Computing and Systems Technology Division Communications

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About This Issue

Peter R. Rony and Joseph D. Wright

This issue continues our tradition of publication of the CAST Computing in Chemical Engineering Award presentation at the Fall AIChE CAST Division banquet. Our thanks go to Jim Douglas, who provided his slides and encouraged the audio taping of his banquet presentation. Your friendly editor has now heard his talk more than anybody in the Western world; it plays well, even after the fifth hearing. The escapades of Archibald the Grim are a useful contribution to the chemical engineering archival literature; we look forward to hearing more about him from Jim.

Our feature article is a contribution from the winner of the 1987 Ted Petterson student paper award, Thomas L. Wayburn, now employed at Chemshare Corporation. We are pleased to be able to include the entire manuscript of Tom's article in this issue. On behalf of CAST members, we thank Tom for writing this special contribution to CAST Communications.

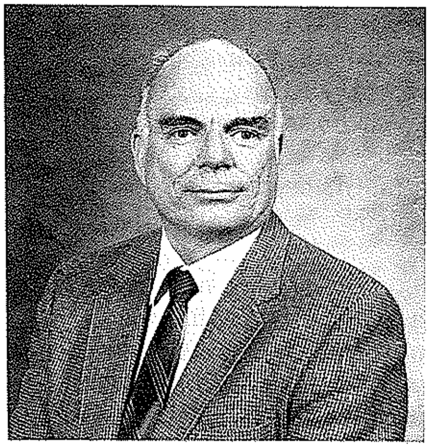
The CAST Division banquet last November was a memorable occasion. Jim Douglas was in excellent form, and two other division members received well earned awards. Your editor probably needs to make a formal apology to Dick Cavett for asking him what he did for a living, but blames the incident on his viewing of too many American Express commercials.

Your editors welcome the new CAST Division officers and wish them productive tenures in office.

Chairman's Message

W. McMaster Clarke, Olin Engineering

As I write this message, it looks like a good year for CAST. To summarize:



Awards: Joe Wright should have selections for 1988 about finished by the time that you read this. It is not too early to be thinking about nominations for 1989 awards.

Programs: Rex Reklaitis and his Chairman and Vice Chairman for each of the four (4) areas (Design, Control, Operations, and Applied Math) have plans for future AIChE meetings and for special conferences well in hand. The next conference is FOCAPD-89.

Publications: Peter Rony and Joe Wright are maintaining the quality of CAST Communications. We are trying to get AIChE approval to carry paid advertising in the Newsletter.

Membership: Like AIChE, Division membership is down, in our case to 1800 from 2000. Our new membership brochure (by Gary Blau et al) and increased promotion budget are an attempt to reverse this trend. You can help. Get out there and promote CAST membership.

Finances: We have a balance of more than one year's expenses, which is great. We are budgeting a deficit for 1988, but less than 5% of our balance. In 1987, we had a deficit of $50 in spite of the unexpected decrease of $1700 in member dues. Congratulations to Herb Britt and the entire executive committee.

Elections: Welcome to our new officers Joe Wright, 2nd Vice Chairman; Maria Burka, Secretary/Treasurer; Herb Britt and Tom McAvoy, Directors. Only about 1/3 of you voted. Let's hear from more of you in 1988.

If there is anything that CAST can do for you, or if you want to do for CAST, please contact any of our officers.

Special Acknowledgments

The Editors would like to thank Fern Lackenbauer for taking a lead role in collating and putting together the many sections of this newsletter. She did this with very little extra direction and greatly facilitated the preparation of the manuscript. Of particular note is the major amount of re-setting of equations in the article by Tom Wayburn. One of the unsolved issues of moving between word processors is adequate handling of technical type.

We also wish to thank the staff at AIChE for their valuable behind-the-scenes role in printing and distributing the newsletter each issue.

Editorial

Those Ubiquitous Computers

by Joseph D. Wright

Did you know that applications in chemical engineering of computers and computing technology were so commonplace that no one talks about them anymore? Every engineer has a computer (or access to one) these days. Don't you agree? Look around you. It's that big box-like thing beside the telephone. Who doesn't have one? The boss? His secretary? The CEO? Who? Everyone has one! Many of you have two – one at home and one at work – and crazy addicts have one for the airplane. That's where this note was written! Yet what do you do with these wondrous machines? Could you do your job without one? Why? Why not? How?

The application of computers and computing technology in chemical engineering was the topic at the recent CAST Division Board of Directors meeting in New Orleans. All agreed that without these tools chemical engineers could hardly do their jobs any more. And yet when we tried to name the most important applications of this technology in industry, there was silence. Surely the large scale system simulators are number one, was one thought. But what about pipe design systems, heat exchanger network design, individual unit operation packages for distillation, reactor design, physical property packages, finite element analyses, fault diagnoses, statistical analyses, etc., etc.? What about optimization? Everyone optimizes plant operations. What about smaller packages for mass and energy balancing using spreadsheets? What about computer control systems? How about analysis and measurement systems? Electronic mail? Report writing?

Which of you, or your engineers have made major contributions in your companies through the creative use of computing technology? Who has made a difference? What have they done? Write to us. We'd like to hear your opinions.

Virus Infects a State University's PCs

by Peter R. Rony

The appearance of computer code, called a computer virus, which has many of the characteristics of a biological virus, has started to plague organizations that have significant concentrations of computers, whether networked or not. Given below is the full text of a message that was recently published at a major state university.

"A very contagious virus has infected the local PC community. Although no cases of data loss have yet been reported, extreme caution should be exercised: the virus may permanently destroy data on diskettes and hard drives. The virus is known to have infested large diskette collections.

"A PC will become a host for the virus if it is booted from an infected diskette or hard drive. A PC will also become a host for the virus if a program that carries the virus is executed on the PC. The identify of the carrier program(s) is not yet known. Once a PC becomes a host, it will contaminate any disk it has access to.

"A disk can become infected by a host PC even if the disk is not written to. A disk can be contaminated just by looking at its directory, for example. A virus-infected PC can be detected by a conspicuous loss of 7 kilobytes of total memory. Disks infected with the virus may have a volume of "(C) Brain." However, if a disk does not have this label, it may still be infected.

Prevention

"To ensure that your PC, hard drive, and diskettes do not become infected, carefully observe the following precautions:

- TURN OFF the PC before you begin to use it. A soft reset (CTRL-ALT-DEL) is NOT sufficient.
- Boot from a diskette that is known to be clear of the virus. (A fresh copy of your original DOS diskette is best).
- Place a write-protect tab on your boot diskette and always boot from this same diskette.
- Place a write-protect tab on all diskettes except diskettes that must be written to.
- DO NOT execute a program unless you are absolutely sure it is safe.
- If you do execute a program you are not sure about, use a special test diskette containing only the unknown program. Remove all other diskettes before this program is run. When the program has completed, TURN OFF the PC before inserting any other diskettes. Boot from a diskette that is known to be clean. Format or discard the diskette containing the unknown program. NEVER test an unknown program on a system with a hard drive.
- PCs with hard drives are especially vulnerable to a virus. In general, hard drive users should keep unknown diskettes away from their PCs.

Detection

"If the directory of a diskette is viewed with the DIR command and the first line returned is:

Volume in drive D is (c) Brain

then the diskette is infected with the virus. If you do not get this message, the diskette could still be infected with the virus.

"If you suspect a diskette or a PC to be infected with the virus, the DOS utility CHKDSK can be used for diagnostic purposes. (CHKDSK.COM is a program on your original DOS diskette(s). A disk containing CHKDSK.COM must be in the default drive before the command can be executed.) Execute CHKDSK giving the drive specifier of the suspected diskette as a parameter. For example, the command,

chkdsk b:

will analyze the diskette in drive B and report the amount of memory contained in the PC.

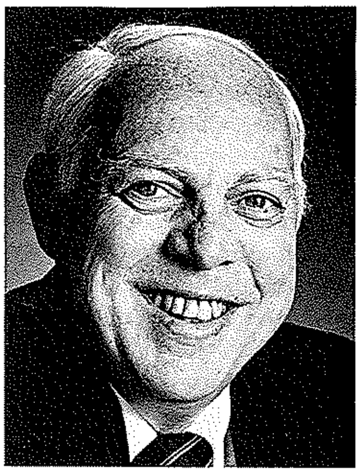
"If the diskette has bad sectors, it may be infected with the virus. Bad sectors on a hard drive are not as conspicuous since hard drives commonly have bad sectors anyway. However, if a diskette or hard drive develops bad sectors that did not previously exist, the likelihood of viral contamination is high."

"If the PC is infected with the virus, CHKDSK will report 7168 bytes less memory than that actually in the machine. Remember that a machine known to contain 256K, for example, should actually contain 256 x 1024 = 262,144 bytes as reported by CHKDSK."

A Different Perspective on Design

by James M. Douglas

1987 CAST Computing in Chemical Engineering Award Lecture



I greatly appreciate the honor of winning this award, and I would like to thank the Awards Committee. In addition, I owe a great debt to my lovely wife Betsy, for her loving support over the years, and to my colleagues at the University of Massachusetts who work in the areas of design and control – Mike Doherty, Mike Malone, Ka Ng, and Eric Ydstie – for numerous stimulating conversations.

Since the inception of this award, the winner has been asked to give a technical talk on his/her research area after the banquet dinner. As most of you know David Himmelblau won the award last year for his work in optimization theory, and, in my opinion, David gave the optimum after-dinner speech. He presented a number of cartoons illustrating the conflicts that arise when people attempt to interact with computers, and since all of us have had the same ridiculous experiences we had a good chance to laugh at ourselves.

Unfortunately, David's talk was so successful that the Awards Committee decided that all future winners would be asked to give "entertaining" talks. I must admit that in all of my professional career I never expected that I would be asked (required) to give an entertaining talk. Moreover, when I started working on a talk to present, trying to make it different and hoping that you might find it somewhat entertaining, I had no idea that Bob Cavett from Monsanto would win the industrial award and that his cousin, Dick Cavett, the widely known New York TV entertainer, would come to see his cousin presented with an award. Hence, I find myself in the bizarre position of being asked to present an entertaining talk, not only to this group but also to Dick Cavett.

The previous winners of this award in Computers and Systems Technology have received recognition for their work in computer methods, numerical analysis, optimization etc., and I am probably the first to win for research on *systems* technology. There is a much smaller group of people working in the *systems* area, as compared to computers, and so I thought that I would talk about *systems* technology, with the hope of stimulating a greater interest in this area.

However, I have recently been working with some of my graduate students, primarily Bob Kirkwood and Dave Nelson, to write a computer code that rapidly develops a conceptual design for a limited class of processes. I hope that the code will be a useful teaching tool, and so we plan to distribute it to universities through CAChE. If any of you would like to see the code, Dave Nelson will give a demonstration after my talk.

Scope of the Talk

Systems technology is a very broad concept. In order to discuss it would be beneficial if we could agree on what we mean by technology and what we mean by a system. Each of us has some *fuzzy*, intuitive notion of what these terms mean, but I intend to spend some time seeing if we can come to a more common agreement. In particular, I would like to talk a little about the impact of technology on society. Then I would like to see if we can agree about the relationship between technology and science. Both of these issues have been discussed extensively in the past twenty years, but my plan is to change the perspective of the discussion, and therefore, hopefully, to change your perspective. After this introduction, I will make some comments about *systems* technology and design, and finally, I would like to discuss how your culture influences the way that you view technology.

"High" Technology versus "Low" Technology

Almost all discussions of technology in today's popular press emphasize *high* technology, and much of the discussion seems to be centered around the idea that technology is applied science. However, to gain a better perspective of what we mean by technology I think that it is better to focus on what we might call *low* technology, and to look at technology in prehistoric times.

Archaeologists and historians make it clear that technology is as old as man. All of you have seen artifacts in the form of tools from these very early times, or artist's representations of cave men and women working with a variety of tools. In fact, historians often describe the period as "Man, the Tool Maker."

If we reflect on the lives of the people in prehistoric times, most would agree that survival demanded a relentless search for food, clothing and shelter. Moreover, there seemed to be an instinctive characteristic in men and women that led them to invent tools that helped them to cope with survival. Thus, we can say that technology does not have its roots in science, but it arises from an instinctive characteristic of men and women to invent material artifacts that help them cope with their material needs.

We still say today, "there must be an easier way to do this job," which I maintain is the essence of technology. Moreover, there is the equivalent of 'primitive' technology still practiced today, and home inventors with little formal training in either science or engineering, but a strong interest and a good understanding of how to make things work, continue to patent inventions which make others' lives easier.

It seems likely that prehistoric men and women focused on the job of surviving and not on the development of better tools, although some of them would be on the lookout for better sticks and stones that could serve their needs. Thus, new artifacts would be conceived as a complete entity and then improved by evolutionary modifications, so there was no design as we would call it today. Similarly, most artifacts had only one or two parts, so there was no *systems* technology.

Impact of Early Technology on Society

Of course, the artifacts used by man became more complex over the centuries, and these artifacts came to have a profound impact on society. I would like to mention two inventions which had a major impact that I doubt many people have thought about – the invention of Archimedes' screw and the invention of the stirrup.

Archimedes' Screw

Archimedes' screw, which probably was not invented by Archimedes, was an early screw pump that made it possible to raise the level of water, and therefore to irrigate land. According to Peter Drucker, the discovery of irrigation led to the first industrial revolution in about 5000 BC. That is, when land became irrigated, the nomadic tribes settled down in a particular area, and living together in a settlement required a complete change in society. In particular, when nomadic life was given up it became necessary to develop specialization of labor, a standing army, a codified legal system, social classes (farmers, soldiers, and a governing class), and a bureaucracy. Hence, a seemingly innocuous invention had a dramatic impact on the future of society.

Of course, many factors had to be present for the growth of the great city-states and the basic model that we still use for what we call civilization. However, it is interesting to extend Drucker's arguments to the role played by the screw pump. In addition, it always surprises me that the anti-technologists in our society don't point out the fact that technology is responsible for the establishment of bureaucracies, because bureaucracies seem to be the bane of Man's life.

The Invention Of the Stirrup

Time went on and the great city-states evolved, and then came another apparently minor invention that had a great impact on society, i.e., the stirrup. A wonderful little book by Lynn White presents the following argument. Before the invention of the stirrup a soldier had to hold a lance straight out at the end of his arm, so that when he speared his opponent he would not be knocked off of his horse. Even this fighting strategy was not very successful so that most soldiers would dismount from their horses to fight, and horses were primarily used to move troops quickly from one place to another.

However, after the invention of the stirrup, soldiers could hold their lance close to their body and spear their opponents with a straight blow. This change of fighting style caused the introduction of shock combat from horseback. As the technique was developed, the idea of adding armor to the horse and rider was adopted, but an armored cavalry also required a different type of field support. That is, a group of retainers were needed to lift the fighter onto his horse, so that each fighter needed a large support staff.

In order to develop a large, shock combat, cavalry force Charles Marte in the early 700's took land from th church, gave it to his followers, an made them nobles, with the provisio that they would fight for him when h needed them. The peasants wh worked the land would then go to wa with the noble and act as the suppo force. Thus, the dark ages we created, and a new type of society wa to last for about 1000 years, primari because of the invention of the stirru

Relationship Between Science ar Technology

Of course, science became an acti activity of mankind starting with t early astronomers and developing ir other areas. In contrast to technolo most of this scientific activity w fairly divorced from the activity of t common man until around the 160 There is a very interesting example the growing interrelationship betw technology and science that started the 1600's in James Conant's bo although it was not discussed Conant.

Scientific Discoveries

The goal of Conant's book is to m the teaching of science m interesting by presenting an histor perspective on the developmen some of the basic concepts. One chapter is entitled, "Illustrations from the 17th Century - Touching the Spring of the Air," and it is focused on the discovery of the gas laws. Conant attributes the origin of the problem to the fact that mining engineers were having difficulty in removing water from deep mines. The lift pump had been invented, but for some unexplained reason the lift pump could only lift water 34 feet.

Galileo tried to explain this problem by saying that the water column would break of its own weight after the water was raised 34 feet, similar to the way a copper wire would break when you added too much weight to the wire. However, two of Galileo's students in 1643 recognized that air pressure might provide a better explanation. In order to test their theory, they took a glass tube 3 feet long and sealed at one end, filled it with mercury, and then, while keeping a finger over the open end, turned the tube upside down in a pool of mercury. The mercury dropped down from the sealed end of the tube, so that a vacuum was created at the sealed end. The mercury did not fall down to the level of the pool but remained a little over 2 feet from the surface. The experiment demonstrated both that it was possible to create a vacuum, which everyone at that time thought was impossible, and that air had weight (the weight of the air on the surface of the pool of mercury was balancing the weight of the mercury in the column), which was generally accepted at the time but had never been measured.

With this background, Conant describes the development of vacuum pumps, the experiments that indicate that sound will not travel through a vacuum, von Guericke's wonderful experiment of the two teams of horses attempting to pull apart two hemispheres after a vacuum had been created within the sphere, etc. He also discusses Boyle's Law relating pressure and volume (1662), and Charles' Law relating temperature and volume (1787), both of which we still teach our students. Conant is a excellent writer, and his account of these scientific discoveries is truly delightful.

Technological Discoveries

However, for engineers there is another message that can be gained from Conant's account. When Conant describes the problem of removing water from deep mines he includes a woodcut from 1556 that shows that mining engineers had already solved the problem. The solution was simply to pump the water from the bottom of the mine to a pool 30 feet above the bottom. Then a second lift pump was used to pump the water up another feet to a second pool, and a third pump was used to raise it another 30 feet, and so on, until the water could be removed from the mine. Hence, the mining engineers had found a perfectly good "engineering" solution, and they had no need to rely on any solution proposed by scientists.

I think a careful examination of most of the scientific discoveries of the 1600's to 1800's came about from an attempt to explain the behavior of technological artifacts that already existed. In other words, technology led science, and the techniques used by technology were developed independently of science. It is still true today that there are significant problems in technology that do not seem to have a science base, but these problems are seldom discussed in universities.

The Current Debate

There is also a great debate going on today, related to the Amundson Report, as to whether chemical engineering should move much closer to biology, materials science, etc., and become more scientific. The debate often becomes confusing to me because there is such a great science emphasis in today's engineering curricula and so few open-ended, engineering problems are addressed, that an appropriate perspective on science vs. technology seems to have been lost. A very interesting discussion of the relationship between science and technology has been presented in the prologue and epilogue of H.G.H. Aitken's book, and I would like to raise some of the issues that he discusses.

The Primary Conflict - Understanding

I think that most would agree that the goal of physical science is to understand the nature of the physical universe. That is, scientists produce conceptual frameworks capable of explaining how nature works. In contrast, the goal of technology is to create physical artifacts (I use the word artifacts in its widest sense to include transportation networks, chemical plants, etc., as well as small, identifiable objects) that people will purchase because they make their lives easier in some way.

It is not really necessary to understand why these artifacts work the way that they do in detail, and normally we are satisfied if the behavior is reproducible, if the artifact can be made on a large scale, and if the production is profitable. For example, we still do not understand turbulent flow in detail, but most of the processes that we build have turbulent flow. Similarly, we do not understand the behavior of the internal combustion engine well enough to predict what additives will prevent knock, but we continue to make internal combustion engines. I present some examples for *high tech.* problems later, but first I want to point out some of the other similarities and differences between science and technology.

Other Similarities and Differences Between Science and Engineering

As Aitken points out, science tries to create a universal truth about the nature of the universe, independent of the culture of any society, and a scientist works to be the first to publish results that involve new understanding. In science there is a free flow of information, and the published results are meant to belong to everyone in every society. In contrast, technology tries to create new wealth, an invention belongs to the inventor, and the invention is protected by a patent. The emphasis on proprietary information and trade secrets in industry clearly demonstrates some of the profound differences between science and technology.

New results in science receive an impartial review from peers, and any qualified peer should be able to reproduce the experiments. In contrast, results in technology are reviewed by the marketplace to see if a new product is better and cheaper. In science you must be able to explain every available piece of evidence, whereas in technology understanding is not even necessary. Thus, the basic value systems are different.

It should also be noted that most of the public does not really understand the details of science. Instead, the only understanding the public has normally comes through the implementation of science in technology. Hence, the public gives science the credit for the best results of technology, but blames technology whenever unfavorable results arise. The support of science always come from donors, whereas new technology in industry is supported from the profits of previous successes.

Despite the fact that there are significant differences between science and technology there are also a large number of similarities. Both have a highly specialized division of labor, both have hierarchies of status and reputation, and both develop conceptual frameworks, although engineering science allows empirical factors to be introduced. There is a high mobility of both science and technology, and no matter what background a person has, there is a good chance of success if you are willing to compete and play by the rules of the game. Thus, even though the value systems are different, Aitken notes that science and technology are very close cousins or mirror image twins.

Understanding "High" Technology

When we consider what is called *high* technology, which includes electronic chip manufacture, biotechnology, specialty polymers, etc., we can again recognize the differences between science and technology. In most cases the discoveries were made by scientists or applied scientists in a laboratory, and the scale-up to a commercial process was undertaken by a similar group of people, although some of them had industrial experience. In most cases the scale-up was based on intuition and some experience with analogous processes. However, almost any chemical engineer who has looked at these processes would say that we do not really understand many (most) of the individual operations. The scale-up would never be considered to be a part of science, but obviously it fits our description of technology.

There is a great temptation to say that because the *designers* did not understand the phenomenon involved in the scale-up, that the processes that were developed were not as good as they could have been. In fact, almost all academic research proposals in these areas, as well as most other areas, include the statement: "If we understood it better, we could do it better." Of course, this academic statement is seldom valid, because the more we learn about a new problem, the more we realize how many more things we need to learn before we can really understand it. Hence, in most cases, the results of an academic research program are presented in terms of a request for more money to study the problem further. Additional understanding soon becomes the dominant goal, and improvements of the current technology soon become irrelevant.

Fortunately (for the US economy), industry continues to ignore 'understanding' and continues to build whatever is useful and makes a profit. If industry had waited until they completely understood all of the details of the scale-up, none of the existing products would yet be on the market. Of course, engineering academics want to understand problems better so that they can teach their students in a more rational fashion. However, this emphasis on understanding causes them to act like scientists, and often causes conflicts with industry.

"Systems" Technology

From the discussion above, we note that we do not expect *systems* technology to be a part of science. Instead, we are talking about the design of artifacts and systems that contain many subsystems. Both types of design problems date back to very early times, e.g., early war machines, the Roman aqueducts, etc. In *systems* problems we are normally concerned more with the interaction between the subsystems than the behavior of a particular subsystem. The importance of these interactions is perhaps best understood in terms of a particular example.

Building a Better Mousetrap

One of the greatest challenges of mankind in modern times has been to build a better mousetrap. In my opinion the best, or at least the most innovative, mousetrap was invented by Rube Goldberg. The first step in his trap starts when a mouse sees a magic lantern projection of a piece of Swiss cheese. When the mouse jumps up to grab the cheese it hits a projection screen and drops into a rowboat sitting in a little tub. The mouse rows around in the rowboat until it becomes seasick. When it jumps out of the rowboat, it falls into a can filled with yeast. The heat of its body then causes the yeast to rise, and the yeast lifts the mouse up until it hits its head on a steel plate. Its head gets squashed against the plate, thus softening the brain, and driving the mouse crazy. The mouse thinks it is a stream of water, runs through an available fire hose, and drops onto a round platform. The record players surrounding the platform make noises resembling a whole bunch of cats. The mouse is afraid to go over the edge of the platform, and it cannot fly, so it remains in one spot and dies of old age.

This is a typical design problem. There is a task that you want to perform, and this task can be subdivided into a number of subtasks. There are a large number of alternatives that could be used for each one of the subtasks, and the *systems* design problem is to develop a systematic procedure for finding the set of alternatives that give the best mousetrap.

It might interest you to know that Albert Einstein was Rube Goldberg's patent examiner. After handling many of Goldberg's inventions, Einstein decided to quit the patent office and become a theoretical physicist. Einstein's career path provides another illustration of the differences between attempts to develop artifacts and attempts to understand the nature of the universe. It is a perfectly natural response for anyone who was supposed to issue a patent on Rube Goldberg's inventions to dramatically change career paths.

The Saga of Archibald the Grim

I would like to consider one other design problem that illustrates the cultural bias that a society may have towards technology. I selected this example because it comes from the roots of my family history, and it is the design problem of Archibald the Grim. Archibald the Grim was the Third Earl of Douglas and Lord of Galloway in the 14th century. He was the bastard son of the Good Sir James Douglas, who won his fame because he carried the heart of Robert the Bruce to the holy land (it is difficult to imagine a more disgusting task, but times have changed).

If you know anything about Scottish history in the 14th century, the main occupation of the Scots seemed to be slaughtering their neighbors. Then, on weekends and holidays, the Scots would ride south to rape and pillage in the English border villages. Since Archibald the Grim was a bastard son, he had to become a particularly good fighter, and in fact, he was able to accumulate a considerable amount of spoils at a relatively young age. When he sought a way to protect his wealth, he decided that he needed to build a new type of castle. Thus, his design problem became:

How can I build a castle so that no matter where an enemy soldier crosses the wall, he will have to fight his way uphill?

Archibald the Grim had never seen a castle that had this desirable characteristic, so he went to the great university of the land and talked to the physicists and mathematicians of his day. In typical academic fashion, they all told him that it was impossible to build such a castle. Moreover, to show how smart they were, they gave him topological proofs showing why it was impossible. Of course, Archibald the Grim could not understand the proofs and he certainly did not want to hear that his dream was impossible. He seriously considered slaughtering all of the academics, but, instead, he stormed out of the university.

He stood fuming in the hallway when a young assistant professor followed him out and told him that he was in the wrong place. "Don't you realize that design is an art and it is not a science?" the assistant professor said. "You should not talk to scientists; rather you should talk to artists." Archibald the Grim thought that this was a hell of a good idea, and so he sponsored a nationwide art contest to design his castle. Surprise of surprises, he received a solution to his problem, which was submitted by a young artist named Escher. When you look at Escher's famous painting, Ascending and Descending, there is a continuous line of soldiers that are climbing a continuous staircase in a clockwise direction.

Some of you might have the 'feeling' that there is something wrong when you look at the picture. The reason it seems to be strange is due to a cultural bias in your background. Let me attempt to explain this cultural bias.

All of you know that Americans drive on the right-hand side of the road. The reason they do is because they are right handed. As most of you know, the Scots and the English drive on the left-hand side of the road. The reason they drive on the left is because they are right handed.

To understand the distinction that I am making here, you have to go back to an earlier culture, and to realize that the Scots and the English learned to fight on horseback with swords. A Scot had to wear his sword on his left hip, because he could not swing his right leg over the horse if the sword and scabbard were on his right hip. When two Scots wearing swords passed each other on a road, their scabbards would bang into each other if they were riding on the right-hand side. Hence, they rode on the left-hand side of the road, and today they drive on the left.

In contrast, Americans learned to fight on horseback with six shooters. They could wear their six shooters on their right hips and still mount a horse with no problem, because the six shooter is so much shorter than a sword. When Americans wearing six shooters passed each other on a road, there was a great advantage in riding on the right-hand side to make certain that your gun hand was always free. Thus, they rode on the right-hand side of the road, and today we drive on the right.

This tradition is so strong that if you walk into an American cocktail party, you notice that everyone circulates around counterclockwise (to the right to keep your gun hand free). In contrast, in Scotland or England if you go to a cocktail party, you see everyone circulating clockwise (to the left to prevent your sword scabbard from banging into that of a passerby). Now, if you look at the Escher castle again, you can understand that the reason it seems to look wrong is that Escher should have drawn the picture the other way around for an American audience, i.e., the soldiers should be climbing a continuous staircase in a counterclockwise direction. Otherwise, if an American enemy attacked Escher's castle the way he has it drawn, the American would naturally turn to the right after he had crossed the castle wall and then he would be attacking down the staircase all the way around the castle.

Conclusion

In conclusion, I would like you to consider one other Rube Goldberg invention: how to get rid of an after-dinner speaker. The session chairman, Bruce Finlayson, pulls a string, the string opens the lid on the jack-in-the-box, the jack-in-the-box pops up and hits a flashlight, and the flashlight wakes up a bird that flies away because it thinks it is morning. The bird flying away releases a balloon, the balloon rises and hits the trigger of a canon, the canon goes off and shoots a small statue of Napoleon, and the statue falls on a string. The string tilts a trough that contains a large sponge soaked with chloroform, the sponge slides down the trough and into the speaker's mouth. The speaker passes out, falls into a garbage can, and an attendant wheels him away. Before Bruce Finlayson starts to assemble the components of this invention, I think I had better sit down. Thank you for your attention.

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A Review of Continuation Methods and Their Application to Separations Problems

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Introduction

Many chemical process design problems require the solution of n nonlinear equations in n variables, e.g., simulation of separation systems. By nonlinear equations is meant equations involving algebraic and transcendental functions but not operators such as differentiation and integration.

Methods for finding the zeroes of nonlinear equations can be divided into local methods, which rely on information about the equations at particular points in their domain of definition, and global methods, which depend on some property of the equations that holds throughout their domain. The quasi-Newton methods, simplified Newton's method, and Newton's method itself are local methods; i.e., a good approximation to the solution is required as a starting point. The Levenberg-Marquardt-type methods, including Powell's dogleg method and the trust-region methods, expand the domain of attraction somewhat by combining Newton's method with the method of steepest descent, but the homotopy continuation methods are true global methods in that they utilize a genuine global property of the mapping that is preserved under homotopy, namely, topological degree. Global methods are candidates for a method that never fails.

A *homotopy*, $h(x,t)$, is a continuous blending of two functions, $f(x)$ and $g(x)$, by means of a *homotopy parameter*, t. With the exception of a few cases, where t is a natural or artificial parameter of the original equations, the homotopies discussed here belong to the class of *convex linear homotopies*, $tf(x)+(1-t)g(x)$, i.e., $h(x,t)=tf(x)-(1-t)g(x)$. Different members in this class correspond to different choices of $g(x)$. The *homotopy equation* $tf(x)+(1-t)g(x)=0$ breaks down, at $t=0$, to $g(x)=0$, an *easy problem* whose solution, x^0, is known. At $t=1$, it breaks down to $f(x)=0$, a *difficult problem* whose solution, x^*, we seek. Since the homotopy equation consists of n equations in $n+1$ unknowns, under reasonable assumptions the solution set will contain a one-dimensional component, known as a *homotopy path*, connecting x^0 with x^*.

Differential homotopy continuation is the method by which we follow the homotopy path from the solution of the easy problem to the solution of the difficult problem. (It is analogous to the way a prudent person lights a gas stove by first lighting the gas burner with a low flow rate of gas and, then, turning up the gas.) The path is followed by differentiating the homotopy equation, as first discussed by Davidenko[1] and further developed by Keller,[2] to obtain an initial-value problem (IVP), which, in the sequel, is referred to as the *Davidenko IVP*. This IVP usually solved by a predictor-corrector algorithm.

In this paper, we give a brief history of the homotopy continuation methods followed by a discussion of a number of homotopies that have been used or could be used to solve separations problems. We then illustrate a few of the many possible implementations of the method by means of two examples so small that arithmetic details can be given. Next, we review the use of homotopy continuation to solve separations problems. This is followed by a discussion of the topological theory behind the method. Some sample problems of low dimension are presented to illustrate various difficulties and how they might be overcome. Finally, some references are given to topics not covered.

Mathematical History

Embedding, homotopy, or continuation methods, referred to here as homotopy continuation methods, go back at least to the work of Lahaye,[3] who in 1934 developed numerical methods based on the theorems of Leray and Schauder[4] and Schauder.[5] In 1950, K. O. Friedrichs[6] suggested a globalization of Newton's method. Early work in this area is summarized in the 1951 review paper of Ficken,[7] who continued the work of Friedrichs and got an upper bound on the number of steps required for the classical homotopy continuation method.

Apparently Davidenko,[1] in 1953, was the first to differentiate the homotopy equation to get an initial value problem. According to Allgower and Georg,[8] the idea of stabilizing the integration of the IVP by applying Newton's method to the homotopy equation is due to Haselgrove.[9] According to Yamaguchi et al,[10] Riks[11] was the first to employ arclength parameterization, however Klopfenstein[12] appears to have had the idea earlier. These ideas were refined by H. B. Keller,[2] who imposed an additional constraint upon the problem in such a way that: (i) solutions are parameterized by an approximation to arclength, (ii) turning points "disappear," (iii) bifurcations are easy to detect, and (iv) it is easy to switch branches.

The state of the art of homotopy continuation up to about 1970 is summarized in the book by Ortega and Rheinboldt.[13] The two reviews by Wacker[14] in 1978 and by Allgower and Georg[8] in 1980 cover developments up to their respective dates.

Kubicek[15] provided a computer code, available through ACM for the price of a tape, for continuing with respect to an actual parameter of the problem. Watson, who with Fenner[16] implemented the algorithm of Chow and Yorke,[17] applied homotopy methods to a number of engineering problems.[18] Den Heijer and Rheinboldt[19] suggested selecting a local continuation parameter corresponding to the component of the tangent whose absolute value was the greatest on the previous iterate. Also, den Heijer and Rheinboldt proved that no nonzero lower bound and no upper bound for the radius of convergence of the Newton correctors can be computed from previous iterates. Rheinboldt and Burkardt[20] provided an implementation, PITCON, of the methods of Rheinboldt and his coworkers, also available from ACM, that can be employed to solve small general problems. A computer code, HOMPACK, also available through ACM, was developed by Watson, et al.[21] This code can be obtained by sending a message to NETLIB@ANL-MCS on ARPANET/CSNET as discussed by Dongarra and Grosse.[22]

Varieties of Homotopy

A number of homotopies have been applied or could be applied to the so-called MESH equations used to model distillation columns and other complex, counter-current separation devices. First we discuss the homotopies then the applications.

The simple function, $g(x)=f(x)-f(x^0)$, a root of which is x^0, leads to the Newton homotopy, $h(x,t)=f(x)-(1-t)f(x^0)$, where $f(x)$, $f(x^0)$, x, and x^0 are n-dimensional vectors, and t is a scalar. The Newton homotopy has two desirable properties: (1) it is easy to implement, and (2) the differential homotopy continuation method based on the Newton homotopy is invariant with respect to variable changes of the form $y=Ax$ and $g=Bf$. This is proved in Appendix C of Wayburn and Seader.[23]

Unfortunately, it has two undesirable characteristics: 1) The function $g(x)$ could have an even number of roots resulting in a homotopy path composed of disjoint segments that connect the roots of $g(x)$ in pairs but do not penetrate the hyperplane $t=1$. Such a $g(x)$ would not satisfy the hypotheses of the Leray-Schauder theorem, discussed in the section on theory. (2) The Leray-Schauder theorem requires also, that there be no solutions on the boundary of $\Omega \subset R^n \times [0,1]$, the domain of definition of $h(x,t)$. Unfortunately, the distillation equations are not defined for negative component molar flows and temperatures, but they could exhibit steady states with molar flows very close to zero. Therefore, the Newton homotopy, $f(x)-(1-t)f(x^0)$, could have solutions on the boundary of its domain of definition, $\Omega = D \times [0,1]$, where D is the domain of definition of the distillation equations.

These defects could be corrected by complexification. It is well known that all solutions of polynomials or equation whose leading terms behave like polynomials can be found by complexification.[24,25,26,27,28] The distillation equations may not belong to this class, but complexification could result in finding some steady-state solutions that would otherwise be missed. The idea is to write one equation for the real part and one equation for the imaginary part of each distillation equation. Then, each independent variable, molar flow or temperature is considered to have a real and an imaginary part. The number of equations and variables is doubled and each scalar in the Jacobian matrix is replaced by a 2x2 block with the elements related by the Cauchy-Riemann equations if they are continuous.

Following Garcia and Zangwill,[29] one could apply the all-solutions homotopy. In the all-solutions homotopy, the simple function, $g(x)$ with x replaced by the complex variable z, is chosen to be $g_i=(z_i)^{q(i)}-1$, $i=1,n$. It is unlikely, though, that the complexified version of the distillation equations could be shown to satisfy Garcia and Zangwills' path-finiteness conditions. Satisfying these conditions amounts to getting a handle on the algebraic degree of the distillation equations. Roughly speaking, the path-finiteness conditions require that the distillation equations behave like polynomials or have leading terms that behave like polynomials. If all solutions are to be found, the simple equations are required to have algebraic degree equal to or greater than the distillation equations on an equation-by-equation basis.

Even if the degrees could be found, the number of solutions, according to Bezout's theorem, would be so great that the homotopy paths would form a hopelessly tangled skein, incapable of being unraveled by even the most precise path-following algorithms. The step size would have to be extremely small to avoid accidentally switching to a neighboring path, and the cost of following all of the paths would be prohibitive. Moreover, by far the majority of the paths would lead to complex solutions. These are the difficulties encountered by Kearfott[30] when he attempted to find all solutions to a local minimization problem on the surface of a sphere as part of a branch switching strategy for bifurcating paths. Nevertheless, despite the tremendous amount of work necessary to complexify distillation equations including the thermodynamic property correlations, and, despite the four-fold increase in computer storage requirements, it might be worthwhile to experiment with complexification.

A simpler remedy was proposed in Ref. 31. Instead of the Newton homotopy, try the affine homotopy, discovered by Fisher et al[32] and rediscovered independently by the author. Replace the simple function of the fixed-point homotopy, $g(x)=x-x^0$, by the affine function, $g(x)=f'(x^0)(x-x^0)$. The particular form of the scaling matrix, $f'(x^0)$, recaptures the scale invariance inherited by the Newton homotopy from Newton's method itself. Moreover, if $f'(x^0)$ is nonsingular, which, by Sard's theorem, it should be for all x^0 except for a set of measure zero, $g(x)$ has a unique solution, so that homotopy paths that "turn back" to $t=0$ without penetrating the hyperplane $t=1$ are ruled out. In addition, one may replace the vector x by the vector $|x|$ whose components are the absolute values of the components of x, viz., $h(x,t)=f(|x|)+(1-t)f(x^0)$. The domain of definition of this homotopy is of the form S x [0,1], where S is a large sphere surrounding the origin in R^n. The conditions of the Leray-Schauder theorem could be satisfied in this new domain. (If the absolute value had been substituted into the Newton homotopy, the paths could return to a reflection of the starting guess in a coordinate plane. This behavior is ruled out by the uniqueness of the solution to $g(x)=0$.) Alternatively, following Lin et al,[33] one could replace each component of x, x_i, by y_i^2. This avoids the nondifferentiability of the absolute-value function, but it increases the algebraic degree.

We have not ruled out a path extending to infinity. For many problems, it is possible to show that the homotopy path is bounded for the Newton homotopy, since, in the Newton homotopy, $f(x)$ equals something that does not depend on x. Also, if x is close to x^k, $f'(x^k)(x-x^k)$ is close to $f(x)-f(x^k)$, the simple function in the restart version of the Newton homotopy, whose behavior is indistinguishable from the Newton homotopy itself; therefore, the following restart version of the affine homotopy might have interesting properties:

$$[(t-t_k)/(1-t_k)]f(x)+$$

$$+[(1-t)/(1-t_k)]f'(x^k)(x-x^k)=0$$

Restart algorithms have the advantage of using the latest information.

All of the above homotopies belong to the class of convex linear homotopies. The following example is just barely outside this class. Brunavsky and Meravy,[34] Li and Sauer,[35] and Li et al[36] employ variations of the homotopy, $h(x,t) = tf(x) + (1-t)g(x) + t(1-t)k(x)$, where, since the $k(t)$ term vanishes at both $t=0$ and $t=1$, $k(t)$ can be anything you please, perhaps something that keeps the homotopy path bounded.

Brunavsky and Meravy,[34] Li and Sauer,[35] and Li et al[36] have developed homotopies whose paths lie in projective space so that the point at infinity is an ordinary point. Their methods apply only to polynomials so far, but, perhaps, in the future, they will be applied to more general functions. We can be encouraged by the fact that every continuous function can be approximated arbitrarily closely by a polynomial.

Many investigators, including[24-28] mentioned above, are working on homotopy continuation methods to obtain all solutions. Clearly, there are tremendous difficulties, particularly if it is desired to use but one starting point. One must arrange matters so that the homotopy path has a single connected component. Homotopy paths with disjoint components can arise and multiple paths can become hopelessly tangled; nevertheless, Kuno and Seader[67] have proposed a method for selecting a starting point that is guaranteed to lie on a path that reads to all real roots.

In order to be certain that a continuation method does not encounter difficulties with physically meaningless values of variables while solving intermediate problems, a method could be designed so that the equations $h(x,t)=0$ are physically meaningful for any value of the continuation parameter. Parametric continuation methods automatically meet this requirement. For example, one could continue with respect to an actual parameter of the problem, such as the reflux ratio, R, of a distillation problem, except that t would be replaced by R and the starting guess, x^0, would be replaced by a steady-state solution of the distillation equations, which, presumably, has been obtained in some other way.

A number of investigators have introduced an artificial parameter into separations problems in order to take advantage of special characteristics of the equations. Their work is discussed in the applications section, which was taken, in some cases nearly verbatim, from Vickery's contribution to Vickery, Wayburn, and Taylor.[37] Clearly the use of problem-dependent methods can be advantageous, but the work of finding a suitable parameter will have to be repeated for each new problem type.

Implementation

In this section, a few of the many possible implementations of the homotopy continuation method are worked out in detail for two simple examples.

Path Parameterization by Homotopy Parameter

Assuming that the conditions discussed in the theory section are satisfied and the homotopy path exists, it is the object of the homotopy continuation method to follow the path from x^0, the arbitrary starting point and the zero of $g(x)$, to x^*, a desired solution of $f(x)=0$, the original problem. We shall illustrate the procedure by applying it to the very simple function plotted in Fig. 1a. Let us pretend that the problem $f(x)=x^2+3x-4=0$ is difficult to solve, but the problem $g(x)=x^2-4=0$ is easy to solve. We could embed the two functions in a homotopy by taking a convex linear combination. Thus,

$$h(x,t)=t(x^2+3x-4)+(1-t)(x^2-4)$$

or

$$h(x,t)=x^2+3xt-4 \quad , \tag{1}$$

which could have been arrived at directly by contriving to cancel out the middle term at $t=0$.

According to the implicit function theorem, if $\partial h/\partial x$, the n x n Jacobian matrix, is nonsingular on the homotopy path, Γ, then Γ can be parameterized by t, in which case the classical homotopy continuation method is guaranteed to succeed. This was proved by Wayburn[38] in Appendix 3 using the well-known Newton-Kantorovich theorem. In the classical homotopy continuation method, the interval [0,1] is broken up into N parts with $t_{i+1}-t_i=1/N$ *for* $i=0, \ldots, N$; $t_0=0$, and $t_N=1$. Newton's method is applied to $h(x,t_{i+1})=0$, $i=1, \ldots, N$, with the solution of $h(x,t_i)=0$ as a starting point. The solution of $h(x,t_0)=h(x,0)=0$ is x^0, the known solution of $g(x)=0$.

In our sample problem, the homotopy path connecting +2 to +1 and the homotopy path connecting -2 to -4 can be solved for directly as shown in Fig. 1b. The number of equations, n, equals 1 and the 1 x 1 Jacobian matrix $\partial h/\partial x=2x+3t$ is nonzero on both homotopy paths, therefore the classical homotopy method is bound to succeed. (Normally, one would not know this unless the problem were already solved.) At $t=0.5$, say, one could apply Newton's method to the equation $h(x,0.5)=x^2+1.5x-4=0$ with a starting guess of +2 and converge to the point (0.5,1.386) on the upper homotopy path in Fig. 1b. For that matter, Newton's method will converge to +1 from a starting guess of +2 and to -4 from a starting guess of -2; so t_1 could have been taken as 1. The classical homotopy method could be improved by choosing the t_i's so as to minimize computational expense.

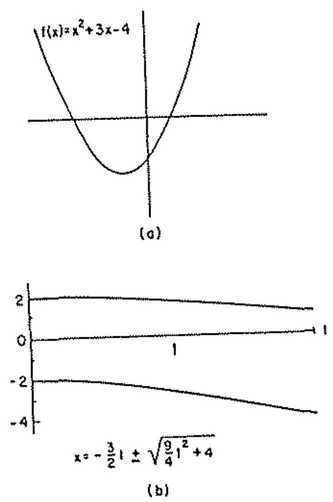


Fig. 1: For $f(x) = x^2 + 3x-4 = 0$: (a) graph of function; (b) homotopy paths with $g(x) = x^2-4$.

Strangely enough, in the case of most realistic problems, the amount of computation can be reduced substantially by converting the algebraic problem into an initial value problem (IVP) for an ordinary differential equation. Since the solution set of $h(x,t)=0$ can be parameterized by t, the homotopy equation defines, implicitly, a function $x=x(t)$. Substituting this into Eq. 1 and taking the total derivative with respect to t, we get

$$\frac{d}{dt}[h(x(t),t)] = 2x\frac{dx}{dt} + 3x + 3t\frac{dx}{dt} = 0,$$

which leads to the IVPs

$$\frac{dx}{dt} = -\frac{3x}{2x+3t}\ ,\ x(0) = \pm 2 \tag{2}$$

These can be solved analytically to obtain

$$x = -\frac{3}{2}t \pm \left(\frac{9}{4}t^2+4\right)^{\frac{1}{2}}$$

the familiar formula for the roots of a quadratic equation, which is plotted in Fig. 1b.

As long as we are pretending that $f(x)=x^2+3x-4=0$ is difficult to solve, we might just as well pretend that the IVP of Eq. 2 is difficult to solve. We could employ Gear's package, which of course would work. Alternatively, we could employ Euler's method, but that would not take advantage of the fact that we have at our disposal the actual function that was differentiated to get the IVP. We can arrange matters so that the calculation does not depend on its history and eliminate all questions of stability by applying Newton's method to the homotopy equation with the point predicted by Euler's method as a starting *guess*. We could use a higher order predictor, but the experience of many workers, cf, Salgovic et al,[39] has shown that the additional cost is not justified. Some experts disagree with this conclusion and higher-order predictors are being studied.

Returning to the general case, we differentiate the homotopy equation with respect to t while thinking of x as a function of t:

$$\frac{dh(x(t),t)}{dt} = \frac{\partial h}{\partial x}\frac{dx}{dt} + \frac{\partial h}{\partial t} = 0\ .$$

Normally, $\partial h/\partial x$ is an n x n matrix; dx/dt is an n x 1 column vector: and $\partial h/\partial t$ is an n x 1 column vector. To implement Euler's method, we need to solve the matrix equation

$$\frac{\partial h}{\partial x}\frac{dx}{dt} = -\frac{\partial h}{\partial t}$$

for dx/dt. For the case of $h(x,t)=x^2+3xt-4$, $\partial h/\partial x$ is a nonsingular 1 x 1 matrix; therefore, to solve for dx/dt, it is necessary only to divide $-3x$, the single element in the column vector $-\partial h/\partial t$, by $2x+3t$, the sole element in the 1 x 1 matrix $\partial h/\partial x$. This amounts to solving for dx/dt by Gaussian elimination. At $t=0$, we get $dx/dt=-3\times 2/(2\times 2)=-1.5$, the same as we would have gotten from Eq. 2. (In the general case, of course, it would not be feasible to compute a formula like Eq. 2, which explicitly exhibits the dependence of dx/dt on the data.) The predicted value of x is $x^0+\Delta t(dx/dt)$. This value will be used to start Newton's method. If Δt is taken to be 0.5, the predicted value of x is 1.25.

In general, the Newton correction vector, Δx, is obtained by solving the matrix equation

$$\frac{\partial h}{\partial x}\Delta x = -h(x,t)$$

The 1 x 1 Jacobian matrix of the example contains the single element $2x+3t$ evaluated at $x=1.25$ and $t=0.5$; i.e., $\partial h(x,t)/\partial x=4$. The homotopy, $h(x,t)$, evaluated at $x=1.25$ and $t=0.5$ equals -0.5625; therefore, the Newton correction is $\Delta x=0.140625$ and the corrected value of x is 1.390625, which equals the correct value up to two decimal places. Of course, one could do another Newton iteration; but, since we need an accurate computation of the homotopy path only at $t=1$, it is probably not worthwhile. To complete the procedure, one would compute the tangent vector at $x=1.39$, $t=0.5$, take another Euler step, correct with Newton's method, etc.

Path Parameterization by Arclength

The case where the function $f(x)=x^3-30x^2+280x-860$ is embedded in the homotopy $h(x,t)=f(x)-(1-t)f(x^0)$ is discussed in Wayburn and Seader.[23] Newton's method fails for this function if x^0 is less than about 12.6. Also, for choices of x^0 less than about 12.6, the homotopy paths, which are plotted in Fig. 2 for a number of choices of x^0, cannot be parameterized by the homotopy parameter, t, over their entire length. They exhibit what are known as turning points. The turning points in Fig. 2 are identified by TP.

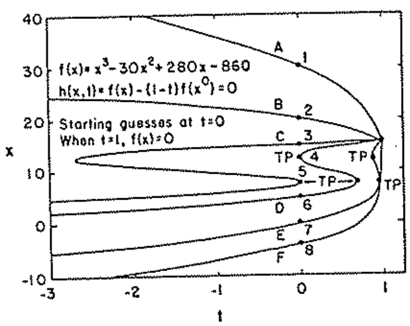


Fig. 2: Homotopy paths for $f(x) = x^3-30x^2+280x-860 = 0$ with $g(x) = f(x)-f(x^0)$.

The methods of the previous section will fail if $x^0=0$, for example, in which case the homotopy equation is $h(x,t)=x^3-30x^2+280x-860t$. To accommodate this case and other cases that exhibit turning points, x and t are taken to be functions of arclength and the homotopy equation is differentiated with respect to arclength to obtain the following IVP.

$$\frac{\partial h}{\partial x}\dot{x} + \frac{\partial h}{\partial t}\dot{t} = 0\ , \tag{3}$$

$$\dot{x}^T\dot{x} + \dot{t}^2 = 1\ , \tag{4}$$

$$x(0) = x^0\ ,$$

$$t(0) = 0\ ,$$

where dx/ds is represented by $\dot{x}$ and dt/ds by $\dot{t}$.

This IVP can be solved conveniently by a simple Euler predictor with Newton corrections in the hyperplane orthogonal to the Euler predictor. Alternatively, the Newton corrections can be taken in the hyperplane orthogonal to the coordinate axis corresponding to a suitable local parameter, which can be either t itself, or, in case $\dot{t}$ is close to zero, some x_i such that $\dot{x}_i$ is not close to zero. Even though $\partial h/\partial x$ is singular, one expects $Dh = [\partial h/\partial x \mid \partial h/\partial t]$ to be of full rank, n, because of Sard's theorem and the parameterized Sard's theorem discussed in the theory section. Identify t with x_{n+1}; let H'_{-i} be the $n+1$ x n matrix, Dh, with the i^{th} column removed; and let $\dot{x}_{-i}$ be the $n+1$-dimensional column vector $\dot{x}$ with the i^{th} component removed. Then, it is easy to show (see Ref. 23) that H'_{-i} is singular if and only if $\dot{x}_i$ is zero. In other words, far from a turning point with respect to x_i, i.e., far from a point on the homotopy path where $\dot{x}_i = 0$, H'_{-1} should be far from singular, and x_i can be used as a local parameter for purposes of solving Eqs. 3 and 4 for the unit tangent vector. Also, Newton corrections can be made safely in the hyperplane orthogonal to the x_i-axis, provided only that the predicted point lies within the tube T discussed in the theory section. (Alternatively, we could employ the deflation methods implemented by Lin et al.[33])

The above remarks can be illustrated by the example. The homotopy equation, $h(x,t) = x^3 - 30x^2 + 280x - 860t = 0$, can be differentiated with respect to arclength, s, to obtain

$$\frac{dh}{dt} = \frac{\partial h}{\partial x}\dot{x} + \frac{\partial h}{\partial t}\dot{t}$$

$$= \left[\frac{\partial h}{\partial x} \middle| \frac{\partial h}{\partial t} \right] \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix}$$

$$= \left[3x^2 - 60x + 280 \mid -860 \right] \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix} .$$

At $x=0$, $\partial h/\partial x = 280 \neq 0$. To compute the unit tangent vector, u, we first solve

$$280\,v_1 - 860\,v_2 = 0$$

corresponding to Eq. 3, where v_1 and v_2 are placeholders for $\dot{x}$ and $\dot{t}$. Since $\dot{t}$ does not vanish, we may set $v_2 = 1$. Then, $v_1 = 860/280 = 3.0714286$. Therefore,

$$u = \frac{(v_1, v_2)^T}{\|(v_1, v_2)\|} = \frac{(3.07, 1)^T}{\|(3.07, 1)\|} ,$$

which satisfies both Eq. 3 and Eq. 4.

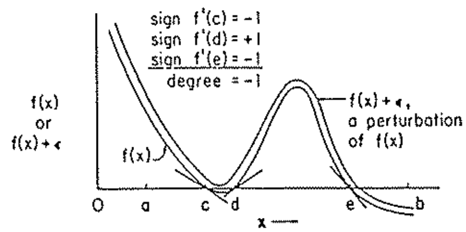


Fig. 3: Motivation for definition of degree.

Given a steplength, the Euler predictor step can be taken followed by a Newton corrections parallel to the x-axis with t fixed. This procedure can be repeated until t equals about 0.97. At $t = 0.9702634$ and $x = 7.4180111$, the 1 x 1 matrix representing $\partial h/\partial t$ is singular; i.e., $3x^2 - 60x + 280 = 0$. This is a turning point with respect to t; and, at such a point, $\dot{t} = 0$. In this one-dimensional case, it is clear that the unit tangent vector is just $(0,1)^T$; nevertheless, let us go through the formalities. We must change the local continuation parameter from $i = 2$ to $i = 1$, since x_1 is to be identified with x and x_2 is to be identified with t. The 1 x 1 matrix H'_{-1}, consisting of the single element -860, is nonsingular and the scalar $\dot{x}_1$ is nonzero. Normally, we would set v_1 equal to 1 and compute the remaining components of v other than v_{n+1}, the placeholder for t. In this one-dimensional case, there are no additional components of v (other than v_{n+1}, which is zero). Therefore,

$$u = \frac{(v_1, v_2)^T}{\|(v_1, v_2)\|} = \frac{(1, 0)^T}{\|(1, 0)\|} = (1, 0)^T$$

There are a number of stepsize algorithms[40,19,41,42] that could be used to select the length of the next step. Suppose that we decide to take an Euler step of length 0.5. The predicted value of x is $7.418 + 0.5 = 7.918$. To compute the first Newton corrector at $x = 7.918$ and $t = 0.9703$ in the direction orthogonal to the x-axis, i.e., with x fixed, we solve the *matrix* equation

$$\frac{\partial h}{\partial t}\,\Delta t = -h(x, t) .$$

Since $h(x,t) = -1.8114974$, $\Delta t = +1.8114974/(-860)$ and the corrected value of t is $0.9702634 - 0.0021064 = 0.968157$, which is equal to the correct value on the homotopy path up to calculator accuracy. Calculations can proceed with a sequence of Euler steps and Newton corrections with either x or t as the distinguished local parameter, whichever is convenient.

Applications to Separation Problems

The homotopy, which, so far, has been used most often for solving distillation equations is the Newton homotopy (Salgovic et al.,[39] Wayburn and Seader,[23] Chavez et al,[43] Lin et al,[33] Bhargava and Hlavacek,[44] Hlavacek and Van Rompay,[45] Kovach and Seider,[46,47] Frantz et al,[48,49] Ellis et al,[50] Burton,[51] Burton and Morton[52]). The first to use the Newton homotopy for problems of separation process origin were Salgovic et al.[39] They solved the homotopy equations in a number of different ways. They integrated the Davidenko IVP from x^0 at $t=0$ to x^1 at $t=1$ and, then, applied Newton's method to $h(x,1)$ starting with x^1. Also, they used a high-order differential equation solving technique and sufficiently small step sizes to ensure that, after integrating the IVP, no significant buildup of error had occurred (i.e., $x(1)$ was indeed the solution to $f(x)=0$). They found that while this method was reliable, the number of function evaluations became quite large.

Another strategy they employed was to integrate the IVP by Euler's method from x^0 at $t=0$ to x^1 at $t=1$ and then to repeat this process with x^1 as the new starting point at $t=0$. The much lower cost of doing the simple Euler predictions compensated for the required looping through the parameter value. It should be pointed out that no corrector steps were used anywhere in this algorithm.

Salgovic et al also solved their test problems switching to Newton's method to solve the final problem after a prescribed number of Euler steps for solving the homotopy equations. No correction was used for the intermediate problems; Newton's method was used to solve only the final problem. This method was found to be quite effective as long as the differential equations were solved to an appropriate accuracy. Unfortunately, the appropriate number of steps and the size of each step could not be determined a priori.

Wayburn and Seader[23] used the Newton homotopy in their solution of the MESH equations for interlinked distillation columns. They parameterized the problem in terms of the arclength of the curve being traced out in the solution space. They used an Euler step to proceed from one intermediate problem to the next and corrected the resulting estimate of the solution vector using Newton's method in the plane orthogonal to the unit normal vector at the point being considered. Problem specifications included the purity of the three product streams as well as a bottoms flow rate for the Petlyuk configuration, for which they found two solutions.

Using these same procedures, Chavez et al[43] found additional multiple solutions for a Petlyuk system and for a fractionator with side stripper used to separate a mixture of benzene, toluene, and o-xylene. While it was not possible to find all the solutions at a given reflux ratio by Newton's method, the homotopy method was successful in all cases. Lin et al,[33] using deflation methods to negotiate turning points, found all of these solutions from a single starting point. In deflation, computations are carried out in the orthogonal complement of the null vector or approximate null vector of the Jacobian of $f(x)$. Deflation methods have been developed by Stewart,[53] Keller,[54] and Chan.[55]

Bhargava and Hlavacek[44] made use of an implementation of the Newton homotopy that they found to be both effective and efficient for the nonideal problems with which they dealt. In it, they do only one Newton correction on the problems leading to the final problem to be solved. The estimate of the solution to the next problem is taken to be the result of that iteration; there is no attempt to use a predictor step to obtain the solution to the next problem (classical homotopy continuation). In their paper, they found that an even step length in the range 0.2–0.5 was sufficient to solve their problems. However, this suggestion was based upon the results of some problems that could be solved by Newton's method without any particular difficulty.

Kovach and Seider[46] used the Newton homotopy for solving azeotropic distillation problems in conjunction with another homotopy for the liquid-liquid equilibrium and three-phase equilibrium problems arising in the distillation calculations. They used the Newton homotopy to find a solution to the azeotropic distillation problems in much the same way that Wayburn and Seader did. From this solution they defined another homotopy that allowed them to look for multiple solutions to the mesh equations and, effectively, to perform parametric sensitivity calculations. This second homotopy as well as the homotopies used for the liquid-liquid equilibrium calculations fall more appropriately in the section on physically-based homotopies and will be discussed there.

Burton and Morton[52] (see, also, Burton[51]) modified an equation-oriented flowsheeting system so that the Newton homotopy could be called upon. A number of example problems involving distillation were solved using essentially the methods described by Wayburn and Seader.[23] The method was not able to find solutions in every case.

Ellis et al[50] used a parameterized form of the Newton homotopy: $h(x,t)=f(x,m)-(1-t)f(x^0,m_0)$ with $t=(m-m_0)/(m_f-m_0)$. They integrated the IVP using Euler's method and a semi-implicit Runge-Kutta method both with and without a Newton corrector. In addition, Gear's method was applied directly to solve the IVP. Step size was adjusted as the integration proceeded. The results of three test problems show that Euler's method required fewest steps, but Gear's method took the least time. The performance of the Runge-Kutta method was disappointing.

Frantz et al[48,49] and Vickery and Taylor[56,57] have also used the Newton homotopy. Their work will be discussed below.

Bhargava and Hlavacek,[44] Hlavacek and Van Rompay,[45] and Frantz et al used the homotopy $h(x,t)=f(x)-exp(-At)f(x^0)=0$, which reverts to the Newton homotopy if $1-t$ is substituted for $exp(-At)$. In fact, differentiation of this homotopy with respect to t, where x is taken to be a function of t, gives $f'(x)dx=-exp(-At)f(x^0)Adt=-Adt\ f(x)$, which shows that following the Newton homotopy path with Euler's method (and no correction) is equivalent to Newton's method with damping. (The product Adt plays the role of the damping factor.)

The affine homotopy, discussed above, has been employed by Wayburn and Seader,[31] Lin et al,[33] and Frantz et al.[48,49] It has good properties, but requires storing an extra copy of the Jacobian matrix.

Vickery and Taylor[56,57] designed a homotopy in which the K-values and enthalpies are simplified for the initial problem. Then, as the homotopy parameter is increased, the thermodynamic quantities are brought back to their original forms, until, finally, the original problem has been solved. Here, we generalize their formulation by writing

$$K_1(T,x,y,t) = (K_{i,simple})^{1-g(t)}(K_{i,actual})^{g(t)}$$

$$H(T,x,y,t)$$

$$= (H_{i,simple})(1-w(t)) + (H_{actual})w(t)$$

where $K_{i,simple}$ is a simple model for the K-value and $K_{i,actual}$ is a rigorous expression. H_{simple} is a simple model for the enthalpy and H_{actual} is the rigorous model. The functions $g(t)$ and $w(t)$ are zero at $t=0$ and one at $t=1$ but are otherwise arbitrary. Possible choices for $K_{i,simple}$ include: (i) unity, (ii) a real, positive number, different for each component, and (iii) an ideal solution K-value. Using $g(t)=w(t)=t$, Vickery and Taylor found the thermodynamic homotopy outperformed the Newton homotopy on separations problems.

Frantz et al[49] used analogous techniques in developing physically-based homotopies for application to hydrometallurgical solvent extraction models. In their work, they describe the development of custom imbedding techniques that allow a physically-realistic model for the chemical equilibrium in the process flowsheets they consider. The method they develop is shown to be superior to any of the mathematical homotopies they employed.

Since they were dealing with hetergeneous azeotropic systems, Kovach and Seider[46] had to consider liquid-liquid phase splitting. To solve these problems, they started by assuming the two phases were pure species with the remaining components added as the homotopy parameter was changed. Kovach and Seider also showed that the two-phase envelope for ternary systems could be traced easily by parameterizing the feed composition and following the phase split as the homotopy parameter is changed.

A parameter occurring naturally in the MESH equations that makes a good continuation parameter is the stage efficiency, E. The maximum separation possible on a given stage is obtained with an efficiency of unity. On the other hand, for a vanishingly small stage efficiency, the stage performs no separation worth mentioning and the streams leaving the stage have essentially the same flow rates, composition, and temperature as the combined feeds. This fact can be exploited in a continuation method. Muller[58] appears to have been the first to use the Muphree efficiency as a continuation parameter. Each problem in the sequence was solved using a stage-to-stage procedure. Sereno[59] used the efficiency as a continuation parameter for solving liquid-liquid extraction problems. Vickery et al[60] used efficiency as a continuation parameter to solve multicomponent distillation problems in single and interlinked systems of columns.

Homotopy continuation methods are quite closely related to parametric continuation methods, a class of methods in which a parameter that occurs naturally in the model equations is varied. Parametric continuation methods are most often employed to investigate the sensitivity of a model to a particular quantity. The reflux ratio and bottoms flow rate are parameters that have been used in parametric solutions of the MESH equations (Jelinek et al[61]). Parametric continuation also has also used to detect multiple solutions of the MESH equations (Ellis et al,[50] Kovach and Seider,[46] Burton[51]).

Theory

Preliminary Discussion

In this section, we show that the differential homotopy continuation method can be guaranteed to follow a homotopy path from an arbitrary starting point, x^0 (a solution of $g(x)=0$), to a solution of $f(x)=0$, provided that: (1) certain regularity conditions, discussed below, are satisfied; (2) x^0 is the unique solution of $g(x)=0$; and (3) the homotopy path does not strike the boundary of D, the domain of definition of $f(x)$ or, stated differently, there exists a bounded set E, a subset of D, such that the homotopy equation has no solutions on the boundary of E.

The vector-valued function f is a mapping from the closure of an open set D, a subset of R^n, into R^n. The problem we wish to solve can be stated mathematically as follows: Find a zero of f; i.e., find a vector, x^*, belonging to D such that f maps x^* into the n-dimensional vector all of whose components are zero. (A brief review of the few mathematical terms used in this paper is provided in Appendix A of Wayburn and Seader.[31]) Before we can discuss the homotopy continuation method and its probability of success for this general problem, we must introduce two important concepts, namely, topological degree and sets of measure zero. Topological degree is the closest one can hope to come to an actual count of the number of zeroes of f in D *that depends continuously on the mapping* f.

Topological Degree

Let f be a continuous mapping from D, a subset of R^n, into R^n; let E be an open and bounded subset of D; and let y be an arbitrary vector in R^n. In this application, y is usually taken to be the zero vector, represented in this paper by 0. Then, the degree of f with respect to E and 0, written $deg(f,E,0)$, can be motivated by looking at a one-dimensional example. Consider the function, f, plotted in Fig. 3. We would like an integer measure, that depends continuously on f, of the number of solutions of $f(x)=0$ in the open interval, $E=(a,b)$. There are no solutions of $f(x)$ on dE, the boundary of E, i.e., $f(a)\neq 0$ and $f(b)\neq 0$. Apparently a simple count of the zeroes of f is unsatisfactory as that number can change discontinuously from 3 to 2 to 1 if f is perturbed slightly.

Returning to the n-dimensional case for a moment, suppose that: (i) f is continuously differentiable on the open and bounded set, E, (ii) the closure of E is within D, the domain of definition of f, (iii) $f(x)=0$ has no solutions on dE, the boundary of E, and (iv) $f'(x)$, the $n \times n$ matrix representation of the Frechet derivative of f, is nonsingular on, ψ, the set of all x belonging to E such that $f(x)=0$. Then a valid formula for the degree of f with respect to E and 0 is

$$deg(f,E,0)=\sum_{x\varepsilon\psi} sgn\, det\, f'(x)\,. \qquad (5)$$

According to the inverse function theorem, the zeroes of f are isolated, and, since E is bounded, they are finite in number. (If there were an infinite number of zeroes, there would be at least one accumulation point, thus contradicting the fact that the zeroes are isolated.) So, the sum in Eq. 5 is well defined and can be applied to the situation in Fig. 3. The sign or signum of a real number, x, is -1 if x is negative, +1 if x is positive, and 0 if x is zero. In the one-dimensional case, the matrix representing the Frechet derivative of f consists of one real number, the slope of the tangent to the curve. Therefore, the root at c contributes -1, the root at d contributes +1, and the root at e contributes -1. So, $deg(f,E,0) = -1+(+1)+(-1)=-1$. Since the degree is nonzero, even if we know nothing else about the function, we know that there is at least one root in (a,b). If the degree had been zero, there may or may not have been a root in E.

Ortega and Rheinboldt[13] give a definition of degree that is independent of whether $f'(x)$ exists or is singular or not. This definition of degree can be shown to have a number of important properties not the least of which is invariance under homotopy. So, not only does degree theory play a role in homotopy but homotopy is crucial in developing the properties of degree. In the subsequent discussion, however, only the solution property of degree will be used.

It can be shown that, if $f(x)=0$ has no solutions in the interior of the open set E, the degree of f with respect to E and 0, written $deg(f,E,0)$, is zero. This is logically equivalent to the following: If $deg(f,E,0)\neq 0$, there exists an x belonging to E such that $f(x)=0$. This is the solution property of degree. Notice that, if $deg(f,E,0)=0$, the solution property says nothing. On the other hand, if there is a unique solution, then the degree is certainly nonzero.

We shall see, in the sequel, that, if the easy problem has a unique solution, the homotopy path is a transversal (connects the starting point to a solution rather than doubling back to $t=0$). If the converse were true, namely, that, if the solution is not unique, the homotopy path is not a transversal, we would not need the concept of topological degree. However, in many important cases, the easy problem does have multiple solutions, but the degree is nonzero and a connecting path can be found.

Sets of Measure Zero

A set of measure zero in R^n is a subset of R^n that can be contained in the union of a countable collection of little balls, themselves subsets of R^n, the sum of whose volumes is less than any positive number one can name. (The members of a countable collection bear a one-to-one correspondence with the ordinary counting numbers, 1,2,3, . . .) Clearly, a subset of a set of measure zero is itself a set of measure zero. An example of a set of measure zero is all the numbers in the computer. These are finite in number. Referring to Fig. 4, imagine that the lowest (most negative) number is contained in a small ball (an interval in R^n) of diameter $\varepsilon/2$ centered at the number, where ε is an arbitrarily small positive number. The next highest (neighboring) number is contained in an interval of diameter $\varepsilon/4$, and so on. Clearly, all the numbers in the computer are contained in a set of intervals the total volume of which is less than ε. (Remember that in R^1 volume is length.)

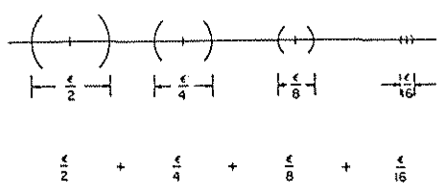


Fig. 4: A set of measure zero.

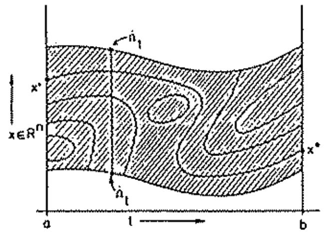
If a real number is chosen at random from the entire set of real numbers, the probability of choosing a member of a set of measure zero is zero. If the success of an enterprise depended on a member of a set of measure zero not being chosen, we could say that the enterprise would succeed with probability one. However, it is not often in real life that a process is truly random.

The Homotopy Path

The idea of the homotopy continuation method is to blend, by means of an artificial parameter, the function f whose root we seek with a function g whose root is known or can be found easily. The homotopy, $h(x,t)$, is defined on the closure of some open and bounded set Ω, a subset of R^n crossed with with the closed interval $[a,b]$, written $R^n \times [a,b]$, as depicted by the shaded region in Fig. 5. A point in Ω is represented by a vector with $n+1$ components. The first n components are those of an n-dimensional vector x belonging to R^n while the last component is a real number t belonging to the closed interval $[a,b]$. The set Ω does not have to be connected, but it usually is; so, we have drawn it as a connected set.

The homotopy equation, $h(x,t)=0$, represents n nonlinear equations in $n+1$ unknowns, the n components of x and the artificial parameter t, a scalar. A typical slice through Ω at fixed t is labelled Ω_t. We shall be interested in the boundary of Ω_t because, in the sequel, we want to rule out solutions of the homotopy equation there. The homotopy, $h(x,t)$, with $t=a$ is $g(x)$, the simple mapping. The domain of $g(x)$ is Ω_a, the intersection of Ω with $R^n \times \{a\}$, the set of all $n+1$ dimensional vectors whose $n+1$st component is a. The set Ω_a is represented by the left-hand boundary of the shaded region in Fig. 5. The homotopy, $h(x,t)$, with $t=b$ is the original function, $f(x)$. The domain of $f(x)$ is Ω_b, the intersection of Ω with $R_n \times \{b\}$, represented by the right-hand boundary of the shaded region in Fig. 5.

The curved lines within the shaded region in Fig. 5 represent a solution set of the homotopy equation, $h(x,t)=0$. This solution set corresponds to a particular choice of $g(x)$, which, in our formulation, depends on the starting point, x^0. If Dh, the total Frechet derivative of h with respect to its variables, represented by the familiar



Ω, open bounded set in $R^n \times [a,b]$

$h(x,t): \bar{\Omega} \longrightarrow R^n$ continuous

$\Omega_a = \Omega \cap R^n \times \{a\}$

$\Omega_t = \Omega \cap R^n \times \{t\}$

$\Omega_b = \Omega \cap R^n \times \{b\}$

$h(x,a) = g(x): \bar{\Omega}_a \longrightarrow R^n$ continuous

$h(x,b) = f(x): \bar{\Omega}_b \longrightarrow R^n$ continuous

$0 \in R^n$ is a regular value of h

Fig. 5: Homotopy paths in the closure of an open bounded set.

$n \times n+1$ Jacobian matrix, has full rank, i.e., at least one nonsingular $n \times n$ minor, then, according to the implicit function theorem, all of the pieces of the solution set will be smooth curves without intersections. A point where Dh has full rank is said to be a *regular point* of h. If, when Dh is evaluated at a point in Ω, every $n \times n$ minor is singular, that point is called a *critical point* of h. If the inverse image of a point y in R^n, i.e., the set of all points in Ω that are mapped by h into y, contains all regular points, then y is said to be a *regular value* of h. If the inverse image of y has at least one critical point of h, y is said to be a *critical value* of h.

The parameterized Sard's theorem states that, if h (twice continuously differentiable) is thought of as a function of x, t, and x^0, and 0 is a regular value of h when its dependence on x^0 is taken into account, then 0 is a regular value of $h(x,t)$ for all x^0 except for a set of x^0 of measure zero. Sard's theorem itself shows that, for most of the convex linear homotopies discussed above, the $n \times n$ matrix representing the derivative of h with respect to x^0 will be nonsingular for all x and t in Ω except for a set of $y^0=f(x^0)$ of measure zero; therefore, 0 can be expected to be a regular value of $h(x,t,x^0)$ and, consequently, of $h(x,t)$ for fixed x^0. Mathematically rigorous statements of Sard's theorem and the parameterized Sard's theorem are given in Appendix C of Wayburn and Seader[31] along with an elaboration of the above argument.

Even though we have encountered multiple solutions for $f(x)=0$ in chemical engineering problems, we do not expect to encounter bifurcation points (points of intersection of two or more branches) on the homotopy path if we continue with respect to an artificial parameter. On the other hand, if t represents an actual parameter of the problem, such as the reflux ratio of a distillation column, the homotopy path might contain a point of bifurcation, i.e. a point where two or more branches of the homotopy path intersect in a critical point of h. When the continuation parameter, t, represents an actual parameter of the problem, the starting point, x^0, is not an arbitrary point. On the contrary, it is a solution of a physical problem.

Now that we know that, with probability one, the solution set of $h(x,t)=0$ is composed of smooth curves, we would like to establish conditions under which one of those smooth curves connects x^0 with x^*, a desired solution of $f(x)=0$. Without loss of generality, we may specialize the interval $[a,b]$ to $[0,1]$ as shown in Fig. 6, where, in addition, the domain of h is taken to be $D \times [0,1]$, where D is the domain of definition of $f(x)$. (In order to prove theorems about degree and homotopy, it is necessary to define h on a domain as general as that of Fig. 5; but, for the purposes of the homotopy continuation algorithm, the simpler domain is adequate.)

For many problems it is possible to choose the boundary of Ω in such a way that $h(x,t)=0$ cannot have solutions on the boundary of Ω_t as t varies between 0 and 1, i.e. such that there are no solutions on the top and bottom borders of the representation of $\Omega=D \times [0,1]$ in Fig. 6. Then, the Leray-Schauder theorem, which is proved in Ref. 23, guarantees that, if there is at least one component of this solution set that starts out at $t=0$ and does not return to $t=0$, there will be a homotopy path connecting x^0 with x^*. The component that starts out at $t=0$ does not return to $t=0$; it cannot cross the sides of Ω; and, finally, the theorem shows that it cannot stop in the interior of Ω. Therefore, it must cross the hyperplane $t=1$ at a solution of $f(x)=0$.

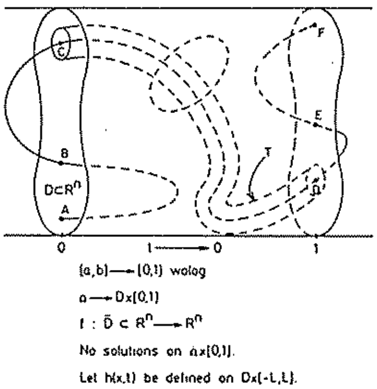


Fig. 6: Existence and regularity of a homotopy path.

A component of the solution set of $h(x,t)=0$ that starts out at $t=0$ and does not return to $t=0$ will exist if the mapping $g(x)=0$ has nonzero topological degree. If the contribution to degree from point A in Fig. 6 is $+1$, the contribution at point B must be -1, so paths like AB do not contribute to degree. Clearly, if the solution to $g(x)=0$ is unique, lies within D, and $g'(x)$ is nonsingular at x^0, then the degree of g with respect to D and 0 is nonzero (either 1 or -1). Suppose now that a path exists connecting x^0 and x^*. We would like to be certain that we can follow the path to a solution of $f(x)=0$.

Since the solution set of $h(x,t)=0$ is closed and bounded, the Heine-Borel theorem can be used to prove that the homotopy path has finite length. As we have seen, in order to follow the homotopy path, it is necessary only to be able to solve linear systems whose matrices are nonsingular $n \times n$ minors of the $n \times n+1$ Jacobian matrices that represent the total derivatives of $h(x,t)$ evaluated at various points inside a tubular neighborhood T of the homotopy path as illustrated in Fig. 6. The parameterized Sard's theorem and Sard's theorem itself lead us to expect regularity on the homotopy path. Using continuity and compactness arguments and the techniques employed in Appendix 3 of Wayburn,[38] we probably could establish the existence of a tube T of radius ε surrounding the path such that the total derivative of h has full rank and the hypotheses of the Newton-Kantorovich theorem hold in the interior of T. That is what is required to guarantee the success of our methods with probability 1, where, it must be remembered, "probability 1" has a technical meaning.

I suspect, though, that our function would be required to satisfy one more condition (in addition to being twice continuously differentiable) to prevent the path from having an infinite number of turning points. We might interpret tightly turning homotopy paths as stiffness; then, we might require that the homotopy equation, including the starting guess and with the function $f(x)$ embedded in it, not be *infinitely stiff*. Of course, highly stiff functions would be bad enough.

It should be pointed out that, sometimes, one can follow a homotopy path outside the region $D \times [0,1]$ to find a desired solution. For example, if x^0 were taken to be point A or B in Fig. 6, a desired solution could be found at point D by going through point C. Solutions at E and F could be found by extending the path beyond $t=1$.

Unfortunately, even if the above line of reasoning were made completely rigorous, there are a number of theoretical details that make it impossible to guarantee the success of the method without reservation. These details, which are discussed in Wayburn and Seader,[31] make it clear what we mean by "success with probability 1." Some of the modes of failure of the method are illustrated by the examples in the next section.

Examples

A simple, single-equation example, given by Garcia and Zangwill,[29] is shown in Fig. 7, where $f(x)=x^2-5x+6=0$, and $g(x)=x^2-1$ whose roots at $t=0$ are -1 and $+1$. The roots $+2$ and $+3$ for $f(x)=0$ at $t=1$ cannot be reached by a real homotopy path starting from $t=0$ because the solution for $h(x,t)=0$ is:

$$x = \frac{5t \pm \sqrt{25t^2-28t+4}}{2},$$

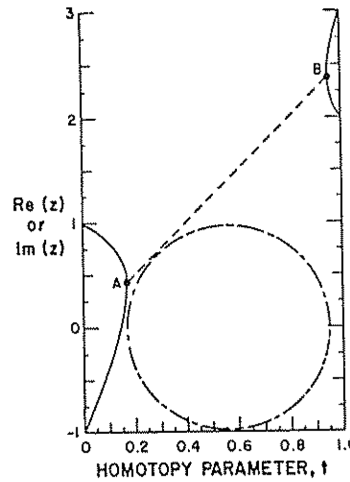


Fig. 7: Complex homotopy path for $f(x) = x^2-5x+6 = 0$ with $g(x) = x^2-1$.

which is real only in the regions $0 \le t \le 0.1681$ and $0.9519 \le t \le 1$. Thus, if only real numbers are used, the two solid-line disconnected paths result. If complex numbers are used, these two real curves are connected as shown by the dashed line for the real part and the long-dash–short-dash line for the complex part. Connecting paths can be obtained also by selecting a different function for $g(x)$, e.g., $g(x)=x-x^0$, with x a real variable. Also, for this example, the Newton homotopy with x real provides a connected homotopy path.

It is impossible to construct, for the Newton homotopy, an example in one variable that exhibits negative solutions of the homotopy equation for $0 \leq t \leq 1$, when both $x^0 = g^{-1}(0)$ and $x^* = f^{-1}(0)$ are positive. However, for two or more variables, negative solutions can occur. A simple example of this phenomenon in the case of two variables is provided by

$$f_1(x_1,x_2) = x_2 - 1 = 0$$

$$f_2(x_1,x_2) = 1.613 - 4(x_1 - 0.3125)^2$$

$$-4(x_2 - 1.625)^2 = 0 \ ,$$

with a starting point of $x_1 = 0.2$, $x_2 = 2.0$. For the Newton homotopy, two homotopy paths are obtained with the projections in the x_1 x_2*-plane* shown in Figure 8a. The left-hand path leads to the root $x_1 = 0.2$, $x_2 = 1$, but the path proceeds into and then out of the negative x_1 region. The right-hand path leads to the root $x_1 = 0.425$, $x_2 = 1$ without entering the negative x_1 region.

Let us focus our attention on the left-hand path. Suppose, for a moment, that for some reason f_1 and f_2 are undefined for negative values of x_1 and x_2, just as the distillation equations are undefined for negative, molar flows and temperatures. A hypothesis of the Leray-Schauder theorem is violated and the homotopy path runs "out the side" of the domain of definition of the homotopy rather than "out the end." A natural modification of the equations, which results in a domain of definition for the Newton homotopy equations that is symmetric with respect to the x_1t and x_2t coordinate planes, is the replacement of $f(x)$ by $F(x) = f(|x|)$, where the symbol, $|x|$, means that the absolute value of each component of f is taken separately, thus:

$$F_1(x_1,x_2) = f_1(|x_1|, |x_2|) = |x_2| - 1$$

$$F_2(x_1,x_2) = f_2(|x_1|, |x_2|) =$$

$$= 1.613 - 4(|x_1| - 0.3125)^2$$

$$- 4(|x_2| - 1.625)^2$$

To differentiate these equations with respect to arclength, for example, one takes

$$\frac{d|x_1|}{dx_1} = \begin{cases} +1, x \geq 0 \\ -1, x < 0 \end{cases} .$$

Unfortunately, if the Newton homotopy is applied to this problem with a starting point of *(0.2,2.0)*, one obtains the disconnected homotopy path whose projection is shown in Fig. 8b.

Since the chief difficulty with this path, namely, its disconnectedness, could be eliminated if $g(x)$ had a unique root, one might consider trying the fixed-point homotopy wherein $g(x) = x - x^0$. For the starting point (0.2,2.0), this leads to the connected homotopy path, whose projection is shown in Fig. 8c, but, for a starting guess of (0.01,2.3), the path goes through a turning point near $t = 0.12$, $x_1 = -0.23$, $x_2 = 2.7$, after which it heads off to infinity in the x_2 direction coming closer and closer to the $t = 0$ plane, which, of course, it can never reach.

The affine function, $g(x) = f'(x^0)(x - x^0)$, however, also has a unique root if $f'(x^0)$ is nonsingular, which, according to Sard's theorem, will be the case, except for a set of $y^0 = f(x^0)$ of measure zero. Intuitively, one expects the affine homotopy, $tf(x) + (1-t)f'(x^0)(x - x^0)$, to have good scaling properties, since, for x close to x^0, $g(x) = f'(x^0)(x - x^0)$ is approximately equal to $f(x) - f(x^0)$, which leads back to the Newton homotopy.

When this homotopy was applied, the homotopy path, whose projection (in the x_1x_2*-plane)* is shown in Fig. 8d, resulted. This path led from (0.01,2.3) to (−0.425,1.0), which, of course, is interpreted as (+0.425, 1.0), the second root of the original problem.

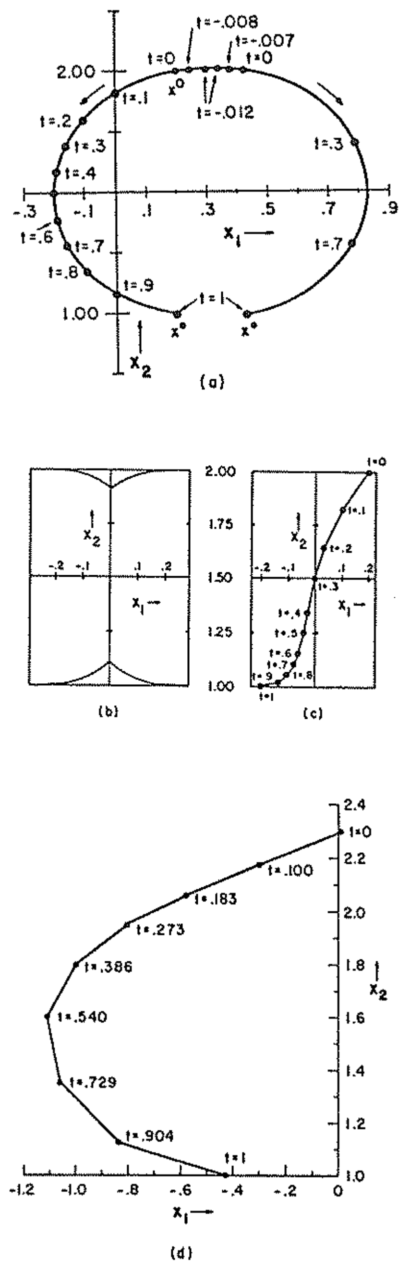


Fig. 8: Projection of the homotopy path for a two-function example: (a) Newton homotopy; (b) absolute value used in Newton homotopy; (c) absolute value used in fixed-point homotopy; (d) absolute value used in affine homotopy.

Differential homotopy continuation applied to this homotopy converged to a root of $f(x)$ from every starting point that was tried. (The starting point farthest from the root was (100,100).)

The following problem, suggested by Westerberg,[62] illustrates some of the pitfalls associated with some of the homotopies discussed above:

$$f_1(x_1,x_2)=x_1^3-30x_1^2+280x_1-860=0$$

$$f_2(x_1,x_2)=x_2^3-30x_2^2+280x_2-860=0$$

We have two completely uncoupled copies of the cubic equation discussed in the implementation section. They are to be solved simultaneously as though they were in a "black box." If the Newton homotopy is applied to a starting guess of (10,14), a homotopy path with two disjoint components results. The path on which the starting guess lies penetrates the $t=0$ plane at four points but does not cross the $t=1$ plane at all. Thus, the method will fail even though there is a perfectly good component that comes from minus infinity in the t direction, crosses the $t=0$ plane five times, and heads off to plus infinity in t after crossing the $t=1$ plane at (15.5,15.5) the correct solution to the problem. (By the way, one might reason that, if the easy problem and the difficult problem were reversed and we started at (15.5,15.5), we would not be able to obtain all solutions by following a single homotopy path.)

When the affine homotopy was applied to this problem, a path resulted that started at (10,14) (this is a requirement of the problem), went through a turning point at $t=0.69$, and went off to infinity in x_1 and x_2 while approaching the $t=0$ plane asymptotically. This is a case of not being able to find a bounded domain with no solutions on the boundary. A number of *new* homotopies were applied to this problem without success and it would be interesting to try some of the projective homotopies even though the problem was solved easily by the affine homotopy with absolute-value function.

Of Things Not Treated

Step size strategies are an important aspect of path following. We have used the algorithm of Georg.[40] Kovach and Seider[46] used the Georg algorithm but got better results with the strategy of den Heijer and Rheinboldt.[19] Other strategies have been suggested by Wacker et al[41] and Deuflhard.[42]

There are many aspects of linear equation solving that could have been discussed here. We have already alluded to the work of Stewart,[53] Keller,[54] and Chan[55] on deflation. Also, there is a recent paper by Watson.[63] The author has experimented with the so-called semi-direct methods for solving linear systems and there are a number of papers on the semi-iterative methods.[64,65,66]

A few references have been given to work in projective spaces,[34,35,36] but this interesting subject deserves more space. Are projective homotopies the wave of the future?

Acknowledgements

Most of this paper is an abstraction and extension of Wayburn and Seader.[31] The material on applications to distillation was abstracted from Vickery et al.[37] The drawings were made by Charles Marton of Potsdam, NY.

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Forum

The Editors are surprised once again that no thoughts, ideas, or items of interest were communicated by CAST members this past six months. Is anything going on out there? Does CAST mean anything to you except a $5 box to check off on your AIChE annual invoice? Are we serving your needs? Write to us. Try using electronic mail.

The Editors

Meetings and Conferences

The following items summarize information in the hands of the Editor by February 15, 1988. Please send CAST Division session information, meeting, and short course announcements to me by August 15, 1988 for inclusion in the Fall 1988 issue of CAST Communications.

Peter R. Rony,
Editor, CAST Communications

Advanced Process Control, McMaster University, Hamilton, Ontario, Canada
(May 9 - 13, 1988)

This intensive short course is intended for persons who already have a background in the basic elements of process control and who are interested in learning more advanced digital methods or in updating their knowledge in these areas. Applications are presented from the collective experience of the lecturers and provide a major emphasis for the course. Laboratories are included and cover design techniques using powerful CAD/CAE tools running on VAX and PC computer systems. Topics in the course include:

- Review of Process Dynamics and Control
- Discrete Time Process Identification
- Process Identification Laboratory
- Introduction to Discrete Control
- Introduction to Univariate Optimal Control
- Statistical Process Control
- Controller Design Workshop
- Advanced Identification and Controller Performance Evaluation
- Closed Group Identification and Controller Performance Workshop
- Plant-Wide Optimal Control
- Adaptive Control
- Tutorial on Adaptive Versus Fixed Control Strategies
- Multivariable Control
- Adaptive Control and Multivariable Design Workshop
- State Estimation and Optimal Stochastic Control

For more information call Dr. P. A. Taylor, McMaster University at (416) 525-9140, extension 4952.

International Workshop on Model Based Process Control, Atlanta
(June 13-14, 1988)

This Workshop will be concerned with the state of the art of model based process control, including but not limited to model predictive, internal model, and dynamic matrix control. The Workshop will provide a forum for the presentation and discussion of papers that describe new model based process control techniques and applications. The first day will consist of invited tutorials and industrial case studies. The second day will consist of contributed papers. The Workshop precedes the three-day 1988 American Control Conference. The registration fee is foreseen to be equivalent to 375 Swiss francs (students, 150 Swiss francs). For further details, contact Thomas McAvoy, Department of Chemical Engineering, University of Maryland, College Park, MD 20742.

1988 American Control Conference, Atlanta
(June 15-17, 1988)

The American Automatic Control Council will hold the seventh American Control Conference (ACC) on June 15-17, 1988 at the Atlanta Hilton and Towers, Atlanta, Georgia. The conference will bring together people working in the fields of control, automation, and related areas from the American Institute of Aeronautics and Astronautics (AIAA), American Institute of Chemical Engineers (AIChE), American Society of Mechanical Engineers (ASME), Association of Iron and Steel Engineers (AISE), Institute of Electrical and Electronic Engineers (IEEE), Instrument Society of America (ISA), and the Society of Computer Simulation (SCS).

Both contributed and invited papers are included in the program. The ACC will cover a range of topics relevant to theory and practical implementation of control and industrial automation and to university education in controls. Topics of interest include but are not limited to linear and nonlinear systems, identification and estimation, signal processing, multivariable systems, large scale systems, robotics and manufacturing systems, guidance and control, sensors, simulation, adaptive control, optimal control, expert systems, and control applications.

The organizing committee intends to arrange workshops to be held in conjunction with the 1988 ACC. Interested individuals should contact the Special Events Chairman, M. K. Masten, (214) 343-7695, or the General Chairman.

For further information, please contact:

Professor Duncan Mellichamp (AIChE Society Review Chairman), Department of Chemical Engineering, University of California, Santa Barbara, CA 93106, (805) 961-2821; Professor Jeffrey Kantor (Program Vice Chairman for Invited Sessions), Department of Chemical Engineering, University of Notre Dame, Notre Dame, IN 46556, (219) 239-5797; Professor Marija Ilic'-Spong (Program Vice Chairman for Contributed Sessions), Department of Electrical and Computer Engineering, University of Illinois, 1406 W. Green Street, Champaign-Urbana, IL 61801, (217) 333-4463; Professor Wayne J. Book (General Chairman), The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, (404) 894-3247; or Professor Hassan Khalil (Program Chairman), Department of Electrical Engineering and Systems Science, Michigan State University, East Lansing, MI 48824, (517) 355-6689.

International Workshop on Adaptive Control Strategies for Industrial Use, Banff, Alberta, Canada
(June 20-22, 1988)

The theme of this conference will be adaptive control strategies for industrial use. The conference will bring together engineers from industry and scientists from universities to focus attention on developments and practical enhancements for using adaptive control in industry. The objectives of the meeting are (a) to provide a three-day long forum for a tutorial introduction to the state of the art in adaptive control, (b) to focus attention on an in-depth view of the problems and needs of adaptive control engineers in industry, and (c) to transfer of current adaptive control technology from universities to industry.

The role of knowledge-based and expert systems in adaptive control will also be a theme for many sessions. The conference organizers plan for active participations from academics as well as practicing engineers from industry. The workshop program will include keynote talks and panel discussions from the leading experts in the field. Registration fees are expected to be approximately U.S. $150.00. For further details, contact Sirish L. Shah, Department of Chemical Engineering, University of Alberta, Edmonton AB, Canada T6G 2G6, (403) 432-5162 or Guy A. Dumont, Pulp and Paper Centre, University of British Columbia, 2835 East Mall, Vancouver, British Columbia, Canada V6T 1W5, (604) 224-8564.

AAAI-88 Workshop on Artifical Intelligence in Process Engineering, St. Paul, Minnesota
(August 25, 1988)

For additional details, please see the Call for Papers near the end of this issue.

Third International Symposium on Process Systems Engineering (PSE '88), Sydney, Australia
(August 28-September 2, 1988)

This Conference is being sponsored by the Institution of Chemical Engineers in Australia and the Chemical Engineering College of the Institution of Engineers, Australia, on behalf of the Asian Pacific Federation of Chemical Engineering, the European Federation of Chemical Engineering, and the Inter American Federation of Chemical Engineering. It is the third in a triennial series entitled PSE, and follows highly successful events held in Kyoto, Japan in 1982 and in Cambridge, England in 1985.

In 1988 Australia celebrates its Bicentenary, and there will be a rich calendar of events throughout the country. PSE '88 is being held in affiliation with CHEMECA 88, Australia's Bicentennial conference on Chemical and Process Engineering, sharing the opening session in the Sydney Opera House and two other plenary sessions at the Sydney Hilton Hotel, where topics of importance to the chemical engineering community will be addressed by speakers of international standing. Delegates will be able to move between the Conferences, gaining a wider appreciation of the Australasian Industry scene, as well as focusing on their particiular technical interests.

Following the tradition of the PSE series, the emphasis in 1988 will be on the presentation of new information on either technology or its application. Papers describing applications will be especially welcomed, particularly where they contain detailed information related to the value of a study.

Six technical sessions are planned, each conducted by a Chairman-Rapporteur, containing presentations of five to six papers of 30 minutes duration, including discussion. Following the successful poster session at PSE '85, a similar session is planned this time. The Conference proceedings will be published. An exhibition relevant to the themes of the Conference will run concurrently.

The main conference themes are:

Process Control and Optimisation

- Benefits Assessment
- Operator/Process Interface
- Plant-wide Systems

Artificial Intelligence

- On-Line Expert Systems
- Design/Synthesis Applications

Batch Process Design and Operation

- Including Operability Considerations
- Scheduling Applications
- Batch Process Control

Industrial Applications

- Case Studies with Benefits Through Applications of PSE

Failure Analysis in Design

- Reliability/Availability Theory for Process Systems
- Applications to Process Design
- Hazard Identification Techniques

Design of Flowsheets

- Retrofitting
- Synthesis
- Operability
- Minerals, Solids and Other Non-Petrochemical Processes

Modelling

- New Models and Algorithms
- Process Identification

Education in PSE

- Undergraduate/Postgraduate
- Continuing Education

The timetable for authors is:
April 30, 1988 Final manuscript

Thinking of Attending?

If you are considering attending PSE '88, whether or not you plan to submit a paper, please return the REGISTRATION OF INTEREST slip (duplicated below) now to ensure that you receive a copy of the Second Announcement and detailed Program.

PSE '88
Registration of Interest

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Affiliation:

Postal Address:

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The Great Barrier Reef ☐ Yes
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Central Australia ☐ Yes

Please mail to:

PSE '88 Conference
The Institution of Engineers, Australia
11 National Circuit
Barton, ACT 2600
Australia

38th Canadian Chemical Engineering Conference, Edmonton, Alberta, Canada
(October 2–5, 1988)

Papers will be presented on topics related to process dynamics, simulation and identification, applications of control theory, adaptive control, LQG control, long-range predictive and receding horizon methods, nonlinear control, and other related areas. In addition, there will be a special session on the applications of artificial intelligence and knowledge-based systems in the process industries. For further details contact R. K. Wood or S. L. Shah Department of Chemical Enginering University of Alberta, Edmonton Alberta, Canada T6G 2G6.

Washington, DC, AIChE Meeting
(November 27–December 2, 1988)

Deadlines: Abstract submission (April 15), Author selection (June 1) Manuscript submission (October 15)

Area 10a Sessions

1-2. **Process Synthesis I and II**
James M. Douglas (Co-Chairman)

Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2252 and Jeffrey J. Siirola (Co-Chairman), Eastman Kodak Compnay, P.O. Box 1972, Kingsport, TN 37662, (615) 229-3069.

3-4. **Design and Analysis I and II.** G. V. Reklaitis (Co-Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4089 and Professor Ross E. Swaney (Co-Chairman), Department of Chemical Engineering, University of Wisconsin, Madison, WI 53706, (608) 262-3641.

5. **Design of Integrated Biotechnology Process Systems.** George Stephanopoulos (Chairman), Department of Chemical Engineering 66-562, Massachusetts Institute of Technology, Cambridge, MA 02139, (617) 253-3904.

6. **Design of Polymer Process Systems.** Michael F. Malone (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-0838 and Kendree J. Sampson (Vice Chairman), Department of Chemical Engineering, Ohio University, Athens, OH 45701, (614) 593-1503.

For further details concerning Area 10a sessions and scheduling, please contact Michael F. Doherty (Area 10a Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2359.

Area 10b Sessions

1-2. **New Developments in Process Control I and II.** John W. Hamer (Co-Chairman), Research Laboratories, Eastman Kodak Company, B82 1st Floor, Rochester, NY 14650, (716) 477-3740 and Professor W. Harmon Ray (Co-Chairman), Deptartment of Chemical Engineering, University of Wisconsin, 1415 Johnson Drive, Madison, WI 53706, (608) 263-4732.

3. **Robustness and Modeling Issues in Process Control.** Professor Ahmet N. Palazoglu (Co-Chairman), Department of Chemical Engineering, University of California, Davis, CA 95616, (916) 752-8774 and Professor Jeffrey C. Kantor (Co-Chairman), Department of Chemical Engineering, University of Notre Dame, Notre Dame, IN 46556, (219) 239-5797.

4. **Unsolved Problems in Process Modeling, Optimization, Control and Operations.** Professor Christos Georgakis (Chairman), Chemical Process Modeling and Control Research Center, Lehigh University, Bethlehem, PA 18015, (215) 758-4781 and Dr. Jorge Mandler (Co-Chairman), Air Products and Chemicals, P.O. Box 538, Allentown, PA 18015, (215) 481-3413.

5. **Adaptive Control.** Professor B. E. Ydstie (Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413) 545-2388 and Professor C. Brosilow (Co-Chairman), Department of Chemical Engineering, Case Western Reserve University, Cleveland, OH 44106, (216) 368-4180.

6. **Expert Systems in Process Control.** Professor Bradley R. Holt (Chairman), Department of Chemical Engineering BF-10, University of Washington, Seattle, WA 98195, (206) 543-0554 and Dr. Carlos Garcia (Co-Chairman), Shell Development Company, Westhollow Research Center, Houston, TX 77001, (713) 493-8873.

Joint Session Between Areas 10b and 15c

7. **Control of Biochemical Systems.** Professor Karen McDonald (Chairman), Department of Chemical Engineering, University of California, Davis, CA 95616, (916) 752-0400 and Prof. Anil Menawat (Co-Chairman), Department of Chemical Engineering, Tulane University, New Orleans, LA 70118, (504) 865-5772.

For further details concerning Area 10b sessions and scheduling, please contact Yaman Arkun (Chairman, Area 10b), Department of Chemical Engineering, Georgia Tech, Atlanta, Georgia 30332, (404) 894-2871.

Area 10c Sessions

1. **The Use of Advanced Computer Architectures in Chemical Engineering Computing.** Professor Mark A. Stadtherr (Co-Chairman), Chemical Engineering Department, University of Illinois, 1209 W. California Street, Urbana, IL 61801, (217) 333-0275 and Dr. Gary D. Cera (Co-Chairman), E.I. DuPont de Nemours and Company, Experimental Station E328/162B, Wilmington, DE 19898, (302) 695-1423.

2. **Computer Integrated Manufacturing in the Process Industries.** Dr. Norman E. Rawson (Chairman), IBM Corporation, DEM-1 5078, 6901 Ruckledge Drive, Bethesda, MD 20817, (301) 564-5959 and Dr. Verle N. Schrodt (Co-Chairman), Chemical Engineering, Science Division/M5773-00, National Bureau of Standards, 325 Broadway, Boulder, CO 80303, (303) 497-6944.

3. **Advances in Optimization.** Professor Ignacio E. Grossmann (Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268-2228 and Professor Christodoulos A. Floudas (Co-Chairman), Department of Chemical Engineering, Princeton University, Princeton, NJ 08544, (609) 452-4595.

For further details concerning Area 10c sessions and scheduling, please contact Ignacio Grossmann, Department of Chemical Engineering, Carnegie Mellon University, Pittsburbh, PA 15213, (412) 268-2228.

Area 10d Sessions

1-2. **Nonlinear Analysis of Chemical Engineering Systems I and II.** Prof. Robert A. Brown (Chairman), Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, (617) 253-4571

3. **Applications of Population Balance.** Professor Doraswami Ramkrishna (Chairman), School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, (317) 494-4066 and Professor Robert Ziff (Co-Chairman), Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan 48109-2136, (313) 764-5498.

For further details concerning Area 10d sessions and scheduling, please contact Doraiswami Ramkrishna, Purdue University, School of Chemical Engineering, West Lafayette, IN 47907, (317) 494-4066.

Houston AIChE Meeting
(April 2-6, 1989)

Area 10a Sessions

1. **Applications of Expert Systems in Process Engineering.** Babu Joseph (Chairman), Department of Chemical Engineering, Washington University, St. Louis, MO 63130, (314)889-6076 and Heinz A. Preisig (Vice Chairman), Department of Chemical Engineering, Texas AM University, College Station, TX 77843-3122, (409)845-0386.

2. **Computer Aided Process Modeling and Simulation** , Lorenz T. Biegler (Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412)268-2232 and Ralph W. Pike (Vice Chairman), Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803, (504)388-6910.

3. **Bioprocess Design and Simulation: Issues and Tools.** Michael M. Domach (Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412)268-2246 and Randy Field (Vice Chairman), Aspen Technology, Inc., 251 Vassar Street, Cambridge, MA 02139, (617)497-9010.

4-5. **Retrofit Design Technique and Applications I and II.** Rajeev Gautam (Co-Chairman), Union Carbide Corporation, P.O. Box 8361, South Charleston, WV 25303, (304)747-3710 and H. Dennis Spriggs (Co-Chairman), Linnhoff March Inc., P.O. Box 2306, Leesburg, VA 22075, (703)777-1118.

For further details concerning Area 10a sessions and scheduling, please contact Michael F. Doherty (Area 10a Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413)545-2359.

Area 10b Sessions

1. **Expert Systems in Process Control**

2. **Control of Separation Operations**

Area 10c Sessions

1. **Innovative Uses of Spreadsheets in Engineering Calculations I and II.** Kris Kaushik (Co-Chairman), Shell Oil Company, P.O.Box 2099, Houston, TX 77252-2099, (713) 241-2098 and Keshava Halemane (Co-Chairman), University of Maryland, Department of Chemical Engineering, College Park, MD 20742, (301) 454-5098.

2. **Plant-Wide Use of Computers in Process Operations.** Ed Rosen (Co-Chairman), Monsanto Co. F2WK, 800 N. Lindbergh, St. Louis, MO 63167, (314) 694-6412 and Irven Rinard (Co-Chairman), City College of New York, 138th St. and Convert Ave., New York, NY 10031, (212) 690-4135.

3. **Personal Computers in Planning and Scheduling.** Mike Tayyabkhan (Co-Chairman), Tayyabkhan Consultants, 62 Erdman Avenue, Princeton, NY, 08540 and Ed Bodington (Co-Chairman), Chesapeake Decision Science, P.O. Box 275, San Anselmo, CA 94960.

4. **On-Line Fault Administration.** Mark Kramer (Co-Chairman), Dept. of Chemical Eng., Room 66-542, Massachusetts Inst. of Tech., Cambridge, MA 02139, (617) 253-6508 and V. Venkatsubramanian (Co-Chairman), Chem. Eng. & Applied Chemistry, Columbia University, New York, NY 20027, (212) 280-2561.

For further details concerning Area 10c sessions and sceduling, please contact Ignacio Grossmann, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268-2228.

European Symposium on Computer Applications in Chemical Industry, Erlangen, Federal Republic of Germany
(April 23–26, 1989)

The conference topic will be subdivided into four subject groups:

- Expert Systems and Data Bank Management Systems
- Computer Integrated Production
- Process Synthesis and Design
- New Developments in Computing

The symposium subjects will be treated in plenary papers, oral (about 40), and poster contributions, plus a round-table discussion. About 30 minutes, including discussion, will be available for every oral contribution, while the time foreseen for the display of posters will be one day. The final decision on oral or poster presentations will reside with the Scientific Symposium Committee.

Authors wishing to present a contribution are asked to submit an abstract of about 300 words (1 page) by April 1, 1988. Other deadlines are:

End of **June 1988:** Information to authors about the acceptance of their contribution.

End of **October 1988:** Distribution of Program.

December 1, 1988: Submission of 6-page manuscripts by authors (including tables, figures, references) ready for offset printing

All manuscripts will be printed and published in one volume and be available for distribution to all symposium participants at the beginning of the meeting. A number of facilities will be available at the symposium for the demonstration of programs and data banks. Interested persons are invited to inform the organizers about their participation by October 1988. Further details will be worked out on the basis of requests received and will be communicated at the beginning of 1989. The symposium language will be English.

The symposium is organized by DECHEMA Deutsche Gesellschaft fur Chemisches Apparatewesen, Chemische Technik und Biotechnologie e.V., Frankfurt am Main in collaboration with members of the Dechema-Fachausschuss Anwendung elektronischer Rechengerate in der Chemischen Technik, and members on the Working Part on use of Computers in Chemical Engineering of the European Federation of Chemical Engineering.

Correspondence and Secretariat: DECHEMA, Attention Mrs. L. Schubel, P. O. Box 97 01 46, D-6000 Frankfurt am Main 97, West Germany. Phone (069) 75 64-235/209.

Foundations of Computer-Aided Process Design (FOCAPD'89) (July 9-14, 1989)

Jeffrey J. Siirola (Chairman), Eastman Kodak Company, P.O. Box 1972, Kingsport, TN 37662, (615) 229-3069 and Ignacio E. Grossmann (Co-Vice Chairman), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268-2228, and George Stephanopoulos (Co-Chairman), Department of Chemical Engineering 66-562, Massachusetts Institute of Techechnology, Cambridge, MA 02139, (617) 253-3904.

Eight sessions are planned. Conference themes include: Design Theory and Methodology, Artificial Intelligence, New Design Environments, Process Synthesis, Mathematical Techniques, Process Simulation and Analysis, Applications of Supercomputers, Chemical Product Design, and Future Outlook.

San Francisco AIChE Meeting (November 5-10, 1989)

Area 10a Sessions

1-2. **Process Design and Analysis I and II.** Krishna R. Kaushik (Chairman),Shell Oil Company, P.O. Box 2099, Houston, TX 77252, (713) 241-2098.

3-4. **Advances in Process Synthesis I and II.** Christodoulos A. Floudas (Co-Chairman), Department of Chemical Engineering, Princeton University, Princeton, NJ 08544, (609) 452-4595 and Don Vredeveld (Co-Chairman), Union Carbide Corporation, P.O. Box 8361, South Charleston, WV 25303, (304) 747-4829.

5. **Computer-Aided Design of Batch Processes.** Iftekhar Karimi (Chairman), Departmenty of Chemical Engineering, Northwestern University, Evanston, IL 60201, (312) 491-3558 and Girish Joglekar (Vice Chairman), Batch Process Technologies Inc., P. O. Box 2001, West Lafayette, IN 47906, (317) 463-6473.

6. **Simulation of Chemical Processes in the Electronics Industry** (Chairman to be Confirmed).

Joint Areas 10a and 10b Session

1. **Integration of Process Design and Control**, Heinz A. Preisig (Chairman), Department of Chemical Engineering, Texas AM University, College Station, TX 77843-3122, (409) 835-0386 and Ahmet Palazoglu (Vice Chairman), Department of Chemical Engineering, University of California, Davis, CA 95616, (916) 752-8774.

For further details concerning Area 10a sessions and scheduling, please contact Michael F. Doherty (Area 10a Chairman), Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003, (413)545-2359.

Area 10c Sessions

Scheduling and Planning of Process Operations I and II. Ignacio Grossmann (Co-Chairman) and Peter Clark (Co-Chairman).

Statistics and Quality Control I and II. Gary Blau (Co-Chairman) and Dick Mah (Co-Chairman).

Advances in Knowledge Representation. Mark Kramer (Co-

Chairman) and Gary Cera (Co-Chairman).

For further details concerning Area 10c sessions and scheduling, please contact Ignacio Grossmann, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, (412) 268-2228.

New Orleans AIChE Meeting
(March 4-8, 1990)

Chicago AIChE Meeting
(November 11-16, 1990)

CALLS FOR PAPERS

AAAI-88 Workshop on Artifical Intelligence in Process Engineering, St. Paul, Minnesota

(August 25, 1988)

Several efforts have been undertaken in the use of Artificial Intelligence in Process Engineering. They include design of process flowsheets, design of chemical or biochemical pathways, design of separation systems, planning of process operations, diagnosis of process faults, analysis of process trends, qualitative simulation, control of processes, etc. Chemical and biochemical processing systems have some special characteristics that make them a challenging domain for Artificial Intelligence research:

- They involve physical systems that share a network-like structure with analog or digital circuits, but the behavior of each component is, in general, much more complicated. For example, the operation of a flash drum or a distillation column depends strongly on nonlinear thermodynamic properties of mixtures.
- Information available on the systems is often qualitative in nature. Challenges arise in the representation of available knowledge at different qualitative levels.
- One never has all the information relevant in carrying out a particular task. One must use partial information aggressively to derive partial results, which are valuable in determining what other information should besought.
- Many tasks, like diagnosis, monitoring, and control, need to be carried out in real time.

Thus, chemical and biochemical processing systems are a fertile domain for the development and testing of methods for dealing with qualitative and incomplete knowledge, reasoning about highly non-ideal real-world systems, and reasoning in real time. This workshop will help both the AI community and the process engineering community evaluate the current state of the field, explore future directions, and initiate joint efforts. We invite papers focusing either on a particular process engineering problem (addressed through AI methods), or a particular AI methodology as it applies to process engineering problems.

The workshop's organizing committee consists of:

Michael Mavrovouniotis (Chairman),
Massachusetts Institute of Technology

George Stephanopoulos
Massachusetts Institute of Technology

Venkat Venkatasubramanian
ColumbiaUniversity

Jim Davis
Ohio State University; and

Rama Lakshmanan,
Massachusetts Institute of Technology.

The Workshop will be held on August 25, 1988, in St. Paul, Minnesota, as part of the National Conference on Artificial Intelligence (AAAI-88). To participate in the workshop, please submit 3 copies of an extended abstract, not longer than 1000 words, including key figures and references, by May 15, 1988. The submissions will be reviewed by members of the organizing committee; authors will be notified of acceptance or rejection by June 15, 1988.

Send submissions to Michael Mavrovouniotis, Chairman, AAAI-88 Workson on AI in Process Enginering, Massachusetts Institute of Technology, Room 66-056, 77 Massachusetts Avenue, Cambridge, MA 02139.

CAST Sessions at AIChE Annual Meeting, Washington D.C.

(November 27-December 2, 1988)

The CAST Division is planning the following sessions at the Washington D.C. meeting:

Area 10a: Computers in Process Design

- Process Synthesis I and II
- Design and Analysis I and II
- Integrated Biotechnology Process Systems
- Polymer Process Design

Area 10b: Computers in Process Control

- New Developments in Process Control I and II
- Robustness and Modeling Issues in Process Control
- Control of Biochemical Systems (joint with Area 15c)
- Unsolved Problems in Process Modeling, Optimization, Control, and Operations
- Adaptive Control
- Expert Systems in Process Control

Area 10c: Computers in Operations and Information Processing

- The Use of Advanced Computer Architectures in Chemical Engineering I and II
- Computer Integrated Manufacturing in the Process Industries
- Advances in Optimization

Area 10d: Applied Mathematics

- Applications of Population Balance
- Nonlinear Analysis of Chemical Engineering Systems I and II

The names, addresses, and telephone numbers of the session chairpersons are given on the next several pages, as are brief statements of the topics to receive special emphasis in soliciting manuscripts for these sessions. Prospective session participants are encouraged to observe the following deadlines:

June 1, 1988: Session chairman reviews Proposals to Present forms, selects speakers.

July 1, 1988: Session chairman submits final session information to Meeting Program Chairman, also sends Presentation Acceptance forms (with extended abstract mat) to speakers.

Sept. 15, 1988: Speakers submit typed abstracts to Session chairman.

Oct. 1, 1988: Session chairman submits abstracts to New York.

Nov. 1, 1988: Speakers submit manuscripts to session chairman.

Nov. 15, 1988: Session chairman submits manuscripts to New York in order to be available for on-site sale.

Nov. 27, 1988: If Nov 15, 1988 deadline is not, bring manuscript to Washington D.C. to be available for on-site sale.

All of these sessions have been confirmed by the Meeting Program Chairman, Henry A. McGee. We are repeating the Call for Papers first published in the Fall 1987 newsletter.

Process Synthesis I and II

Papers are solicited in all areas of chemical process synthesis including design theory, new approaches and techniques, and applications in heat integration, separation trains, reactor networks, and overall flowsheets in both grassroots and retrofit situations, and the like.

Chairman

Prof. James Douglas
Department of Chemical
Engineering
University of Massachusetts
Amherst, MA 01003 (413)
545-2252

Design and Analysis I and II

This session seeks contributions in all areas of application of computing and systems technology to process design and analysis. Topics of special interest include: design under uncertainty, design of batch operations, reliability and availability analysis, design for operability, retrofit design, applications of reduced order models in design, as well as quantitative methods for selecting the layout of process equipment.

Chairman

Professor G.V. Reklaitis
School of Chemical
Engineering
Purdue University
West Lafayette, IN 47907
(317) 494-4089

Co-Chairman

Professor Ross E. Swaney
Department of Chemical
Engineering
University of Madison
Madison, WI 53706
(608) 262-3641

Integrated Biotechnology Process Systems

Papers are solicited in the general area of development, design, operations and/or control of integrated biotechnological systems. The term 'integrated' is used to indicate that the focus of this session is not on the analysis or design of individual units, but that its emphasis is on the unique aspects arising from the integration of several units into a cohesive biotechnological process. Typical examples include:

(a) Interaction between bioreactors and downstream processing systems. (b) Analysis, design, operation and control of the downstream processing system, usually composed of several units. (c) Integrated batch plants carrying out a number of different bioproduction lines.

Chairman

Professor George Stephanopoulos
Department of Chemical Engineering
Massachusetts Institute of Technology
Room 66-562
Cambridge, MA 02139
(617) 253-3904

Polymer Process Design

Studies which focus on processes for polymer production or for the processing of polymeric materials are of interest. The topics may include but need not be limited to: equipment design, the interactions between design and control, physical property measurement and prediction for design, and especially systems interactions in polymer processes.

Chairman

Professor M.F. Malone
Dept. of Chemical Engineering
University of Massachusetts
Amherst, MA 01003
(413) 545-4869

Co-Chairman

Professor K. Sampson
Dept. of Chemical Engineering
Ohio University
Athens, OH 45701
(614) 593-1503

New Developments in Process Control I and II

Papers are invited which demonstrate advances in process control, including advances in the areas of:

- multivariable control
- nonlinear control
- self-tuning and adaptive control
- control of nonsquare systems
- control of heat-integrated processes
- on-line optimizing control

Papers demonstrating advances in the application of process control are also invited.

Co-Chairman

John W. Hamer
Research Laboratories
Eastman Kodak Co.
B82 1st Flood
Rochester, NY 14650
(716) 477-3740

Co-Chairman

Professor W. Harmon Ray
Dept. of Chemical Engineering
University of Wisconsin
1415 Johnson Drive
Madison, WI 53706
(608) 263-4732

Robustness and Modeling Issues in Process Control

This session is intended to address issues of process modeling in control design and analysis. Relevant topics include

- Model identification and reduction
- Characterization of modeling errors in the time and frequency domains,
- Robust control synthesis
- Control analysis of linear and nonlinear process models,
- Incorporation of process models into controller implementations.

Theoretical studies, practical applications and relevant case studies are solicited.

Co-Chairman

Professor Ahmet N. Palazoglu
Dept. of Chemical Engineering
University of California
Davis, CA 95616
(916) 752-8774

Co-Chairman

Professor Jeffrey C. Kantor
Dept. of Chemical Engineering
University of Notre Dame
Notre Dame, IN 46556
(219) 239-5797

Control of Biochemicals Systems
(Joint Session Between Areas 10B and 15C)

The scope of this session includes experimental and theoretical studies involving new on-line monitoring techniques, dynamic process modeling and novel control strategies for bioreactors or downstream processing units. Topics may include applications of new biosensors for bioprocess control, state and parameter estimation techniques, dynamic model development for microbial or cell culture bioreactors and advanced control applications such as multivariable, nonlinear or adaptive control algorithms.

Chairman

Professor Karen McDonald
Dept. of Chemical Engineering
University of California
Davis, CA 95616
(916-752-0400

Co-Chairman

Prof. Anil Menawat
Dept. of Chemical Engineering
Tulane University
New Orleans, LA 70118
(504) 865-5772

Unsolved Problems in Process Modeling, Optimization, Control and Operations

This session aims to solicit presentations by academic and more importantly industrial researchers on what are the most important unsolved research problems in the following research areas:

- Process Modeling
- Process Optimization
- Process Control and
- Process Operations, including:
  Statistical Process Control,
  Safety,
  Scheduling

Presentations will be brief and should not address a problem that has been only partially solved by the authors.

Chairman

Professor Christos Georgakis
Chemical Process Modeling
Control Research Center

Co-Chairman

Dr. Jorge Mandler
Air Products & Chemicals
P.O. Box 538

Lehigh University Bethlehem, PA 18015 (215) 758-4781	Allentown, PA 18015 (215) 481-3413

Successes and Failures of Adaptive Control Systems

Papers are invited on topics related to the application of adaptive control algorithms to chemical process systems. The scope ranges from applied methods and practical views to stability analysis and the nonlinear properties of adaptive control systems. Topics of interest include the issue of persistent excitation, the implementation of dead zones, multivariable and nonlinear adaptive control, constraints and the use of expert systems. Especially desirable are papers that describe, in detail, the application of adaptive control systems to chemical processes. Papers discussing the implementation of adaptive calibration systems and online uncertainty estimation will also be considered.

Chairman	*Co-Chairman*
Professor B.E. Ydstie Dept. of Chemical Engineering University of Massachusetts Amherst, MA 01003 (413) 545-2388	Prof. C. Brosilow Dept. of Chem Eng Case Western Reserve University Cleveland, OH 44106 (216) 368-4180

Expert Systems in Process Control

This is a call for papers demonstrating the use of expert systems in process control. We are particularly interested in theoretical insights or actual applications of expert systems and other artificial intelligence techniques to real time control problems. Papers dealing with the use of expert systems for configuring and designing control systems as well as other applications related to process control will also be considered.

Chairman	*Co-Chairman*
Professor Bradley R. Holt Dept. of Chemical Eng, University of Washington Seattle, WA 98195 (206) 543-0554	Dr. Carlos Garcia BF-10 Shell Development Co. Westhollow Research Center Houston, TX 77001 (713) 493-8873

Nonlinear Analysis of Chemical Engineering Systems I and II

Papers are sought on application of the methods of nonlinear analysis to chemical engineering problems. Applications may cover any area of interest to chemical engineers (such as chemical reaction engineering, fluid mechanics, transpor processes, process control, etc.) and may deal with one or more aspects of nonlinear analysis; for example bifurcatior methods, singularity theory, elucidation of complex dynamics, etc.

Chairman

Prof. Robert A. Brown
Dept. of Chemical Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139
(617) 253-4571

The Use of Advanced Computer Architectures in Chemical Engineering Computing

Advanced computer architectures involving the use of vector processing, multiprocessing (parallel processing), and vector multiprocessing provide the potential to greatly increase the speed of scientific and engineering computing. Topics of interest for this session include the application of advanced computer architectures to solve chemical engineering problems, the development of new algorithms or codes for exploiting advanced computer architectures, and descriptions or reviews of recent technological developments related to advanced computer architectures. Of particular interest are papers involving multiprocessing or vector multiprocessing architectures.

Co-Chairman	*Co-Chairman*
Professor Mark A. Stadtherr Chemical Engineering Dept. University of Illinois 1209 W. California Street Urbana, IL 61801 (217) 333-0275	Dr. Gary D. Cera E.I. DuPont de Nemours Co. Experimental Station E328/162B Wilmington, DE 19898 (302) 695-1423

Computer Integrated Manufacturing in the Process Industries

Papers are being sought that address systems that are being planned and implemented for Computer Integrated Manufacturing in the process industries. They should address computing techniques used for the development and integration of business systems and manufacturing operations. The vision is one that will add to the definition and solution from the business planning, through the process plant to the sale of product.

Chairman

Dr. Norman E. Rawson
IBM Corporation
DEM-1, 5078
6901 Ruckledge Drive
Bethesda, MD 20817
(301) 564-5959

Co-Chairman

Dr. Verle N. Schrodt
Chemical Engineering
Science Division/M5773-00
National Bureau of Standards
325 Broadway
Boulder, CO 80303
(303) 497-6944

Advances in Optimization

Topics of interest include computational methods for large-scale linear, nonlinear and mixed-integer optimization; applications to plant-wide and on-line optimization, planning and scheduling, retrofit design; interfaces with process simulators and modeling systems.

Chairman

Professor Ignacio E. Grossmann
Dept. of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
(412) 268-2228

Co-Chairman

Professor Christodoulos A. Floudas
Dept. of Chemical Engineering
Princeton University
Princeton, NJ 08544
(609) 452-4595

Applications of Population Balance

We solicit papers on the application of population balance concepts to dispersed phase systems in chemical engineering. Applications to biological populations will also be of interest to this session.

Chairman

Prof. Doraswami Ramkrishna
School of Chemical Engineering
Purdue University
West Lafayette, IN 47907
(317) 494-4066

Co-Chairman

Prof. Robert Ziff
Dept. of Chemical Engineering
University of Michigan
Ann Arbor, Michigan 48109-2136
(313) 764-5498

CAST Sections at AIChE Annual Meeting, Houston, Texas

April 2-6, 1989

The CAST Division is planning the following sessions at the Houston Meeting:

Area 10A: Computers in Process Design

- Application of Expert Systems in Process Engineering
- Computer-aided Process Modeling and Simulation
- Bioprocess Design and Simulation: Issues and Tools
- Retrofit Design and Simulation I&II

Area 10B: Computers in Process Control

- Expert Systems in Process Control
- Control of Separation Operations

Area 10C: Computers in Operations and Information Processing

- Plantwide Use of Computers in Process Operations
- On-Line Fault Administration
- Personal Computers in Planning and Scheduling
- Innovative Uses of Spreadsheets for Engineering Calculations I & II

Area 10D: Applied Mathematics

- No sessions are planned

The names, addresses and telephone numbers of the session chairpersons are given below as are brief statements of the topics to receive special emphasis in soliciting manuscripts for these sessions. Prospective session participants are encouraged to observe the following deadlines:

October 1, 1988: Submit an extended abstract of no less than 500 words in length to each of the session chairs.

November 1, 1988: Authors informed of selection and session content finalized.

March 1, 1989: Two copies of the final manuscript submitted to the session chairs.

Authors are reminded that under current AICHE meeting policies, the meeting booklet will only contain titles of papers presented. However, a book of abstracts is distributed to attendees at the meeting. Moreover, hard copy of papers are also made available for on-site sale.

Applications of Expert Systems in Process Engineering

The objective of this session is to provide a current perspective on the use of Artificial Intelligence and Expert Systems in chemical process engineering. Papers dealing with real-world applications are encouraged.

Session Chairman	*Session Co-Chairman*
Professor Babu Joseph Dept. of Chemical Eng. Campus Box 1198 Washington University St. Louis, MO 63130 (314) 889-6076	Professor Heinz Preisig Dept. of Chemical Eng. Texas A&M University College Station Texas 77843-3122 (409) 845-0386

Computer Aided Process Modeling and Simulation

Papers are solicited dealing with advances in computer-based modeling and simulation strategies as well as applications. Topics for this session include, but are not limited to:

- novel solution strategies for unit operations
- numerical methods related to process engineering, including solution of steady-state and dynamic models
- novel strategies for process simulation and optimization
- new computer-based models for process applications

Chairman	*Co-Chairman*
Prof. L.T. Biegler Chemical Engineering Dept. Carnegie-Mellon University Pittsburgh, PA 15213 (412) 268-2232	Prof. R.W. Pike Chemical Engineering Dept. Louisiana State University Baton Rouge, LA 70803-7300 (504) 388-6910

Bioprocess Design and Simulation: Issues and Tools

This session will provide an interface between process design/simulation and biotechnology practitioners. Papers that report on the development of bioprocess design/simulation tools and those that identify critical problems in tool development that are particular to biotechnology are desired. Representative problems include lack of physical property data, theory applicable to product separations, and tractable, but yet high-fidelity kinetic models for reaction processes.

Chairman	*Co-Chairman*
Prof. Michael M. Domach Dept. of Chemical Eng. Carnegie-Mellon University Pittsburgh, PA 15213 (412) 268-2246	Dr. Randy Field Aspen Technology, Inc. 251 Vassar Street Cambridge, MA 02139 (617) 497-9010

Retrofit Design Techniques and Applications

Papers should describe design techniques and methodology for retrofitting plants which lead to improved raw material efficiency, reduced energy consumption, increased capacity, or improved flexibility. Algorithms and procedures and their embodiment in software can also be described provided the focus is on the technology and not on the features of the software.

Papers are also solicited describing experiences in process retrofitting and how retrofit design techniques were used to identify improvements. Application of software tools in specific projects and the benefits thereof can also be described.

Chairman	*Co-Chairman*
Dr. R. Gautam Union Carbide Corp. P.O. Box 8361 S. Charleston, VA 25303 (304) 747-3710	Dr. H.D. Spriggs Linnhoff March P.O. Box 2306 Leesburg, VA 22075 (703) 777-1118

Expert Systems in Process Control

Papers discussing the application of artificial intelligence and expert systems for process control are invited. Of particular interest are papers describing on-line expert systems for process monitoring, diagnosis and supervisory control. Possible topics include interfacing expert systems to process data and development/delivery issues. Details of small-scale control simulation/applications implemented in PROLOG/LISP are also invited.

Chairman	*Co-Chairman*
Jim Langa Process Control and Computer Technology Division Alcoa Technical Center Alcoa Center, PA 15069 (412) 337-2890	S. Atiq Malik Process Engineering Department Petrochehmicals Division Polysar, P.O. Box 3060 Sarnia, Ontario, Canada N7T 7M1 (519) 862-2911

Control of Separation Operations

This session will concentrate on the control of complex separation operations. Papers covering distillation control are of particular interest, but other complex, multi-variable separation operations may also be covered. Potential separation control topics include:

- Single and Multi Variable Model Based Control (IMC, DMC, IDCOM, etc.)
- Pairing Controlled Variables
- Multivariable Model Identification Techniques
- Inferential Control
- Constraint Control
- Optimizing Control.

Chairman	*Co-Chairman*
David A. Hokanson Exxon Chemical Company P.O. Box 4900 Baytown, Texas 77522 (713) 425-5945	Vince Costello SETPOINT, INC. 14701 St. Mary's Lane Houston, Texas 77079-2995 (713) 584-1943

Plant-Wide Use of Computers in Process Operations

This session focuses on uses of computers in process operations (other than in traditional process control). Papers are invited in the areas of computer applications for analysis and improvement of process operations including, but not limited to:

Planning and Scheduling, On-line Optimization, Process Information

Processing, Reliability and Safety, and interfacing

On-line Control with Plant-wide Optimization Models.

Chairman	*Co-Chairman*
K.R. Kaushik Shell Oil Company P.O. Box 2099 Houston, TX 77252-2099 (713) 241-2098	K. Halemane University of Maryland Dept. of Chemical Eng. College Park, MD 20742 (301) 454-5098

On-Line Fault Administration

Timely diagnosis of malfunctions and product quality deviations is critical in maintaining process profitability, safety, and availability. Because of the stochastic nature of process failures, a continuous effort in fault detection, diagnosis, and correction is essential for process operability. This session will focus on computational and management approaches to on-line fault administration, with particular emphasis on:

- Error detection in process data
- Alarm interpretation
- Synthesis of corrective actions
- Design of human interfaces
- Industrial experience
- Novel computational approaches

Chairman	*Co-Chairman*
Professor Mark Kramer Dept. of Chemical Eng. Room 66-542 Massachusetts Inst. of Tech. Cambridge, MA 02139 (617) 253-6508	Professor Venkat Venkatasubramanian Chem. Eng. & Applied Chemistry Columbia University New York, NY 20027 (212) 280-2561

Personal Computers in Planning and Scheduling

This session is intended to explore the opportunities and problems of using PCs in planning and scheduling of plant operations. Papers are invited which deal with:

- Implementation of special methods and algorithms on PCs
- Practical experience of using PCs in actual plants
- Man-machine interfaces for planning and scheduling
- Suitability of PC hardware and software for planning and scheduling

Chairman	*Co-Chairman*
Michael T. Tayyabkhan Tayyabkhan Consultants 62 Erdman Avenue Princeton, NJ 08540	C. Edward Bodington Chesapeake Decision Science P.O. Box 275 San Anselmo, CA 94960

Innovative Uses of Spreadsheets for Engineering Calculations I and II

These sessions will explore some of the innovative ways spreadsheets are being used to carry out chemical engineering calculations and attempt to assess their role in the chemical engineer's toolkit.

Chairman	*Co-Chairman*
Edward M. Rosen Monsanto Co. F2WK 800 N. Lindbergh St. Louis, MO 63167 (314) 694-6412	Professor Irven Rinard City College of New York 138th St. and Convert Ave. New York, NY 10031 (212) 690-4135