that layer. Another thin film is then laid on that layer and another pattern photoengraved on it, and so on for several layers.

About ten years ago Mead decided to try to calculate the physical limits of this technology. How small could you make a transistor and still expect it to function in computer machinery? His astonishing prediction was that transistors could be made a thousand times smaller than those being manufactured at the time. Transistors this small — with the potential of a million or more on a chip — have been built since that prediction and proved to function, but there's a problem. They are incredibly complex. Even if the physical limits do allow a million transistors and the accompanying wiring on a tiny chip, how can human beings cope with something that intricate? The complexity of VLSI is so enormous that it completely overwhelms any other difficulties. Silicon chips no longer present problems in physics but rather in computer science — how to make sure such a system works.

Mead often uses an analogy originated by his Caltech colleague, Charles Seitz, to explain just how complex these integrated circuits become as you scale down the size of the wires and transistors and scale up the size of the chip. If you blow up the scale of one of these integrated circuits so that the distance between the wires is equal to a city block, then you can imagine the whole chip as a street map. In the early 1960s, when the chips were about a millimeter across, or forty-thousandths of an inch, with wires about two-thousandths of an inch apart, the chips would have had to be expanded by a factor of four million to attain city-block size between wires. Then you would end up with something like a street map of Pasadena — a small city where it's not too difficult to remember where everything is and how to get around.

The next round of technology (where things were about two years ago with chips five millimeters across) brought something like a map of Los Angeles, where it's a bit harder to remember how to find everything, and even the map itself is rather unwieldy. And yet to come are chips a centimeter across with wires the size of two wavelengths of visible light. This would translate into an urban street



Carver Mead

map the size of California and Nevada. The analogy goes still further. When we reach the physical limits of transistor size that Mead predicted ten years ago, the silicon chip will resemble a city street map the size of North America. Of course, no one has done this yet, but Mead believes there is every reason to expect that it can and will be done.

How would you plan, lay out, and manage a city the size of North America? The key is design, says Mead. And he's been saying it for ten years, having foreseen that problems of managing the complexity were sure to arise. With a chip the size of Los Angeles, industry realized it also.

Until then almost all the rapid advances in integrated circuit technology had taken place in industry. Where were the universities, the "cutting edge," all this time? Most of academia was left far behind, but at Caltech there were some people in the background doing what universities are good at (and industry often is not) — looking very far ahead, doing research whose outcome is uncertain, taking risks. Industry was thinking about immediate costs, not long-range problems.

But while industry wasn't looking, those costs changed. Along with a profound reduction in the overall cost of computation, which is radically affecting society in many ways, technology has also changed the relative costs of the parts of the integrated circuit. In the earlier days of integrated circuits the logic elements were the expensive part; as more and more computing functions were put on a single chip, whose cost didn't change essentially (about \$10), the cost of the individual logic functions decreased dramatically. For the same \$10 you now have many orders of magnitude greater computing power than a decade ago. Now the costly element has become the wiring — the time and energy it takes to communicate among the increasingly more numerous units of an integrated circuit. Scaling down the size of the wires has also resulted in increased resistance and therefore increased delay.

Another time factor — the time in person-months that it takes to design a very complicated chip — has increased exponentially. And as complexity continues to increase, this design cost will grow out of reach of even the largest companies, Mead maintains.

Industry hasn't changed its method of design much since the time when there were 12 transistors on a chip.

Most semiconductor companies design each of the transistors and the interconnections individually, by hand, a process that at the present level of complexity takes many tens of person-years for complicated microprocessors. The end product of what Mead calls the "spaghetti school" of design is an almost impenetrable maze of random wiring. Other firms, particularly the computer companies, have tried to use computers to simplify the process, arranging the transistors in regular rows with wiring laid down on top. Although chips designed in this way look more rational, they do not efficiently solve the problem of keeping communication distance (and time) at a minimum. As chips get larger, the area used for wiring and the time and energy spent sending signals around the chip increases tremendously.

At Caltech Mead and his colleagues discarded the traditional design methods and started from scratch to restructure the way integrated circuits are designed — to devise a new approach that would exploit the potential of VLSI and would cope with the complexity by using orderly, simplified floorplans, keeping interconnection paths as short as possible to save time and energy consumption. Essential to their approach is the concept of locality — placing elements that communicate with each other (both logic and memory elements) close together so that their messages don't have to travel back and forth over "long" distances across the chip. To accomplish this, Mead's group has developed hierarchical design — progressively splitting the whole system into smaller, simpler parts, or modules, that are independent of each other and of the whole system and that communicate with each other only at well-defined points. As the name implies, hierarchical design approaches the problem from the top down, like a reverse tree (indeed trees and leaves are designations in many of the design ideas devised at Caltech).

Mead's structured approach applies hierarchical design to the particular constraints of VLSI systems — implementing the design in the many-layered construction of the actual chip, placing modules with similar functions next to each other in regular patterns like a tiled floor. Algorithms also simplify the design task, and computers help to determine the optimum arrangement of modules, making it several orders of magnitude simpler than the traditional design methods.

One particularly successful system, devised by graduate student Dave Johannsen, makes a chip design possible in a few minutes rather than in person-years. It's a silicon compiler, a computer program that performs most of the implementation computation to turn out a mask set for all the various layers of the integrated circuit. The designer can specify what functions the modules, or blocks, are to perform, and the computer does the rest — figuring out the circuitry within each block and between the blocks. (The program is called "Bristle Blocks" from the appearance of a rectangular module with interconnections sticking out all over it.) With the Bristle Block program a designer can, in

effect, design a chip by moving around the building blocks, leaving the complicated interconnections to the computer.

With an earlier integrated circuit technology, there were microprocessors (the arithmetic and logic units) and there were memories — separate functions on separate circuits, communicating by a “bus” (usually a cable of wires providing common transportation for data). VLSI makes it possible and efficient to have the two functions together on one chip — many processors and many memories or many processors with a common memory. This leads to the possibility of concurrent processing — lots of calculations going on at once instead of in sequence, the way current computers work. Mead and his colleagues have developed a number of design patterns, including various arrays and trees, to facilitate the fewest and shortest possible interconnections among the units.

The Caltech group is not trying to hide its ideas. In fact, to emphasize the importance of partnership between industry and academia and avoid repetition of the early years of integrated circuits when industry was preoccupied with the immediate future, Caltech’s Silicon Structures Project involves a number of industrial sponsors in a working relationship. These include IBM, Xerox, Burroughs, Hewlett-Packard, Digital Equipment Corporation, Intel, and Honeywell, with more on a waiting list for the informal “think tank.” Each of the companies sends a scientist to Caltech for a year to work on design ideas and methodologies with Mead’s group; thus the participating firms have contact with really innovative research, and the Institute, in return, gets a better understanding of industry’s problems.

Another factor that is returning universities to leadership in integrated circuit technology is Mead’s original VLSI course, developed at Caltech. Out of that course came the only textbook in the field, *Introduction to VLSI Systems*, written by Mead and Lynn Conway of the Xerox Palo Alto Research Center. This extraordinary course has already been adopted at MIT, Stanford, Berkeley, Carnegie-Mellon, Washington University-St. Louis, USC, UCLA, and the universities of Florida, Washington, Illinois, Rochester, Utah, and Colorado. Reflecting Mead’s simplifying approach to design, the course also applies this simplification to instruction, providing the minimum of basic information about fabrication technology, logic design techniques, and system architecture. By limiting instruction to the key concepts, from the underlying physics to the complete VLSI systems, and eliminating all the rest of the “mental baggage,” the course is turning out designers at a surprising rate — and they can walk right out of the classroom and start to work.

One reason for this quickly acquired skill is the “learning by doing” feature of the course. Students work on projects involving architecture, design, layout, and testing of real integrated circuit systems that are then actually manufactured — the chips of a whole class on a single silicon wafer. Originally the Caltech class had to beg for space on

commercial lines to get student designs produced. Now, however, at Caltech’s instigation the Advanced Research Projects Agency (ARPA) has funded a fabrication plant expressly for the innovative designs coming out of universities.

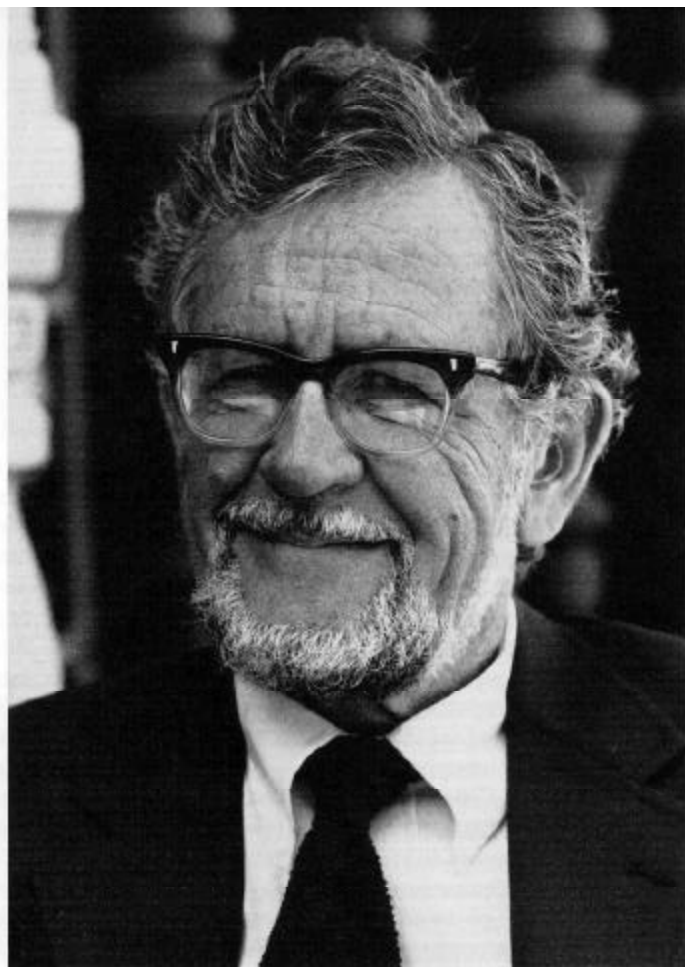
The ARPA-funded silicon “foundry” is a prototype of what Mead considers essential to the future of the industry — the division of labor between the designers and the fabricators, between product creation and product replication. While there are still hard problems to be solved in the technology of processing, the outcome is predictable; industry knows what has to be done and knows that it can be done. Where the startling advances will come now is in the area of design. And the sophisticated developments in design are coming out of the universities and small new firms that have no access to manufacturing. They have insufficient capital to begin making their own chips because fabrication has reached such a capital-intensive stage.

Mead envisions the semiconductor industry in the future with an analogy to writers and printing companies. Designers should create the circuits, and other firms (the silicon foundries) would “print” them, since, as in printing, an unlimited number of system designs can be reproduced by a single process. Only if access to these foundries is provided by well-capitalized firms can the high level of innovation in computer electronics continue.

Here again Mead’s streamlining and standardizing approach to design proves necessary. If the rules of the game are simplified and well defined, designers and manufacturers will have a “clean interface” (with requirements of geometric design rules, standard data format, and standard test chip) and will be able to communicate even though their functions are separated. If the designers can generate the complete layout for the chips (and by the new method they can), then the only information that must be transferred to the “printer” is the patterns representing the various layers. Despite the close cooperation of Institute and industry in the Silicon Structures Project, industry has not wholeheartedly embraced all of Mead’s revolutionary ideas. It has been to some extent unwilling to trade off some of the things that Mead’s approach demands (for instance, maximum number of transistors on a chip) for a simpler design method, and the large semiconductor companies are not enthusiastic about processing competitors’ designs.

Although both the computer and semiconductor industries have been heading toward the same goal, neither has adjusted to the innovations of the other. But there is no question that eventually both are going to have a totally different structure that will require working together. Mead sees the universities, which stress the underlying unity of what sometimes seem to be disparate disciplines, as marriage brokers. Arranging the marriage has been left to the universities, and — although industry may not yet recognize it — if Mead is right, the ceremony has already taken place. □

JDR



Anyone familiar with the initials above also knows something's wrong with them. Over the years "JDR" has been signed to countless memos, reports, and other papers, but seldom in any color but bright red. JDR — John D. Roberts — has never left doubt in anyone's mind about what he thinks or the fact that it is he who thinks it. So his signature and comments tend to be as visible on a paper as his craggy, 6'4" frame is on the campus — and was even before he added the administrative jobs of vice president, provost, and dean of the faculty to his academic position as Institute professor of chemistry.

That many titles and the responsibilities implicit in them should suggest a busy man and one who knows his way around collegiate traffic patterns. Certainly they describe Roberts, who has been steering his way with skill, distinction, and dispatch through the jobs of teacher, researcher, administrator, consultant, and writer almost from the day he graduated from UCLA. It must be a coincidence that the four-level freeway exchange in downtown Los Angeles sits on the site where he was born in 1918, but probably the only more appropriate way of honoring his nativity would have been to construct LAX there.

Of course, juggling jobs and time didn't begin for Roberts on commencement day 1941; he started at least as early as high school by being lab assistant and reading

papers for his physics teacher. For two years at UCLA he carried a full academic load and worked in a bakery six nights a week from 7 until midnight. Fortunately, by the end of his sophomore year, he was doing well enough in chemistry to be offered a part-time research job that paid real money for something he loved doing.

It was no surprise around the Roberts house that Jack was making a mark in science; he'd been pointing in that direction for a career ever since he got his first chemistry set at about the age of 12. Members of the family were tolerant of the occasional noisy and/or smelly episodes in his garage laboratory, but neighbors whose radios couldn't rise above the interference from a highly activated Tesla coil were somewhat more critical.

He was also strongly influenced toward science by the popular books about scientists and their work published in the late 1920s and early 1930s, and he read most of them. In fact, learning about Eddington, Jeans, and Einstein took him on a brief detour in interest from chemistry to astronomy where, he says, the required level of math soon sent him back to earth.

Caltech was an early magnet too, and as a teenager he was a frequent and fascinated visitor to campus on open-house days. He considered coming to the Institute as an undergraduate, and his mother corresponded with Robert

Millikan about the possibilities. But the stringencies of the Depression were very real in the Roberts family. His father's heating business went bankrupt, and there were two other children to get through school. When he balanced monastic Caltech's tuition of \$300 a year against coeducational UCLA's less than \$60, the choice became simple.

The first Roberts research paper was published in 1940 (with William R. Crowell and Caltech's Don Yost), and he received his bachelor's degree in 1941. While he always got A's in science courses, he didn't do so well in some others. English composition was his particular *bête noire* until one of his chemistry professors took the time to show him how to use the English language in scientific writing, in the process instilling in him a respect for its importance. He also taught Jack how to do the meticulous drawings that have become his trademark. Considering the more than 400 research papers and 7 books that now have the Roberts name on them, that pedagogical dedication was a sizable contribution to chemistry.

In 1942 Jack married Edith Johnson, whom he had met in high school. One of the material assets Edith brought to the marriage was a spinet piano, and its presence in their apartment gave Jack the opportunity to experiment with do-it-yourself music lessons. He elected to do this by alternately listening to a recording of the first and second movements of Beethoven's "Moonlight Sonata" as played by Paderewski and then trying to play them himself. The ultimate result was a fair amount of musical accomplishment — at the cost, says Edith, of some cooling of their relations with the downstairs neighbors.

Incidentally, there was no tie-in between his choice of a Polish pianist to emulate and his own maternal Polish connection — a tie that was supposed to show up in his middle name. His mother wanted that name to be Dombrowski, which was her family name and that of a famous ancestor, General Jan Henryk Dombrowski, liberator of Poland in the Napoleonic era. To her sorrow, whoever made out his birth certificate put down only the *D*, so legally JDR has just a middle initial.

Throughout his years at UCLA Roberts worked on reaction mechanisms in organic chemistry, mostly with William G. Young and Saul Winstein, two UCLA faculty members who obtained Caltech PhDs with the much beloved Howard Lucas. He also did war-related research, having been kept out of active military service by a hearing loss — the result of scarlet fever incurred at age 10. He received his PhD in 1944, and in 1945 went to Harvard as a National Research Council Fellow. A year later he became an instructor in chemistry at MIT, and by 1950 he was an associate professor there.

Roberts remembers 1950 for at least two other reasons. He began his association with E. I. du Pont de Nemours as a consultant — an association that still continues — and he first heard about the potential of NMR over a lunch table at MIT. In the eyes of the world, chemical applications of

Nuclear Magnetic Resonance is an area that eventually became almost synonymous with John D. Roberts. Ironically, with his weak background in physics, NMR was just part of the alphabet to him in 1950. It was not until four years later, after he had come to Caltech, that in the course of a consulting visit to du Pont he really became aware of NMR's possibilities for chemical research.

"I came back from that trip," he says, "and went to work persuading the division chairman, Linus Pauling, to buy the equipment, which wasn't easy because Linus had trouble believing that organic chemists could fruitfully use such sophisticated instrumentation. Then when the equipment came, I knew a lot of what it could do, but I didn't really know how it worked."

He soon learned. By 1970 his colleague George Hammond — also a distinguished chemist — could write: "Roberts's work in the field of molecular orbital calculations and Nuclear Magnetic Resonance is of paramount importance in modern organic chemistry. Today, nearly every student of organic chemistry casually feeds secular determinants to high-speed computers and admires the parameters generated by the electronic brain. Roberts was doing the job when one had to diagonalize matrices by direct use of group theory and drudgery. If Roberts had not entered the field of NMR at an early stage, I believe that the field would have developed differently and far less effectively." (In *John D. Roberts: On Thirty Years of Teaching and Research*, a 1400-page volume published by W. A. Benjamin, Inc., in honor of its best-selling author on the occasion of the tenth anniversary of the founding of the Benjamin firm. Further remarks from this book by Benjamin himself and by a Roberts graduate student, George Whitesides, will be found on pages 12 and 13.)

NMR is a precise and comparatively rapid method of studying a wide variety of molecular properties. It is effective only when the molecules contain certain kinds of atomic nuclei, the most important being hydrogen, deuterium, carbon-13, nitrogen-14 and 15, oxygen-17, fluorine-19, and phosphorus-31.

A vial containing a small sample of the substance to be analyzed is placed in a strong magnetic field (nowadays up to as high as 120,000 gauss; the earth's magnetic field, by comparison, is less than one gauss). The strong magnetic field induces the nuclei of the molecule's atoms to line up as compass needles do in the earth's magnetic field. When aligned, these nuclei will "receive" certain radio frequencies that are beamed at them. An NMR spectrum is obtained in effect by tuning across the dial of a radio transmitter and recording which frequencies are absorbed by the sample. This recording appears as a series of peaks on a graph. The locations of the peaks permit identification of the atoms, and the heights of the peaks are proportional to the number of atoms present. By carefully interpreting the data, the investigators can determine the structure of the material in the sample, whether impurities are present, and in what amount.

Some of the "practical" results of NMR research at Caltech have been contributions to understanding the nature of the important industrial polymer polypropylene, the macrolide antibiotics, and the structures of steroids, alkaloids, and enzymes.

The techniques and the instruments have gotten more sophisticated and effective over the years, of course. A fairly new NMR machine in the Roberts lab is now being used to observe the rare isotope nitrogen-15 in enzymes (memorialized as N15 NMR on the license plate for the Roberts Honda). The machine has a cryogenic magnet (that has to be maintained with liquid helium at temperatures within four degrees of absolute zero) with a high magnetic field strength (45,000 gauss) and extraordinary uniformity of field (better than one part in 20 million over a volume of about one cubic inch).

All this was in the future, however. After spending half of the academic year 1951-52 as a Guggenheim Fellow at Caltech, Roberts returned in 1953 as a 35-year-old member of the faculty to fill the hole left by the retirement of Howard Lucas — and brought with him, says Harry Gray, current chairman of the division of chemistry and chemical engineering, "an international reputation as an organic chemist." He also brought with him an MIT woman graduate student, Dorothy Semenow, and a dilemma for all-male Caltech. The story persists that Roberts refused to accept an Institute appointment unless and until Semenow was granted admission, but Roberts labels that a myth. He does say, "I was very pleased to be able to find that the Caltech faculty could make such a drastic change in established policy in just a few months."

In the eyes of many, the ability to persuade demonstrated by Roberts in this instance — and many another thereafter — amounts to genius. Speculation about his methods is laced with both envy and admiration. David Morrisroe, Caltech's vice president for business and finance, thinks he does it "by expecting considerably more from people than people think they can do. This has a very positive effect. He shores it up with a certain tenacity in follow-up that pretty much assures achievement, and he's good at picking a point where a reasonable compromise can be made. Maybe it's the mark of a good experimentalist—that he doesn't persist when the facts overwhelm his ideas."

A case in point for the efficacy of Jack's expectations is the way Robert Ireland, professor of organic chemistry, found himself chairman of the Athenaeum's House Committee in 1976. As Bob remembers the sequence of events, Jack agreed to become chairman of the Board of Governors for the ailing faculty club on condition that Bob would take on the House Committee. "I kept saying no," says Bob, "and Jack kept saying OK and going away — and then he'd bring me stuff about the Athenaeum and its problems. Maybe the basic problem was that I just couldn't say no to Jack. Eventually there I was, running a reorganization-of-the-Athenaeum project."

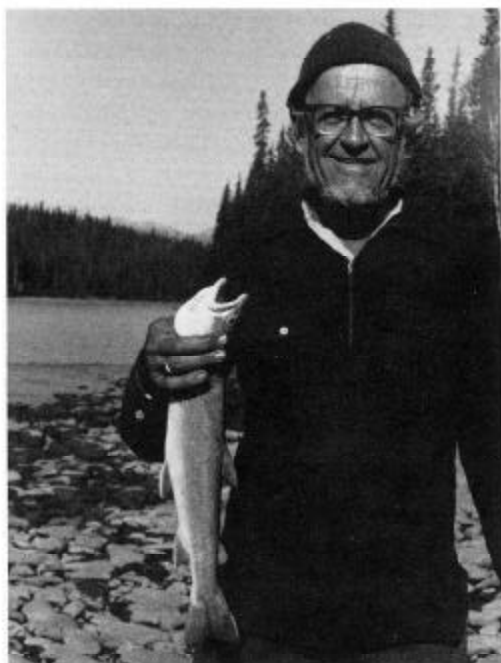
Anyone who has made use of the revitalized Caltech faculty club in the last year or so will testify to the spectacular success of that project and partnership. As a matter of fact, Ireland worries that the Athenaeum is now so overused and overscheduled that the staff and physical facilities may not be able to continue to cope.

Roberts has an intellectual understanding of that problem, but he also wishes more of the faculty would eat lunch at the Athenaeum with their colleagues. "I know some people aren't geared to that kind of socializing," he says, "and I know it isn't easy to sit down at a table with seven strangers. But it's a great way to get to know people. What helped me when I first came here was that Carl Niemann, who was a well-known member of the chemistry faculty, would take me there every day and introduce me to whoever was at the table where we sat."

The 27 years between 1953 and 1980 have seen Roberts reap an astonishing number of honors and awards — in recognition, of course, of an equally astonishing amount of hard work and scientific achievement. "He's without doubt one of the greatest organic chemists in the world," says Gray, "and he's won every award you can think of except the Nobel Prize, which he deserves. He's made very important contributions to chemical education, and his book (*Basic Principles of Organic Chemistry*), written with Marjorie Caserio, is the landmark text in organic chemistry in the last half of this century."

When the first edition of that book was published by W. A. Benjamin, Inc., in 1964, Roberts had been a director-editor of the firm since its founding in 1960. Reminiscing about Roberts's perfectionist attitude and the publication experience, Benjamin wrote in 1970 that "producing a text of that size and scope was the most monumental task a small publisher could possibly undertake. Then add Roberts in the role of senior author, and the adjective 'monumental' is reduced to a feckless pun. I doubt that anyone has any idea of the enormous amount of work that Jack and Marjorie put into this textbook during 1962 and 1963. Much of the manuscript had already been through early drafts, and yet they wrote and rewrote again and again. And we reviewed and rereviewed. Then some 2000 pages of manuscript, roughly the size of three normal books, began to engulf our Broadway headquarters. . . . Once we placed the copy-edited manuscript in the hands of the typesetter, everything began to go wrong. Roberts raged and pleaded, both at long distance, and eventually things began to work. . . . Through one crisis after another Roberts reigned over the entire production process and in the end knew as much about publishing techniques as anyone on our staff."

The teaching of chemistry courses and the care and feeding of graduate students have also occupied a fair amount of his time at Caltech — though his concern for them has not always been evident to the student recipients. This troubles Roberts, but he feels that if he avoids trying to "mother-hen" them, the students are more likely to



JDR's life has not been all slaving over academic obligations or even over a hot (or cold) NMR machine. He's also had some fun. At the left, John Izaak Walton Roberts proves he's a complete angler, and above with wife, Edith, and son Donald he mans the tiller of the family sailboat.

realize — and rise to — their true potential. The results of this attitude have been mixed; a few students have been a bit unhappy, but 46 have earned their PhDs or are at work on them. JDR himself has taken some good-natured razzing about the process, notably from George Whitesides (PhD '64, the Haslam and Dewey Professor of Chemistry at MIT, and a recent recipient of a Caltech Distinguished Alumni Award), who describes the Roberts method of selecting graduate students as “shaking the box to see what falls out.”

The one avenue of communication that graduate students had with him, Whitesides goes on, “was strictly one-way: we wrote monthly progress reports, which, in his absence, we left in his office. We never saw the reports again, and their contents elicited no comment. Our emotional condition as we abandoned these reports on his desk must have resembled closely that in which earlier and (presumably) more primitive cultures tied offerings of chickens in the forest to be eaten by trolls.

“... If Roberts was hard to find in the normal course of events, he compensated by going to considerable effort to read thesis drafts as rapidly as the students could produce them. . . . As drafts were submitted and returned, it rapidly became obvious that, contrary to popular opinion, he *had* followed the progress of the research. In fact, he knew not only the details that had been included in the progress reports, but also details which he had no earthly reason to know. To this day, I have no idea how he came by some of the information he pencilled into the margins of my thesis. Certainly I never told him; perhaps it was divine revelation, perhaps *a priori* reasoning. Regardless, although disillusioning at the time, this final exposure to

the realities of the situation provided a therapeutic conclusion to the graduate educational process.”

It's only fair to point out that there are other equally strong and much more serious testimonials to the Roberts rules of order in regard to critiques. He may — and does — vigorously attack the ideas of a colleague with whom he disagrees; he never opens fire on people.

Now Jack's life has not been all slaving over academic obligations or even over a hot (or cold) NMR machine. There have been trips to most corners of the world (to give lectures, receive awards, attend conferences, vacation, or just to contemplate the scenery while planning and/or writing a book), fishing, sailing (he has his own boat), skiing (two broken legs), whitewater river trips with his sons (who are professional-level boatmen), and tennis (he experiments with new kinds of rackets as they appear on the market and hovers near the top of his division of a most informal Institute tennis ladder). He also continues to be interested in classical music (and still plays the piano now and then), and he does a lot of computer programming and color photography.

Most importantly, there are the four Roberts children, who were born between 1951 and 1955 — Anne, Donald, John Paul, and Allen. “With all the time and energy that my doing science involved,” says Jack, “Edith had to be the major influence with the children, and she's just been fabulous.” However it has been done or by whom, the Roberts child-rearing system has produced remarkable results. (“They're all intellectual giants,” says Ireland.) Two of the boys have just received their MD degrees, and the third is an electronics engineer. Daughter Anne has just begun her third year in medical school, a bit behind

her younger brothers because she got a master's degree in history before deciding to go into medicine.

When Roberts was asked by Caltech President Marvin Goldberger to consider taking over the posts of vice president and provost upon Robert Christy's retirement in January 1980, he already had plenty of experience with administration. From 1963 to 1968 he was chairman of the division of chemistry and chemical engineering and was its acting chairman from 1972 to 1973. He had served on a number of committees at Caltech and for the National Academy of Sciences and the National Science Foundation. So he should have been able to make an educated estimate of what was likely to be involved. He knew, for example, that he would be winding down his research. "There are a lot more things it would be fun to do," he says, "and some that we can still probably do better than anyone else. But the demonstration part of NMR is about over, and this is an appropriate place to start to close things down."

Roberts also had experience being a member of the faculty under the two previous vice presidential provosts — Christy and Robert Bacher — and under their predecessor, Earnest Watson, who did a somewhat similar job under the title of dean of the faculty. Jack respects and admires each of them, and envies what he perceives as their poise in difficult situations.

In speaking at the first faculty meeting after his appointment was announced last December, Roberts defined his concept of the different requirements for wearing each of his new hats. "As vice president," he said in part, "I expect to assist the president by helping to decide controversial issues — through gathering data, opposing points of view, and alternative courses of action. If it should happen that an important decision has to be made quickly, when Murph is not available for consultation, I will be empowered to act for him. The efficiency of modern communication makes this unlikely to be an important function.

"If you ask people what a provost does, you will get different answers. Webster is not much help; among the definitions he offers is 'keeper of a prison.' More to the point but still vague is 'high-ranking administrative official of an American university.' The Caltech provost has been traditionally the chief academic officer, and within the guidelines set by the president I plan to be just that.

"When I came to Caltech 25 years ago, Earnest Watson was dean of the faculty, and the faculty seemed to like the idea of someone fulfilling such a function. I asked Murph to recreate the position because I want the faculty to know that someone represents their concerns in the administration. Furthermore, I know that the greatness of Caltech resides in its faculty, not in its administration, and I want to contribute to the strength of the faculty in the years ahead. It is as dean of the faculty that I expect to work with the division chairmen in matters of appointments, promotions, and salaries.

"Bestowing all of these titles on one person may seem to raise issues of conflict of interest, but it does avoid increasing the administrative bureaucracy and thereby saves money and office space. Furthermore, one telephone extension will suffice for the several functions."

Ten months later, Roberts finds that some of the light-heartedness with which he spoke on that occasion has faded. No amount of previous experience could have prepared him or anyone else for the diversity of issues involved and for the scarcity of money for projects and salaries. Worrying about the rate of inflation, the realities of the economic recession, and the increase in the cost of utilities (double what they were a year ago) is keeping Vice President, Provost, and Dean of the Faculty Roberts awake nights. "There are so many good people here," he says, "with so many good ideas about things to do, it is a terrible responsibility to decide among them. I listen to the proposals and wonder if I can ever get the whole picture into perspective; and I feel pretty defensive about having to be 'encouragingly' negative about so many things. It's tough to have to risk losing any of our good people, and they are good — creative, imaginative, and forward-looking. It's also tough to think about not being able to bring in the best new ones because of space and financial problems."

He is also concerned, as many of the faculty and administration have been before him, about how the Institute can continue to change — as it must if it is to maintain its high academic standing — without substantial growth — a route to change that Caltech has traditionally resisted, though it is used by many universities. He has to be even more concerned than his predecessors about wage and salary guidelines, the high cost of housing for grad students, postdocs, and young faculty, and the recruitment of qualified scientists and engineers from inadequately represented groups, ethnic and female.

One approach he is using to get a better understanding of faculty points of view is to keep an open office door; another is to take faculty members from different divisions to lunch each Friday. He began at the level of the first-year assistant professors and is working up the academic ladder, hoping eventually to have broken the Athenaeum's noontime bread with every professor, including those he's known for years. He has found it particularly rewarding to trade ideas and information with the faculty in this context.

Such exchanges can't help but be beneficial in many ways. Roberts is doing a lot of careful planning these days and making a vigorous effort to enlarge the Institute's resources and capabilities, but he's having to make some thorny choices. JDR may sign his name in red ink, but he doesn't like that color on the bottom line of Caltech's balance sheet. More importantly, he believes that Caltech's strength derives from its faculty being able to work on the things they feel are most significant. His goal is to help them do just that. □

Future Prospects for Low-Pollution Combustion Engines

by FRANCIS H. CLAUSER

During the last three decades the crucial problems in the design of combustion engines have changed radically. Because of air pollution, exhaust emissions from combustion engines have become a dominant factor in engine design. It was Caltech's Arie Haagen-Smit who showed that sunlight produced the photochemical reactions of hydrocarbons and oxides of nitrogen that created the irritating oxidants in our southern California smog. And these, along with carbon monoxide, came principally from the combustion of vast amounts of hydrocarbons here in the Los Angeles basin.

Soon after the mechanism of smog formation was unraveled, it became clear that automobiles were major contributors. Early attempts to clean up the emissions were relatively easy, principally because cars in those days were so bad. The sixties and seventies have seen great progress in legislation governing air pollution, in the organizational problems of managing air quality, and in technological improvements to automobiles that have reduced their emissions by more than tenfold.

Now we have reached a point where improvements are more difficult to come by. Instead of tenfold improvements the struggle is to achieve improvements of tens of percent, and this raises the question of what the future holds. A few years ago optimists believed that the worst was over and that with continued improvements in combustion engines the smog problem would be solved. But the last few summers, with their long stretches of first- and second-stage alerts, have shown that we are barely holding our own.

Has our progress been slowed because we are approaching natural lower limits on the emissions from combustion processes? Or are the natural limits so low that we can expect to make improvements of tenfold several times over in the future? If the latter is the case then the optimists may yet be proven right. No one really knows what the

lower limits are on exhaust emissions, but I believe that improvements of tenfold several times over are indeed still possible.

The business of studying combustion emissions and combustion engines is still largely an empirical one. Great emphasis has been placed on reducing emissions by advancing or retarding the spark, making the fuel-air mixture leaner or richer, getting better carburetion, introducing exhaust gas recirculation, adding catalytic converters, and similar fixes. When I became interested in the problems, it seemed to me it would be foolhardy for a university to compete with a vast industry whose basic approach was to look only a few years ahead to the regulations they would have to meet. Inevitably, their emphasis was on the near-term future. What I could do — and I have found it a matter of keen interest — was to undertake research to ascertain what the fundamental limits of the problem are and how those limits can be approached.

As far as the thermodynamic side of combustion engines is concerned, we know the basic limits and how close we are to them. In fact, it was in elucidating these fundamental limits that Sadi Carnot got classical thermodynamics off to a start more than 150 years ago.

What is the scope of the emissions problem as we now see it? There are five pollutant emissions under legislative control — unburned hydrocarbons (UHC), carbon monoxide (CO), oxides of nitrogen (NO_x), particulates (smoke, or soot), and sulfur dioxide (SO₂). At present, only the first three are of significance here in southern California, and I will focus my attention on them. Sulfur dioxide is of concern in areas where fuels containing a significant amount of sulfur are burned, and particulates will probably be an increasing factor in the future.

To understand the emissions that come from a typical modern internal combustion engine, we first need to know a little of the technical jargon. Whenever any hydrocarbon

fuel such as methane, propane, or gasoline burns in air, there is a critical ratio of fuel to air such that each hydrocarbon molecule can find just enough oxygen partners to form CO_2 and H_2O with nothing left over. Chemists call this the stoichiometric ratio. Different hydrocarbons have different stoichiometric ratios, but for many purposes their behavior is best compared by using for each the relative fuel-air ratio, that is, the actual fuel-air ratio divided by the stoichiometric ratio. A rich mixture is one having excess fuel, and its relative fuel-air ratio is thus greater than one. A lean mixture correspondingly has a relative fuel-air ratio of less than one.

When a lean mixture burns, it does pretty much what is expected — the fuel burns to form principally CO_2 and H_2O , and the excess O_2 appears in the exhaust as just that, excess O_2 . However, when a rich mixture burns, the principal result is not that the excess fuel appears in the exhaust. Instead, there is a rearrangement of partners, and CO and H_2 appear in the exhaust along with H_2O and decreasing amounts of CO_2 . Only for very rich mixtures will significant amounts of fuel and carbon appear in the exhaust.

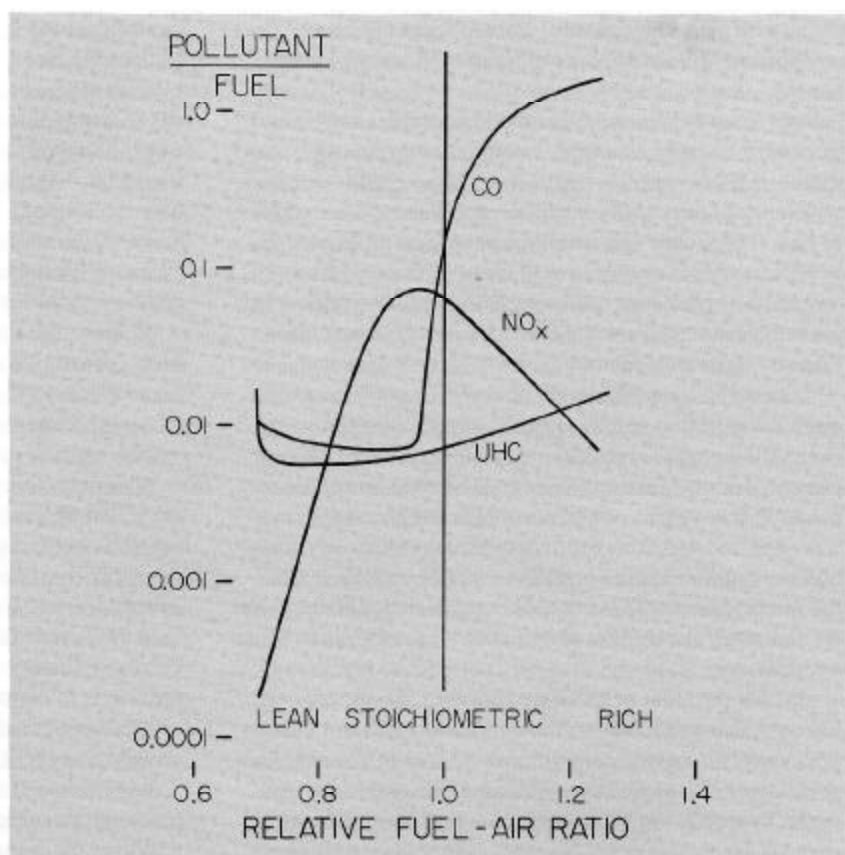
Of the three pollutants CO , UHC , and NO_x , only CO is a primary exhaust product and this only when the mixture is rich. With this one exception, all of the exhaust pollutants are only secondary products, and they occur in

surprisingly small quantities. It is this fortunate fact that permits us to burn hundreds of thousands of tons of hydrocarbons each day and have only hundreds of tons of pollutants discharged into our atmosphere.

In Figure 1, which depicts the emission characteristics of a typical gasoline engine, we have plotted the concentrations of UHC , CO , and NO_x in the exhaust, expressed as ratios to the amount of fuel entering the intake. Each varies greatly as the relative fuel-air ratio is changed. The only one that rises to large values is CO , which — as we remarked earlier — becomes a primary product when the mixture is rich. For lean mixtures, CO rapidly drops to low values and then abruptly levels off. The curve for NO_x rises to a peak on the lean side of stoichiometric and drops to quite low values for both very rich and very lean mixtures. In contrast, the UHC has a minimum fairly well into the lean region. It rises somewhat for rich mixtures, but it abruptly goes up almost vertically for mixtures so lean that the engine misfires. This happens because when firing does not occur, raw fuel becomes a primary exhaust product, appearing as unburned hydrocarbons.

In order to obtain a feeling for what constitutes a "good" engine as far as pollution is concerned, let us relate the levels shown in Figure 1 to the permissible federal and California levels for passenger cars. The federal standards set limits of 3.4 grams per mile for CO , and .4

Figure 1. The exhaust emissions of a typical gasoline engine are plotted here, with the horizontal axis representing the fuel-air ratio divided by the stoichiometric ratio. Along the vertical axis are the concentrations of the pollutants (unburned hydrocarbons, carbon monoxide and oxides of nitrogen) divided by the concentration of intake fuel; this scale is logarithmic (in powers of 10) and thus covers a very wide range of values.



grams per mile for UHC. Here in California we also have limits of .4 grams per mile for NO_x.

How are we to compare these values for vehicles with those we used in quoting engine emissions? For the engine we used the ratio pollutant/fuel, whereas vehicle levels were expressed as pollutant/distance. We can of course write the engine index, pollutant/fuel, as pollutant/distance times distance/fuel, and we recognize that distance/fuel is the familiar gasoline mileage, or miles/gallon of the vehicle. Unfortunately, we have here a strange conglomeration of units — miles, grams, and gallons. Inserting the proper factors to take this into account, we have

$$\frac{\text{(engine)} \text{ grams pollutant}}{\text{grams fuel}} = \frac{1}{3000} \times \frac{\text{(vehicle) grams pollutant}}{\text{mile}} \times \frac{\text{miles}}{\text{gallon}}$$

Let us consider two extreme cases: a gas guzzler that gets 10 mpg and an economy car that gets 40 mpg. Using the above formula, we can translate the legislative vehicle limits into permissible engine limits as follows:

Gas Guzzler		Economy Car	
$\frac{\text{UHC}}{\text{Fuel}}$	and $\frac{\text{NO}_x}{\text{Fuel}} = .0013$	$\frac{\text{UHC}}{\text{Fuel}}$	and $\frac{\text{NO}_x}{\text{Fuel}} = .0053$
$\frac{\text{CO}}{\text{Fuel}} = .011$		$\frac{\text{CO}}{\text{Fuel}} = .045$	

If we apply Figure 1 directly to these numbers, we see immediately that a typical engine, when used in the economy car, can — by operating with lean mixtures — have acceptably low values for all three pollutants. But the gas guzzler hasn't a chance. It would need all the help it can get from a catalytic converter, exhaust gas recirculation, and any other "fix" available. For an engine to be good enough to get the gas guzzler within the standards it would have to be some four times better than the typical engine.

The pollutant scale of Figure 1 covers a range of more than 1000 to 1. It is thus a matter of some wonderment that engine performance and legal standards are currently so neatly matched that the line between pass and fail falls between the gas guzzler and the economy car, which differ in mpg by only a factor of four. This is no accident. Each time engineers have devised a technical improvement, legislators have lowered the limits in such a way that only the best pass.

Now let us look at the problem from a quite different vantage point. A simple hydrocarbon flame (Figure 2) performs fundamentally the same task as combustion in the gasoline engine — burning hydrocarbon. But here the process is far less complex. The flame burns smoothly and steadily in a uniform well-mixed mixture contained in a cylindrical quartz tube. At first glance the flame appears to be urged along by a glowing disk. Actually both the flame and the disk are standing still. It is the mixture that is moving in the tube, and the disk creates a flow field be-

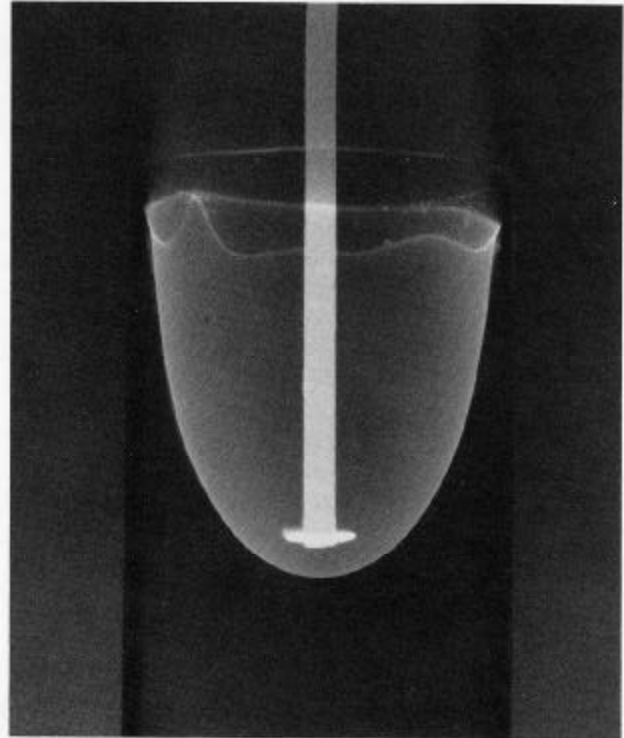


Figure 2. This free-standing flame, produced by a well-mixed mixture of propane and air entering a vertical quartz tube from below, provides an excellent setup for measuring the fundamental characteristics of combustion emissions. In the experiment, the curved flame is positioned by a disk-shaped flame holder. The flow is smooth and steady so the flame stands motionless, striking the quartz tube in a wavy ring around the boundary.

hind the flame that anchors it in place. Such a setup is well suited to laboratory experiments because the free-standing flame can be probed in detail to reveal what reactions are taking place.

How do the emissions from this free flame compare with those from combustion in an engine cylinder? Analogous to the emission levels in Figure 1, we show in Figure 3 the corresponding values for the free flame. A number of startling differences are immediately apparent. The flame has a UHC level that is 1000-fold lower than that of the engine, and this low value extends over a much wider range of fuel-air ratios, including a significant portion of the rich-mixture region.

If we probe the free flame to determine what happens to the hydrocarbon fuel as it passes through the flame, we are immediately struck with what a wonderful thing it is. In front of the flame the hydrocarbon concentration is several percent, or several tens of thousands parts per million (ppm). Immediately behind the flame this drops to a level of a few tenths of a part per million. This abrupt drop of 100,000-fold shows how efficient the flame is in consuming the hydrocarbons.

To put this in perspective, here in southern California the air we breathe usually contains one or two ppm of

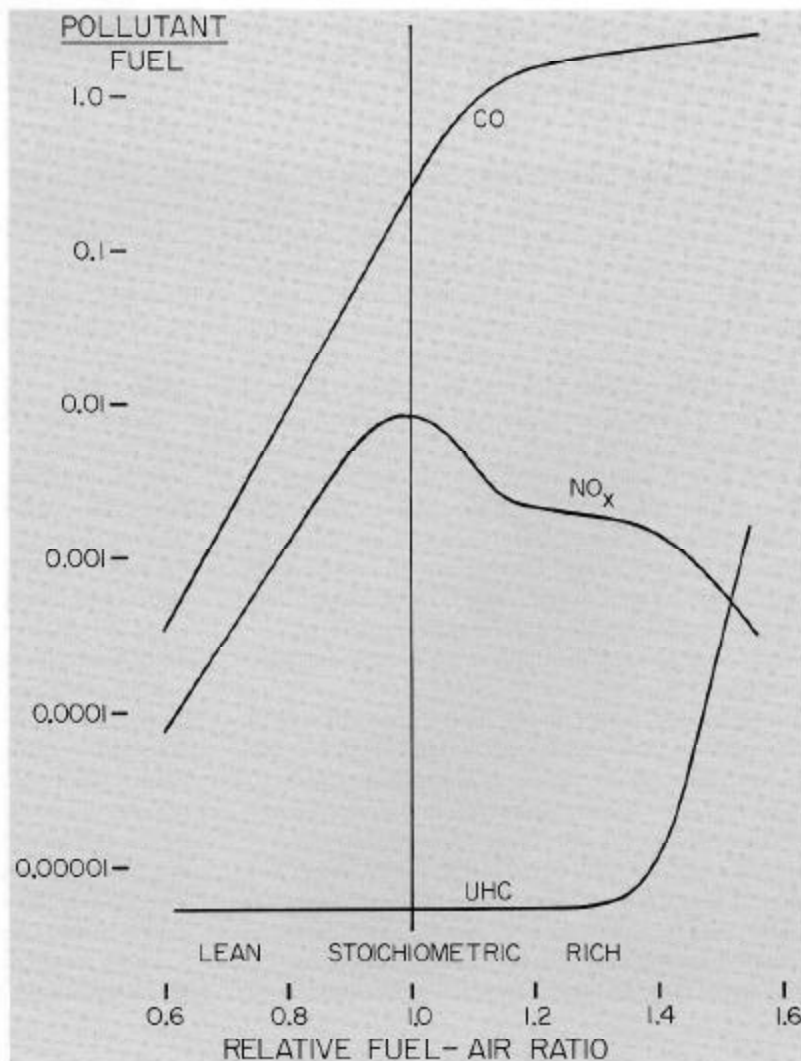
hydrocarbons. In contrast, the exhaust from the free flame has a concentration one-tenth as great. If the engine were as efficient as the flame, our cars would cleanse the air of hydrocarbons instead of contributing to the pollution. Clearly something significantly different is happening in the two cases.

For NO_x emissions, the flame is also significantly better than the engine. Its peak values are approximately one-tenth those for the engine. For CO, in the rich region where CO is a primary product, the flame and engine are, as expected, nearly the same. As the mixture becomes lean, the CO from the flame does not drop as rapidly as for the engine, but instead of leveling off it continues to drop to quite low values.

These comparisons raise a host of questions. Why is the engine worse than the free flame? Does this flame represent the best that can be done; or is it possible to go to even lower levels? Might it be possible to build a useful engine that could approach the levels of the free flame, or achieve even lower values?

In seeking answers to these questions we have to look at the mechanisms that lead to the formation of each of the pollutants individually. First we examine the situation for CO. In the free flame, there is a luminous front that is about one millimeter thick, where the primary reactions take place. First the hydrocarbon molecules break up; almost immediately the carbon atoms unite with oxygen atoms to form CO. If the mixture is rich (that is, oxygen deficient), many of these CO molecules cannot find other oxygen partners, and CO emerges as a primary exhaust product. If the mixture is lean, the CO molecules at a more leisurely pace seek additional oxygen partners (usually stealing them from OH radicals) to form CO_2 . However this second union doesn't always stay stuck. Temperature has a large effect, both on how fast this second union takes place and how fast it comes apart. Both reactions slow down as the temperature decreases, so much so that for ordinary temperatures the time constants are measured in acons. Furthermore, the ratio of the two rates shifts, favoring CO_2 over CO, so that at ordinary

Figure 3. Exhaust emissions from the free flame shown in Figure 2 are plotted here on the same scales used in the Figure 1 graph for the gasoline engine. Striking differences are immediately apparent.



temperatures CO should virtually disappear.

With this picture in front of us we can formulate general principles for obtaining low levels of CO. A prime requisite is that all combustion should be with lean mixtures. At first glance it would appear that the leaner the better. This seems to be borne out by the CO curve in Figure 3, which continues to drop as the mixture becomes leaner. But a closer analysis reveals that the principal effect of leanness here is to lower the flame temperature, shifting the equilibrium from CO to CO₂. Any other means for reducing the flame temperature would also lower the CO level.

This immediately suggests a way of obtaining even lower concentrations of CO than those in the free flame. In almost every combustion process, after combustion has taken place, the temperature of the products is reduced. In some engines this is done by expanding the gases to extract mechanical energy. In others, the heat is transferred to other media (water, for instance). This lowering of the temperature can be used to reduce the CO concentrations, but to be effective it must be done in a carefully prescribed way. As the temperature drops, not only does the equilibrium shift but also the rate of approach to equilibrium drops as well. At elevated temperatures, equilibration times are measured in milliseconds, but as the temperature falls they become seconds, then hours, and finally centuries. If at any point in the cooling process the rate of cooling gets ahead of the equilibration rate, the CO will be "frozen in" and the benefits of further cooling lost. Below 1200K equilibration rates become impossibly slow. For temperatures such that the times are reasonable, however, CO concentrations of the order of five ppm can be reached. On the scales of Figures 1 and 3 this is a level of approximately .0001 for CO/fuel, which is below any of the values for either the engine or the free flame. Here we have a case where it should be possible to build an engine that would do even better than the free flame.

Now let us turn our attention to the problem of NO_x emissions. In the air around us, nitrogen and oxygen have existed together without detectable interaction for billions of years. It's not that they won't react, but rather that such reactions, like the CO reactions, are extremely temperature dependent. Here, very little happens until temperatures of the order of 2000K are reached, and then O₂ and N₂ dissociate into N and O, and a set of reactions gets under way that leads to the formation of NO and NO₂. As the temperature goes up, the pace of these reactions increases rapidly, so rapidly that it appears as though a critical threshold has been passed.

In the case of the free flame, this critical temperature is exceeded only for mixtures with relative fuel-air ratios between .75 and 1.5. In Figure 3, we see that lean and rich flames both produce very little NO_x (that is, either NO or NO₂). But the NO_x curve rises to a peak near a relative fuel-air ratio of one.

For the engine a similar behavior occurs, but there the

peak of the NO_x curve is some ten times higher. This is caused by the much higher temperatures that exist in the engine for two reasons. First, the mixture is compressed before burning, which raises its temperature significantly. Second, the combustion takes place at nearly constant volume rather than constant pressure, which causes an additional increase in temperature.

At this point we see that a portion of the strategy we outlined for reducing CO will also apply in the case of NO_x, namely that of keeping the combustion temperatures low. In the first case, after the rapid initial formation of CO, the slower oxidation of CO to CO₂ is favored by lower temperatures. In the second, lower temperatures inhibit the formation of NO_x.

It is in the cooling portion of the strategy that a discrepancy in goal occurs. For CO, a properly paced cooling rate will cause the CO to be oxidized to CO₂. In the case of NO, the attack of atomic O on the N₂ molecule promotes the formation of NO_x. It is the attack of atomic N on NO_x, however, that causes the destruction of NO_x. Unfortunately, upon cooling atomic N disappears considerably faster than atomic O. This means that it is virtually impossible to get rid of NO_x by a program of cooling. For NO_x, the best strategy is simply never to let the temperature get high or, if it does, to cool it off before the relatively slow NO_x formation reactions have had time to occur. Fortunately, the procedures for obtaining low CO and low NO_x are not completely contradictory. The useful range of temperatures for oxidizing CO lie between 1200K and 2000K, whereas NO_x forms at a significant rate only above 2000K. Hence a proper procedure is to keep the burning temperature below 2000K and then to cool at a properly tailored rate down to 1200K. In this way it should be possible to obtain concentration levels of the order of five ppm or less for both CO and NO_x. On the scales of Figures 1 and 3 this translates into values of approximately .0001 for CO/fuel and NO_x/fuel. This number is more than 100 times lower than those required to meet the CO standard for the gas guzzler we considered earlier, and 13 times less than the NO_x standard. For the economy car, the numbers are even more impressive.

Now we come to the last of the three major pollutants — unburned hydrocarbons. We have seen that in a typical engine UHC levels are 1000 times greater than in a simple flame. Why is this so? For the UHC to appear in the exhaust, some of the incoming fuel must escape being burned, not only during combustion itself, but also during the subsequent expansion and expulsion from the cylinder.

In the early 1960s Wayne Daniel of the General Motors Research Laboratories proposed two ways in which this might occur. In the first the fuel-air mixture enters into crevices such as that around the top of the piston above the piston rings. This takes place during the intake and compression strokes. After combustion, these unburned hydrocarbons emerge during the expansion stroke and are carried out in the exhaust. The second mechanism proposed

by Daniel was that of wall quenching. Since the time of Sir Humphry Davy it has been known that a flame will not pass through a wire screen if the mesh is fine enough. The flame is quenched by heat being drawn away by the screen. Daniel similarly reasoned that a flame near the cooled wall of the piston and cylinder would be quenched and thus unable to burn a thin layer of combustible mixture lying along the surface. This unburned layer would at a later stage be swept off the surface and carried into the exhaust.

Tests by Wentworth of G.M. and by others showed that in fact the crevice around the top of the piston above the rings could be a major source of unburned hydrocarbons. When this crevice was eliminated in tests, the exhaust hydrocarbons decreased by more than half. And then a strange thing happened. Attention became focused on the wall-quenching problem, and nothing was done about the piston crown device. Cars in production today still have that same crevice.

A few years ago two thoughts occurred to me, since my background is in fluid mechanics, and I had come to believe that these quenching phenomena were of a boundary layer kind that can involve significant dynamic behavior. The first thought was that there might be a third mechanism for producing unburned hydrocarbons, namely, the quenching of the flame at the boundary between the fresh incoming charge and the residual charge left over from the preceding cycle. The second was that fundamental research on wall quenching might be worthwhile because the evidence for its existence was largely inferential and no one seemed to have examined in detail what was actually taking place. So I undertook research on both of these subjects.

In the wall-quenching experiments, I set up a situation not unlike that shown in Figure 2 except that I used a water-cooled metal wall instead of a quartz tube. With small probes I was able to explore in detail the regions both ahead of and behind the flame, and in particular the region along the wall. Now according to the wall-quenching hypothesis there should be a layer about a millimeter thick of unburned hydrocarbons next to the wall behind the point where the flame strikes the wall.

Much to my surprise there was no such UHC layer. As mentioned earlier, the flame reduces the hydrocarbon level from tens of thousands of parts per million in the oncoming stream to tenths of parts per million in the region after the flame. Contrary to expectations, this state of affairs was found to hold right up to the wall. In spite of whatever quenching that may be taking place, the flame is able to consume the hydrocarbons near the wall to the same low level that it does in the free stream.

Upon taking stock, I realized that in my original experiment both the wall and the flame were stationary in space, with the combustible mixture flowing through the flame front. In an engine the flame sweeps across the cylinder and moves with respect to the wall. To determine if the



Francis Clauser sets up his laboratory experiments on flame quenching as a source of unburned hydrocarbons.

movement of the flame relative to the wall was affecting the result, I curved the flow channel in such a way that the cooled wall could be part of a large aluminum wheel. Here, with the flame striking the wall, I could have the wall moving in either direction with any speed, essentially duplicating the relative velocities of wall and flame that occurred in an engine cylinder. For small speeds of the wall relative to the flame, there was still no layer of quenched hydrocarbon at the wall. As the speed of the wall increased, however, either with or against the flow direction, such a layer did begin to appear, and at large speeds it was comparable in size to that predicted by the empirical theory (which contained no notion that speed would be a factor).

These experiments show that wall quenching does play a role in producing UHC, but less of a role than formerly believed. Perhaps more importantly, they show that wall quenching can be eliminated in engines that are designed in such a way that the flame front is stationary, or nearly so, with respect to the surrounding wall (as occurs in steam engines, stirling engines, and gas turbines). This almost certainly will prove to be an important factor affecting the design of engines of the future.

In the second series of experiments, those on UHC pro-

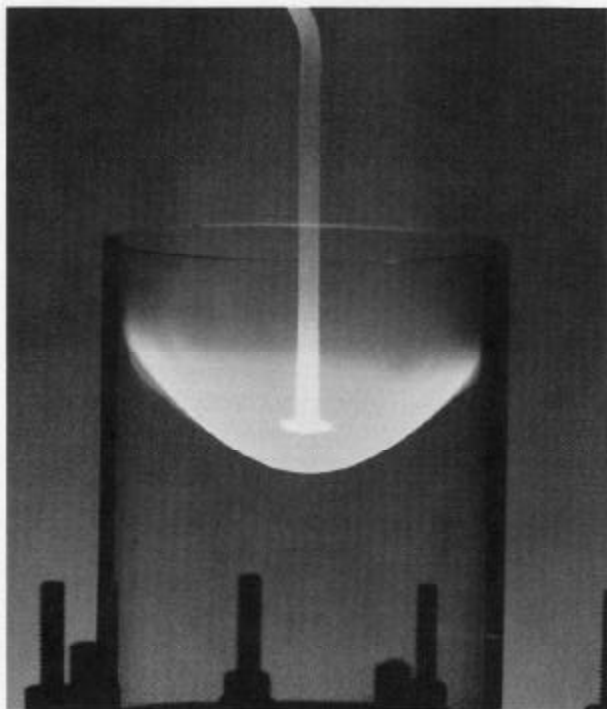


Figure 4. In this experiment the setup is similar to that in Figure 2 (the rod is the same size) but with the central stream surrounded by an annulus of incombustible gas also rising vertically. The flame in the combustible cone spreads outward and upward until it strikes the incombustible stream where it is quenched, leaving in its wake a surprisingly large amount of fuel that emerges as unburned hydrocarbons.

duced by incombustible gas quenching, the setup shown in Figure 4 was employed. Here the combustible mixture coming from below is surrounded not by a quartz tube as in Figure 2, but by an annulus of incombustible gas (such as exhaust gas or air) that is also moving upward. When the flame strikes the boundary between the combustible core and the surrounding annulus, it is extinguished. The question is how much UHC will be left over along the boundary after the combustion is over. The results were dramatic. Hydrocarbons were found to exist in large quantities along the boundary in the wake of the flame. All of this indicated that incombustible gas quenching can in fact be a major source of UHC in combustion engines. A second part of this experiment is now under way. We have designed and built an engine that almost completely scavenges the residual charge after each cycle. We hope to find out soon if this can lead to a significant reduction in exhaust hydrocarbons.

As yet we do not know the full story of the origin of all of the exhaust hydrocarbons. Some as yet unknown source mechanisms may be found. In the laboratory, however, we have built combustion chambers that yield UHC levels comparable with the values of the free flame, indicating that it may be possible to build an engine having these

same remarkably low values.

Again, why is the typical gasoline engine so much worse than the free flame? The gasoline engine, like all combustion engines, performs three basic thermodynamic acts. It compresses its working medium, here a mixture of fuel and air; it adds heat to this medium, in this case by combustion of the medium; and finally it expands the medium to extract useful mechanical work. The gasoline engine, in company with the diesel, does all three acts in the same chamber. This puts rather severe time constraints on the combustion and post-combustion processes. At an engine speed of 3000 rpm, the combustion itself must be completed in about two milliseconds and the subsequent expansion in about ten. When flame temperatures are high, combustion is fast, but as temperatures are reduced, by leaning the mixture or dilution with exhaust gas, combustion slows to rates well below those needed to meet the two-millisecond requirement. This constitutes a major obstacle in reducing temperatures enough to insure very low concentrations of NO_x . Further, the restricted expansion times militate against obtaining the low concentrations of CO that are possible in a properly paced cooling program.

Because of the repetitive nature of combustion in the compression chamber of the gasoline engine, ignition must be initiated each cycle, and the flame must sweep across the chamber at relatively fast speeds. As a result there appears to be no way to avoid UHC produced by wall quenching since the flame cannot be held stationary relative to the cooled walls. With the present configuration of gasoline engines it may be found that the intermixing of the residual gases from one cycle with the fresh mixture of the next leads to quenching that cannot be avoided. If so, this too will prevent the achievement of very low levels of UHC. In addition, there is evidence that both wall quenching and residual gas quenching cause the CO to freeze in before it has been oxidized to CO_2 .

All of the above stand as significant obstacles that make it difficult for the gasoline engine to achieve very low pollution levels. What are the prospects for other combustion engines? The whole class of "external" combustion engines, which includes the steam engine and the Stirling engine, has a significant advantage as far as low pollution is concerned. Since the combustion process takes place independently of the compression and expansion processes, much greater freedom exists in design to meet the requirements for low pollution. If this is so, why haven't these engines demonstrated such potential? Recently I measured the emissions from the large steam boilers here at Caltech. I found that both the CO and the UHC were in fact reasonably close to the very low values I have indicated above should be possible. In contrast, it was the NO_x that was unacceptably high. In these boilers, combustion takes place at a leisurely rate. Neither wall quenching nor incombustible gas quenching is a problem. Heat is extracted over a long flow path. As a result, both the hydrocarbons

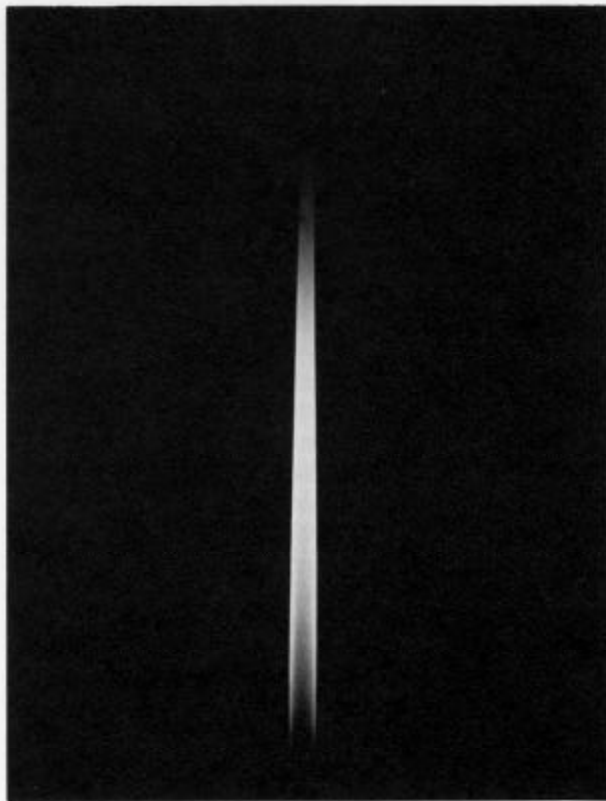


Figure 5. Setting a bad example, this flame is typical of a large number of current combustion devices that, because of ease and simplicity, mix and burn at the same time. Here the air and fuel enter separately from below and begin to burn as they begin to mix. In the central bright stream, the mixture is extremely rich (almost entirely fuel), releasing a great deal of carbon as smoke; the burning mixture in the surrounding sheath is quite lean because little fuel has diffused out that far. In between these two regions, burning is occurring with a broad range of fuel-air ratios, producing large amounts of exhaust pollution at the unfavorable ratios (where the curves reach high levels in Figure 3).

and the CO are oxidized to concentrations of a few parts per million.

I believe the reason for the high NO_x lies in an affliction that plagues a wide variety of combustion devices, namely, the act of mixing and burning at the same time. This affliction has a long history, dating back to the camp fires of earliest man and continuing today in the vast majority of combustion devices we use.

The problem lies in the wide range of fuel-air ratios that occur in a mix-and-burn flame. In the emissions for the free flame shown in Figure 3 we see that for each of the pollutants there are certain fuel-air ratios that produce unusually high values of the pollutant. Clearly these fuel-air ratios should be avoided if at all possible. But consider a flame such as that shown in Figure 5. Here the fuel and the air are introduced separately, and they burn as they mix. If we examine what is happening locally, we find that near the core of the fuel stream, combustion is taking place at very rich mixtures. Out in the airstream combus-

tion is taking place at very lean mixtures. In between, all other fuel-air ratios can be found. For each pollutant there are local regions where that pollutant is being produced in unacceptably large quantities. Clearly it does no good to keep pollution levels low elsewhere if some regions are producing excessive quantities.

Now let us reverse the thrust of the question and ask why mix-and-burn is so widely used if it is so bad. The alternative, of course, is to mix the fuel and air thoroughly and then, and only then, to burn it. The difficulty is that, given half a chance, the flame will either strike back into the mixing region or, worse, be blown out. For the premixed flame, control becomes a major issue. In contrast, the mix-and-burn configuration is a highly stable one that requires little if any control. In nature's scheme of things, mix-and-burn is the lowest of combustion denominators, the configuration of last resort.

The Caltech steam boilers also have burners of the mix-and-burn type. Within the main fire box large quantities of all the pollutants, including soot, are produced. Fortunately for all except NO_x , the process of extracting heat and cooling the mixtures is so leisurely and the intensity of mixing so great that they are eventually oxidized to very low levels. Initial local hot spots, however, produce relatively large amounts of NO_x . As we saw earlier, cooling and mixing do not reduce NO_x significantly. If the Caltech boilers are a reasonably good case study, then the indications are that "external" combustion power plants have good chances of achieving very low pollution levels if they can master the problems of premixed burning.

Finally, let us take a brief look at the problems of jet engines and gas turbines. Here too combustion takes place as a separate and specialized function, so these engines should enjoy many of the advantages of the external combustion engines. Further, the temperature limitations of the turbine are low enough to make the achievement of very low values of NO_x quite favorable. However, all conventional gas turbines and jet engines employ mix-and-burn systems that hinder the achievement of these potentially low levels of NO_x . Experimental jet engine combustors using burners with premixed fuel and air have demonstrated that significantly lower levels of CO, UHC, and NO_x are possible. Here again, the problem is one of preventing strike back and blowout over the wide operating range of the jet engine.

And what of the engine of the future? Almost certainly we shall soon be able to build combustion systems that use premixed mixtures having precise fuel-air ratios and that can operate stably over a wide range of conditions. With this accomplished, exhaust emissions should experience a dramatic decrease. Engine designers can then employ a wide variety of compressors and expanders to assemble engines that can be tailored for many different uses. All should be able to enjoy exhaust emissions levels powers of ten less than our present engines. And we should be able to have our cars and breathe clean air too. □



Sir Francis Bacon

The Scientific Method

by DAVID and JUDITH GOODSTEIN

How did the scientific method develop and do practicing scientists really use it?

Judith Goodstein: Two major philosophical schools of thought about the nature of the scientific enterprise are, first, that of the 17th-century philosopher of science, Sir Francis Bacon, and, second, that of the 20th century's Sir Karl Popper. Bacon's ideas on this subject have, of course, dominated Western scientific thinking for more than 300 years. In fact, it is Bacon to whom we owe the idea that there *is* a proper way to approach the study of science.

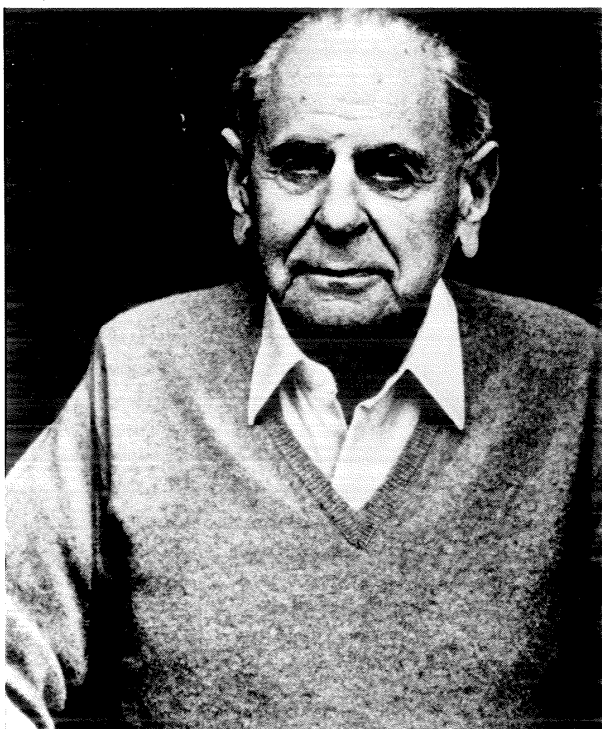
Francis Bacon was born in England in 1561. He was

educated at Trinity College and then entered Gray's Inn, where he studied law. He was also something of a politician, and he became chancellor under James I in 1618. Three years later he was dismissed after being convicted of taking bribes. His scientific contemporaries included Gilbert, Galileo, and Kepler, but he remained isolated from the scientific developments associated with them. He attacked both Copernicus and Ptolemy for producing only "calculations and predictions" instead of "philosophy, what is found in nature herself, and is actually and really

true.” His knowledge of the sciences, it turns out, was largely based on literary sources, and on this solid foundation he built his famous theory of the scientific method.

Bacon held the view that the scientist starts his research by recording observations. If these observations were correct, he believed, they would lead to equally correct judgments, or generalizations, about nature. In the application of this inductive process, Bacon outlined a necessary sequence of steps to be followed. To make true inductions, one must begin by purging the intellect of “idols” that obstruct man’s unprejudiced understanding of the world. If this is accomplished, the mind becomes, in Bacon’s phrase, “a clean slate,” on which true notions can be imprinted by nature itself.

Bacon’s inductive method started with observations that would lead to the construction of systematic tables of the presence, absence, and comparisons of properties. From these, inferences would be made that could then be “put to the question” by artificial experiment. While the ascent from particular observations to generalizations is a very complicated process, Bacon felt that done properly it would result in a number of inferences whose conclusions would be infallible. Furthermore, he was aware that infallibility would depend on there being only a finite number of properties — and on the scientist’s ability to list all of them in any given instance. Since some properties are “hidden,” he was amenable to the use of “aids to the senses,” which included the telescope, for example, and



Sir Karl Popper

many other kinds of laboratories and instruments.

Bacon invented a scientific Utopia in which there is a division of scientific labor. Those who do experiments and collect information form the first group; a second determines the significance of the information and experiments and carries out new ones; and a small third group, known as the interpreters, “raises the former discoveries into greater observations and axioms.” Bacon assigned 33 experimentalists to the first two tasks. He didn’t see the need for more than 3 interpreters.

Bacon’s scientific methodology can be summarized as follows: 1. The scientist must start with a set of unprejudiced observations; 2. these observations lead infallibly to correct generalizations or axioms; and 3. the test of a correct axiom is that it leads to new discoveries. Three hundred years later, Sir Karl Popper arrived at a different view.

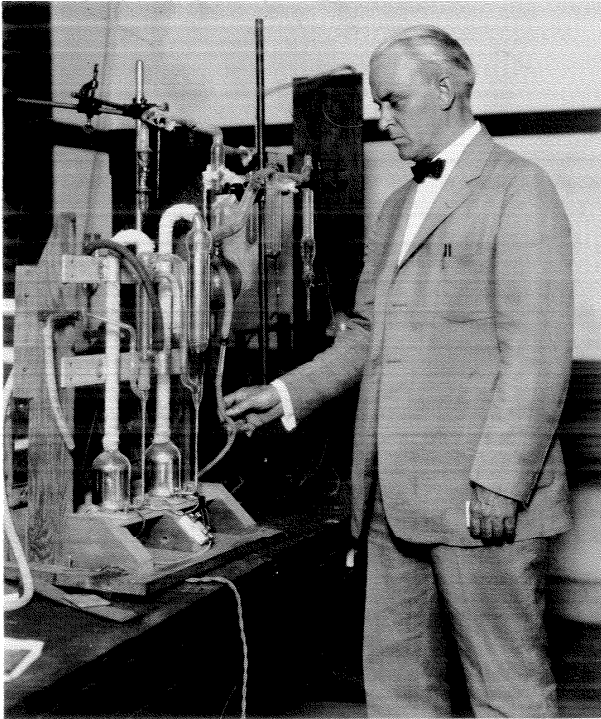
Popper is a contemporary philosopher of science. He was born in Vienna, where he received his university and graduate training and published his major work, *The Logic of Scientific Discovery*, in 1934. Popper’s scientific contemporaries include Einstein, Heisenberg, Bohr, and Born.

No one has ever accused Popper of learning his science through novels and plays. It was Einstein’s 1905 paper on special relativity that prompted him to begin studying the philosophy of science — because of the implications in that paper of what it means to say that two events at different points in space occur simultaneously. He was curious as to how one “verifies” this. As it turns out, he made “falsifiability,” rather than “verifiability,” the cornerstone of his ideas about how science operates.

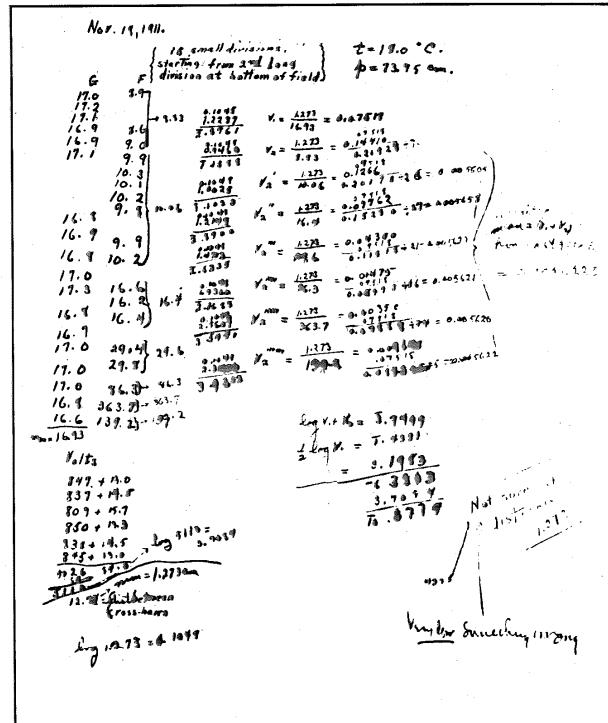
According to Popper, a scientist, whether theorist or experimentalist, puts forward statements (or systems of statements) and tests them step by step. The initial stage — the act of conceiving or inventing a theory — doesn’t interest him because that is a creative act that cannot be analyzed logically. Popper focuses his analysis on the next step, which consists of showing the proposal to be wrong. He says, in effect, that all scientific discoveries are refutations of past theories.

Philosophers say science is something that follows the scientific method. Yet philosophers Bacon and Popper present two opposing views of what the scientific method is. For Bacon, the unprejudiced, systematic observer is led infallibly to generalizations that in turn produce new discoveries. Popper says instead that theories are the product of inspiration, and progress consists in falsifying them by showing their predictions to be wrong. To find out which one of them is right, we turn to a practicing scientist.

David Goodstein: Sir Francis and Sir Karl certainly have very different views of how science — and scientists — operate, but we can compare them at two points. We can compare the two views of the process of creating theories, and we can ask what happens once the theory has been created. What does the experimentalist do? I’ll leave the



The instrument Robert Millikan is inspecting in this photograph taken in the 1920s at Caltech was used for spectroscopy and cosmic ray research. The famous Millikan oil drop experiment was performed



much earlier at the University of Chicago. Above is a page from Millikan's lab notebook dated November 18, 1911, and with a comment on the results in the lower righthand corner.

question of how theories are created for Madame, the archivist, to take up later. Right now my job is to discuss what experimentalists do once they have a theory to test.

As my first example, let me tell you about one of our own patron saints, Robert A. Millikan, and his oil drop experiment. Millikan had two things to find out with that experiment — whether the electric charge came in quantized units, and if so what the size of the unit was. And so, good, Baconian, dispassionate observer that he was, he had to go into the laboratory with no preconceived notions, look at his oil drop, make his measurements, and report *all* of the results, which — he says in the *Physical Review* — he did.

Now I've looked at some of Millikan's laboratory notebooks (written only for himself) to see how he worked. On December 20, 1911, he shows his readings — the voltages, the rate at which the drop is falling in gravity, measurements of what happens when the drop is in the field — and then he does his calculations. And what do we find at the bottom? His comments. "This is almost exactly right," he says. "This is the best I ever had." On another day his comment was, "Very low. Something is wrong." Another one says, "Beauty! Publish!"

If this seems shocking, let me assure you I am not trying to tell you that Millikan was being a bad scientist. He was one of the very best scientists. But he was doing what scientists always do when they're in the laboratory,

which is to look for the result that they want. To tell you about that, I'm going to analyze in a very general way a hypothetical, but realistic, experiment.

If you have a liquid like water, it can exist in equilibrium with its own vapor, and the curve along which it exists in that state is called the vapor pressure curve. If you warm the water and steam up, they can still be in equilibrium, but at a higher pressure. At higher pressure the vapor is more dense, and because the temperature is higher, the water is less dense. As you warm the system, the densities of these two fluids get closer and closer, and finally they become equal to each other — at what is called the critical point.

About 20 years ago it was discovered that at the critical point of any substance its heat capacity (the amount of heat put into the system divided by the change in temperature) becomes infinite. Various other properties were also found to behave peculiarly at the critical point, and a theory grew up to explain these so-called critical phenomena.

The theory makes a definite prediction about how the heat capacity becomes infinite. What is important is how far we are from the exact critical temperature (that is, the temperature at the critical point). Suppose we make a measurement near the critical temperature, but at a small temperature difference away from it that we can call ΔT . The theory says that, if ΔT is sufficiently small and we

plot the log of the heat capacity versus the log of ΔT , we will find a straight line. Moreover, if we make these measurements both just above and just below the critical temperature, we should get two straight lines, and they should have the same slope. That is the prediction we are going to set out to prove.

Now, no matter how carefully we do our work, we immediately run into a severe problem. In order to find ΔT at each point, we must know not only the temperature at which we are working, but also the critical temperature, to a very high precision. It is not good enough to look the critical temperature up in a book — probably we will need to know it more accurately than it has ever been measured. We must deduce it from our own experiment.

The critical temperature is just the temperature at which the heat capacity we are measuring becomes infinite. Of course, we cannot really measure an infinity in the laboratory, but we can accomplish the same purpose by assembling our data and using them to choose a critical temperature that makes those two curves into parallel straight lines. If we do that, to be sure, we are not really testing the theory, but there may be no other way to do it.

There are other problems as well. The theory only applies, strictly speaking, to a sample of infinite size, in the absence of gravity. We can use the theory itself to correct our data for the size of our sample and the presence of gravity, but those corrections, in more subtle ways, amount to doing the same thing we did with the critical temperature: They make it easier to make the experiment agree with the theory.

There is more we could say, but the point should now be obvious: Experiments don't give clear answers; they are ambiguous, and the art of collecting and interpreting experimental data is subtle and complex.

What happens after we've done our experiment and evaluated our results? Seemingly, the first possibility is that the theory will turn out to be all wrong. We've made our measurements, and it's clear that nothing will make them come out to be two straight parallel lines. Now that's not going to be the outcome, because some of the data were available before the theory was formulated. In fact, the theory grew out of that data, so you know it is approximately true.

The next possibility is that we make our measurements, plot our data, get two straight parallel lines, write the paper, and send it off to be published.

The third possibility is that we go through all of this action — and we don't get two straight parallel lines. At that point we start examining the experiment to find out what went wrong — just as Robert Millikan did. Note that if we do get those two straight parallel lines we don't examine the data to find out what went right. That effect alone builds in a strong bias for the experimenter to get the results he wants.

You may say, "That's ridiculous. We're good Baconians; we go into the laboratory with a clean slate in our

heads. We have unprejudiced minds. We just make our measurements, and nature tells us the results — and that's all we want. Isn't that true?" And the answer is, "Of course not."

To do this experiment, to make these measurements, some guy worked 70 hours a week for a solid year. Did a passion for the dispassionate collection of data drive him to work that hard? It's nonsense to think the human animal works that way. Whatever the motives that drive us to do science, they are not the dispassionate collection of data. It follows from that that the experimenters always want something from their results, and we have to know what that is if we are going to analyze the scientific process in a reasonable way.

I think this is the way it works: When a theory first comes out, the experimenter prefers to confirm that it is correct. The reason for that is very simple. Suppose the theory comes out and you do a brilliant experiment that shows clearly, unambiguously, once and forever that the theory is wrong. Well, that's the end of the story. The theory is gone forever, and so is your experiment. On the other hand, if you show that the theory is right, you've made a contribution to the growth of knowledge, and it will be remembered and be important. So which do you want — to show that it's right or that it's wrong?

What happens over a period of time is that a number of experiments are done showing that the theory is right. After a while, the theory becomes a law of nature, a part of the received wisdom. Now, it would be really exciting to be able to show that it was wrong, to tear down a crusty prejudice standing in the way of new knowledge. If you can do that, you've made a contribution. Furthermore, all of the things that made it possible to show that it was right now make it possible to show that it was wrong.

This is the Popper stage — the stage of falsifiability — when a theory is tested and ultimately found false. Sometimes, however, all attempts to disprove the result fail, and the theory stands — as in the case of the critical point theory I have described.

That's the way I see the scientific method operating experimentally. The other part of the story is how the theories arise. Is it by the Baconian inevitable generalizations from dispassionately gathered facts or by some sort of a mystical act of creation, as Popper thinks? For an answer to that, we turn to the archivist, who will give us a historical example.

Judith Goodstein: We've talked about what two philosophers say the scientific method is, and Monsieur, the physicist, has told us how it works today — which seems to indicate that neither Bacon nor Popper is all-powerful in the minds of 20th-century scientists. How did it work in a simpler, more classical past, around the turn of the 19th century, for example?

In 1807 the English chemist Sir Humphry Davy, who had impeccable scientific credentials, isolated the chemical



Sir Humphry Davy

elements potassium and sodium and, in 1808, the metals of the alkaline earths, barium and calcium. Two years later he established the elemental nature of chlorine and predicted the existence of fluorine. Soon after, he and Gay-Lussac established iodine as a third halogen. He also did extensive and diverse other research, but did he have a scientific method?

To his public he certainly preached the methods of Bacon. "The legitimate practice, that sanctioned by the precepts of Bacon," he said, "is to proceed from particular instances to general ones, and to found hypotheses upon facts to be rejected or adopted as they are contradictory or conformable to new discoveries."

What about the genesis of Davy's ideas? Did he follow his own advice? The answer is, almost never. He held many unorthodox ideas, and he clung to them tenaciously. He embraced theories not in vogue. He speculated, for example, about the composition of ammonia and water, two compounds considered by his fellow chemists to be well established experimentally. He also argued that the chemical elements were not the simplest obtainable units of matter, and he spent many research hours trying to decompose nitrogen into a metallic base and oxygen.

This was a period of time in which the ideas of Lavoisier and Dalton dominated chemistry. Lavoisier believed that he could systematize chemistry around a simple

principle, namely oxygen, which would explain all chemical phenomena. He divided substances into elements and compounds, defining an element as any body that could not be further decomposed. He assumed, further, that elements maintained their individuality when they combined to form compounds.

Davy, on the contrary, believed that a few fundamental particles of matter composed all the simple substances that were commonly called elements. To him, Lavoisier's definition of an element did not offer any clues as to the internal nature of matter. Davy was always careful to distinguish between Lavoisier's "simple bodies" and the "true elements of bodies" — the fundamental particles of matter composing all substances.

Davy also quarreled with the atomic theory of matter proposed by John Dalton. Dalton's theory of matter incorporated the historical idea that the "ultimate particles of matter" were best expressed by the word "atom" because it signified indivisibility. His theory offered an explanation of what was going on when chemical combinations occurred. Although it was an internal explanation of the behavior of matter, it put great stress on the individuality of the elements, whose relative atomic weights were tabulated. The theory, in Davy's opinion, sacrificed the idea of a unity of matter. If there were discrete atoms for each element without any possibility of their further reduction, then the explanation of the properties of substances required as many different kinds of atoms as the number of known elements. And that number kept growing. Between 1800 and 1812 chemists added 15 new elements to the list of 18 previously known. Davy viewed this trend with alarm. Dalton's use of the term "element" in his theory precluded Davy's dream of a "real indestructible principle" of matter ever being realized.

Davy's speculations turned on his assumption that the elements of Lavoisier and Dalton were complex bodies. His announcement of the discovery of potassium and sodium was coupled with what he called a "phlogistic" theory of matter because he thought this theory better expressed his belief that the metals all contained a common substance and because he sought a simple system of chemistry. Davy's assumptions belie all of his Baconian admonitions about the role that facts play in advancing the progress of a science. The adoption of a theory which assumes that the elements are *not* simple is Davy's first requirement for chemistry's inclusion as a "true science."

Many of the experiments Davy performed after 1806 bore the mark of his search for the few fundamental particles that compose all matter. His researches were not based on random analogies. The analogies were inspired by the idea that speculations about the unity of matter must be translated into laboratory experiments.

The fact is that Lavoisier and Dalton as well as Davy indulged in speculation. All three chemists paid lip service to the Baconian idea that the scientist does not start his research by speculating and forming hypotheses. Yet, judg-

ing from the historical record, each of them allowed his work to be guided by unsupported philosophical assumptions about nature.

Well, where does that leave us? Is there a scientific method? For an answer to that question, we turn again to the physicist.

David Goodstein: It seems to me that a number of questions arise from this discussion. The first is, what would be the purpose of a theory of the scientific method that we really believed in? What would we use it for?

It certainly is not needed by the scientists. Nobody needs to tell them what to do when they go into the laboratory. They may give lip service to Bacon or even to Popper, but they don't really pay any attention to them because they know exactly what they want to do.

One purpose for which a theory of the scientific method is used is as an objective test to distinguish between sciences and pseudosciences. It gives us a way of ruling out astrology, for example, as a candidate for being a science. Of course, we don't really need it to rule out astrology as a science, but such a test becomes significant when it is applied to marginal cases as, for example, psychoanalysis. There was a seminar here on campus a couple of years ago at which a philosopher of science discussed whether psychoanalysis is a science. His analysis was purely in terms of Popper; that is, it is a science if it makes falsifiable predictions and tests them experimentally. It is not a science if it doesn't do that.

By contrast, we have the case of physics, which is treated differently from the pretenders to science. An excellent example is the critical point theory we discussed earlier. It is intrinsically unfalsifiable because we are not told just how small ΔT must be before the theory becomes valid. In a marginal science, the philosophers would rule out such a theory as being unscientific. But the physicists had no doubt they were dealing with good physics, and they proceeded to incorporate it into their body of knowledge.

I think this fact points out that the philosophers are really saying, "Science is what physics does, and other things are sciences to the extent that they do the same things that physics does. So we should figure out what physics does, and then present it so that other things can imitate it and thereby become sciences." It shouldn't need very much thought to see that it would be destructive to another field for it to force itself to follow a methodology that is nothing but a mistaken notion of what physics does.

The second question that arises is, if we don't believe Popper or Bacon gave us the true scientific method, does such a thing exist? I suppose the answer to that is yes. Furthermore, Bacon and Popper each have a piece of the truth, I think, but neither of them has cornered the market, as he thinks he has.

Something identifiable does go on in science by which some sort of empirical information gets put together; in some way theories or generalizations are formulated; and

they are then tested in some way by experiments that either prove them to be wrong — that is, falsify them — or lead to new discoveries and deeper and larger theories. That's the way science works, but that really describes everything from solid-state physics to French cooking. Is there a more precise, objective criterion that distinguishes between sciences and pseudosciences?

I think there is, and it is this: What characterizes a science is the absolute unswerving belief by its practitioners that they are dealing with laws of nature. I don't mean approximate truths or generally true things; I mean hard, real laws, whose consequences arise from direct causal links. The consequence of that belief is the conviction that if you did an experiment somebody else could repeat it and get the same result.

We've already seen that the result of an experiment is so subtle that its repeatability is in some doubt. Yet the scientist must believe in repeatability because that belief gives science its integrity. One reason a scientist doesn't cheat is that cheating obviously doesn't pay if somebody else can easily find him out by duplicating his experiment.

Let me repeat — the thing that keeps this whole balky, complicated machine on its tracks is the absolute unswerving belief by every practitioner that there are laws to be discovered. Now any philosopher can prove to you that there is no way of distinguishing between laws as constructs of the human intellect and laws that exist objectively in nature. Nevertheless, every scientist must believe in the depths of his soul that those laws exist and that the results of his experiment arise from those laws by direct causal chains that can't be broken.

I think that belief in those laws exists in physics and chemistry and in some other disciplines in which the objects of study are vastly more complex and less well understood than they are in physics and chemistry — biology, for example. Those are real sciences. On the other hand, I don't think those laws exist, for example, in psychoanalysis. Far more importantly, I don't think that the practitioners of psychoanalysis believe that they are dealing with hard laws that are connected by direct causal links to the results of what they do. And because they don't believe it, regardless of what methodology they use, what they do is not a science.

Much the same can be said for most of what we call the "social sciences," which does not mean that they are useless or unimportant. It just means they should not try to succeed by imitating physics. Real scientists sometimes pretend to have followed one or another "scientific method." In other fields, practitioners sometimes actually modify their methods in the hope of satisfying the philosophers and thereby being accepted as real scientists. All of this does little good and may sometimes do real harm. The huge success of the scientific enterprise is not due to its method but rather to the fact that its methods match its substance. There is no magical prescription for other fields of knowledge to be as successful. □

Research in Progress

Signs of Life

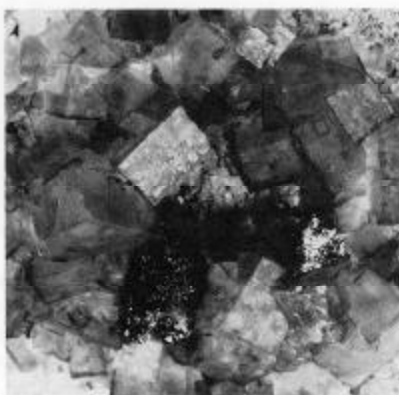
When Heinz Lowenstam, professor of paleoecology, discovered the first evidence of biologically produced magnetite ("The Case of the Iron Teeth," *E&S*, June 1964), many scientists found the idea too far-fetched to accept. But in the nearly 20 years since Lowenstam first noticed the gouge marks made by the teeth of chitons (a group of the mollusks) on rocks in a Bermuda tidepool, the iron oxide mineral magnetite has been discovered in numerous other forms of life — from bacteria to honeybees and dolphins. Recent research has also shown that magnetite in the tissues of homing pigeons acts as a compass utilizing the earth's magnetic field (*Caltech News*, August 1980).

Lowenstam and others have also found many more organically produced minerals besides magnetite, and more are being discovered all the time. Although he hasn't counted lately, Lowenstam says there are, for example, many more phosphate and carbonate minerals than previously thought, as well as numerous iron and manganese oxide minerals. Furthermore, organisms that make minerals are widely distributed throughout the five kingdoms of life — bacteria, protozoa, fungi, plants, and animals.

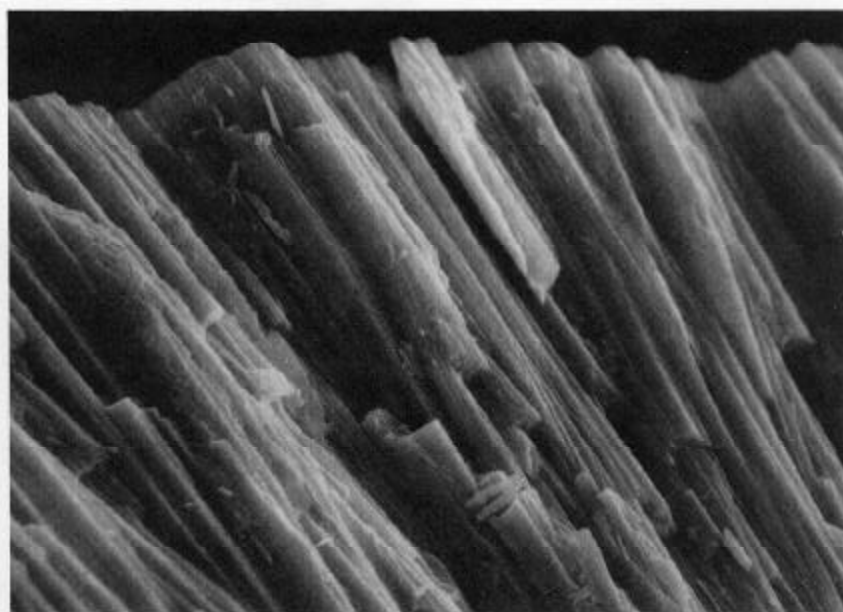
What is particularly striking about finding many of these organically produced minerals is that they shouldn't exist at all where they are formed. They are either not ever produced by inorganic processes in the biosphere or are there only in a particular environment. Magnetite, for instance, is found only in material extruded from the earth's mantle and is not actually precipitated in the biosphere except by such biomineralization processes as the chiton's teethmaking. The animal apparently accomplishes this by an enzyme-conversion process from hydrous

iron oxide (ferrihydrite), which is easily produced inorganically in the biosphere.

If certain mineral compounds cannot be easily formed inorganically, how can animals manage it? The answer seems to be that some organisms have "ion pumps," and they can concentrate and localize elements that exist in low concentrations in the external environment. The mineral compounds must be formed in an internal chemical milieu isolated from the outside environment. Some of these compounds, when exposed to the external world, dissolve in minutes. For example, the strontium sulfate mineral celestite produced in the biosphere only by the planktonic Acantharia, which create a beautiful lattice structure of the mineral, has left no



Naturally occurring fluorite (CaF_2) crystals, such as these precipitated from ore-bearing fluids, are formed only at very high temperatures and have a characteristic cube shape.



Needle-shaped fluorite crystals (magnified 250 times in this scanning electron micrograph) are biologically formed in the balancing organs (statoliths) of the opossum shrimp at less than room temperature.

fossil record because the surrounding unsaturated seawater dissolves it.

Because of the organic matrix into which these minerals fit as they are formed, they end up with crystal habits distinct from their counterparts in the physical world. They can then be distinguished from inorganically produced minerals by their morphology and, as a rule, also by their chemistry.

As a paleoecologist, Lowenstam is chiefly interested in studying the history of the evolution of life, and these biologically formed minerals often provide important clues — benchmarks at which life started to elbow its way into competition with inorganic processes in the biosphere. His recent paper, written with Lynn Margulis, professor of biology at Boston University and Sherman Fairchild Distinguished Scholar at Caltech in 1977,

challenges the commonly held view that solidly mineralized structures suddenly appeared at the end of the Precambrian Era, 580 million years ago. The two hypothesize that skeletal mineralization was initiated earlier in the late Precambrian in the form of "pinpoint" mineralization of organic hard parts. The oldest fully mineralized hard parts were calcareous throughout, indicating that this process was somehow related to improvements in calcium modulation, transport, and sequestering. The appearance of predators produced selection pressure on prey to develop more efficient nerve and muscle action, which required improvements in calcium modulation and reserves. This may have led to overshooting in calcium supply, with the excess transported to or near the body surface to initiate and later perfect skeletal mineralization.

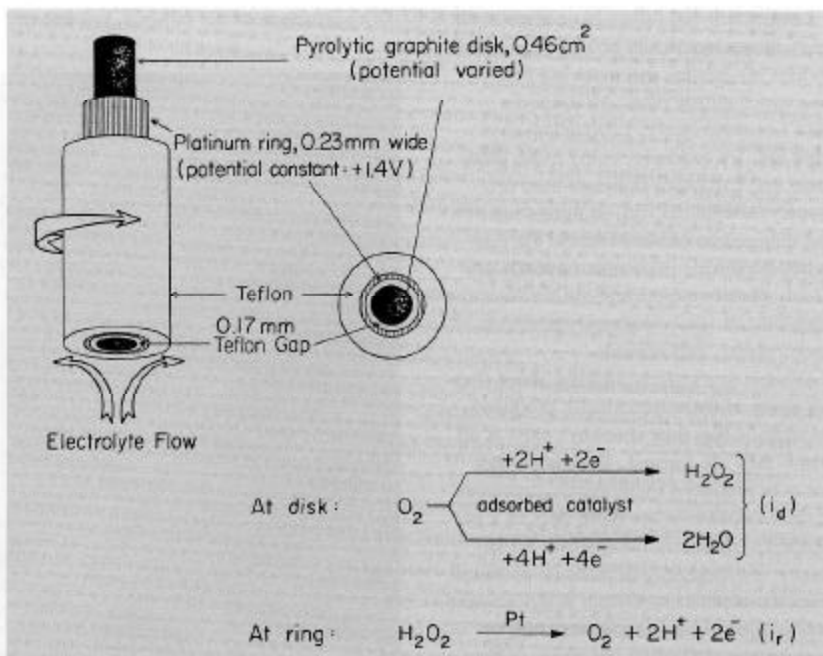
Other recently published research puts forth Lowenstam's theory that organically produced magnetite contributes significantly to the ocean floor sediments that have retained the magnetic pattern of the earth's reversing polarity.

But the applications of his work in biomineralization are not limited to the ancient history of our planet. Lowenstam also suggests that the presence of certain minerals might give a hint of the existence of some sort of life on other planets. Instead of just looking for life as we know it, scientists should perhaps instead look for minerals that "shouldn't be there." Further analysis, if it is possible, might show the presence of characteristic crystal shapes of biologically formed minerals, proving that some kind of biological process is at work in these seemingly "hostile" environments. □

Catalyst Converter

The fuel cells that powered the Apollo and Gemini spacecraft (at a cost of about \$100 per watt) were efficient, non-polluting, and easily located near the site of their use; they had no moving parts and responded well to large changes in demand. Unfortunately, \$100 per watt is somewhat steep for the average consumer of electric power. But improvements since the 1960s and the rising cost of fuels make fuel cells increasingly attractive as alternative power generating systems.

One of those improvements has been the discovery of better catalysts for the electrode reactions that occur in fuel cells. Professor of Chemistry Fred Anson and his students have been testing some of the complex molecules that have been fashioned to act as catalysts. Although these molecules may be complex, the fuel cell itself is quite simple in concept, similar to a battery. It has positive and negative electrodes immersed in an electrolyte;



A rotating ring-disk electrode assembly was used to determine catalyst efficiency. As the rod rotates, the electrolyte flows upward and outward across the electrodes. The reactions at the ring and the catalyst-coated disk are shown at right.

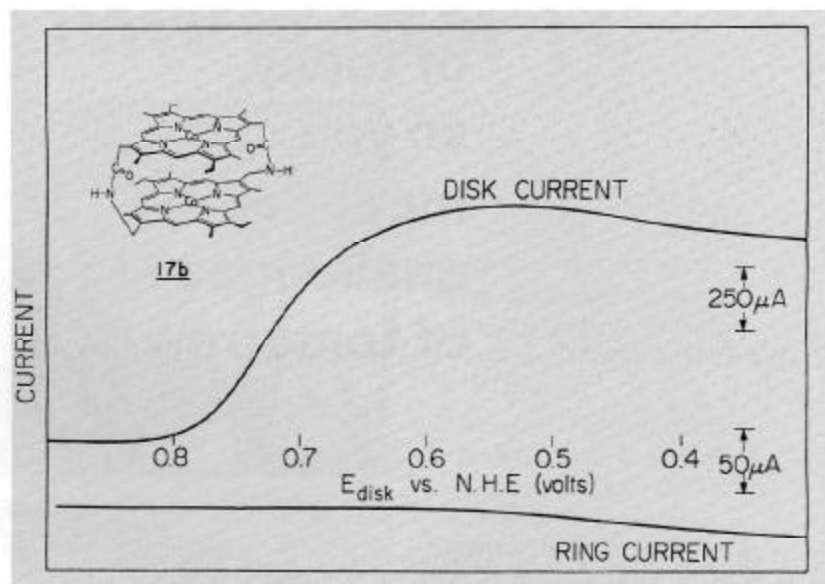
at the cathode (positive pole) it consumes oxygen from the air, and at the anode (negative pole) it consumes hydrogen produced from hydrogen-rich fuels such as hydrocarbons. The electrochemical transformations occurring at both electrodes cause oxygen and hydrogen to combine to form water, and electrons flow spontaneously from the hydrogen to the oxygen electrode through an external circuit to deliver electricity.

Problems occur in this neat arrangement at the oxygen electrode, where the chemistry is somewhat complicated. The bond must be broken between the two oxygen atoms in gaseous oxygen, and four new bonds between oxygen and hydrogen must be formed. Unfortunately, instead of proceeding to water, the reaction often stops at the point where hydrogen peroxide (H_2O_2) has been formed, which avoids breaking the oxygen-oxygen bond; but this is a wasteful reaction pathway that yields only half as many electrons. Better catalysts are needed to induce the reaction to go along the more energy-rich path to water.

Catalysts, such as the finely divided platinum used in the Apollo fuel cells and in a 4.8 megawatt pilot plant being built in New York, are expensive. A high initial cost of a catalyst might be tolerated, however, if it retained its activity while present on the surface of the electrode — where all the action is. But platinum does eventually become less active.

Devising ways to attach catalysts to the surface of the electrode was one of the first problems attacked by Anson's group at Caltech. They found that aromatic molecules (containing benzene rings) bind strongly to graphite electrodes. As a group of chemists in J. P. Collman's laboratory at Stanford synthesized possible catalyst molecules, Anson's group tested them to determine how well they clung to the graphite electrode and whether they directed the oxygen reduction reaction toward the production of water rather than hydrogen peroxide.

To break the bond in the oxygen molecule, the researchers hoped to stabilize the oxide ions being formed by letting them interact with positive metal ions. The Stanford group prepared a series of metalloporphyrins — flat, ring-shaped, aromatic molecules with a hole in the middle where metal ions, specifically cobalt, could be placed. Two of these flat molecules were strapped together "face to face" with chemical bridges.



Disk and ring current versus the potential of the graphite disk coated with catalyst — the double porphyrin molecules containing two cobalt ions and strapped together face to face by four bridge atoms. The flat curve of the ring current indicates that little H_2O_2 is being formed (and reoxidized to produce current) and the main product is the desired end, water, which gives no response at the ring.

Having aromatic character, these porphyrins stick to the graphite electrodes very nicely. To determine how efficient they are as catalysts, Anson's group used an instrument with a graphite disk electrode (coated with the catalyst) and a concentric ring electrode, both mounted on a cylindrical rod. The two electrodes are insulated from each other so that electrochemistry can be carried out separately at each electrode. Rotation of the rod about its axis causes the electrolyte to flow up and then radially across the disk and ring. Since the voltage at the ring and disk can be independently controlled, the product of oxygen reduction at the disk can be monitored at the ring. Water gives no response at the ring, while hydrogen peroxide is reoxidized so that an anodic current is detected.

The single, unbridged porphyrin molecule, when tested, yielded only hydrogen peroxide; the face-to-face molecule connected by six bridge atoms and containing two cobalt ions was an improvement but still produced a substantial amount of peroxide. But the same double porphyrin

connected by only four bridge atoms produced very little H_2O_2 , most of the reaction proceeding directly to the desired product, water.

Anson and his colleagues speculate that the four-bridge porphyrin catalyst works as it does because the two cobalt ions react rapidly with both of the oxygen atoms in the oxygen molecule as it moves inside the cavity separating the bridged porphyrin molecules. This happens only if the separation of the cobalt ions is precisely correct. There is evidence that the active form of the catalyst is that in which the oxidation state of each cobalt ion is +2. A perfect catalyst would allow each fuel cell to yield about 1.2 volts; Anson's best value is about 0.7 volt, while the target voltage for the platinum catalyzed fuel cell is 0.6 volt.

Many more experiments are necessary to improve the catalyzed reaction, but the recent progress coming from Anson's laboratory and his associates at Stanford is quite encouraging. It suggests that fuel cells may be able to supply a larger portion of our power needs in the future. □

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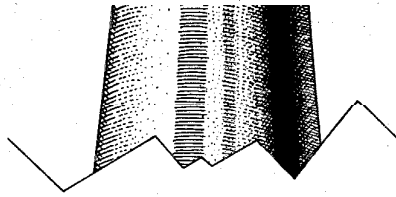
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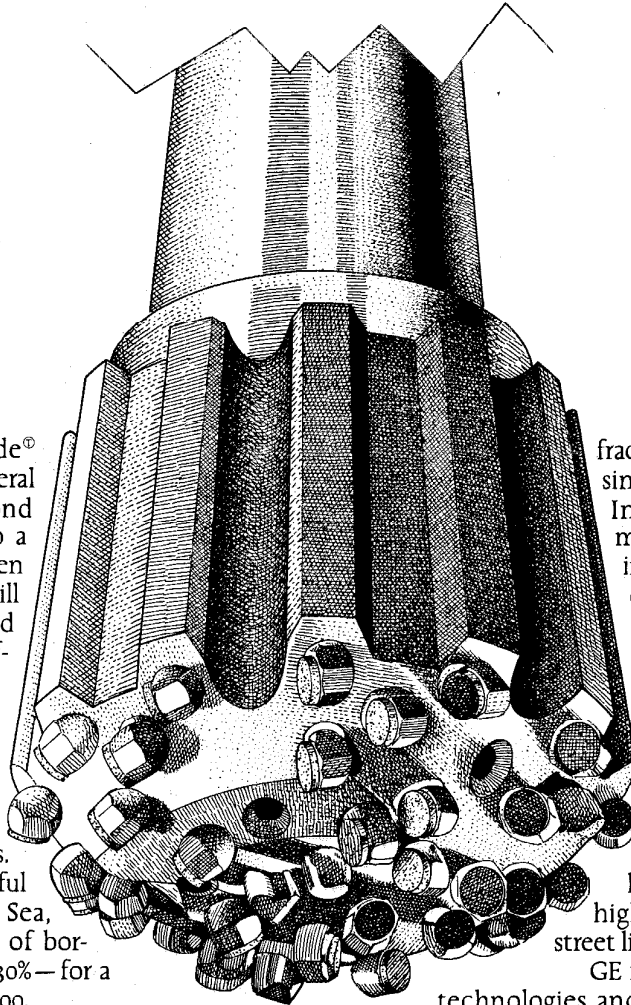
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The polycrystalline diamond blank microfractures because of its structure. Natural cleavage planes of mined diamond (right) cause it to break off in larger pieces.

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