



NEWSLETTER

COMPUTING AND SYSTEMS TECHNOLOGY DIVISION

American Institute of Chemical Engineers

VOLUME 2: NUMBER 1

MARCH 1979

CHAIRMAN'S MESSAGE

In the last twenty years, computer technology has created new directions within chemical engineering. Companies have matured to provide software systems for process design, hardware costs have been reduced to permit routine data-logging in laboratories, textbooks have been written, and a journal was created to routinely report advances in our field. Since many of these developments were initiated at universities, a new generation of young engineers has been educated to better appreciate the role of computers in the technical and managerial aspects of chemical engineering.

These developments were destined to occur, but the rate of progress surely was catalyzed by the work of a few individuals who created a forum for technical discussions within AIChE. The founding members of the Machine Computation Committee provided direction at a time when temptations existed to coordinate through the Association for Computing Machinery, mathematical societies and simulation groups. Credit for the many fine technical sessions goes to these persons and others who participated through the National Programming Committee to organize sessions in Applied Mathematics and Information Processing (formerly Area 1d), Process Control (formerly Area 2L) and Computers in Management (formerly Area 5c).

It is twenty years later and I am delighted to begin 1979 as Chairman of the AIChE Computing and Systems Technology Division. In its first year over 430 chemical engineers joined CAST and many continue to join monthly. We owe much to Bob Morris and his organizing committee for coordinating the transition from Machine Computation Committee to CAST and to Charlie Ware,

last Chairman of MCC, and Vern Sterba, first Chairman of CAST. To Vern and his Executive Committee, we are especially indebted for solving many of the early problems that faced CAST.

Our new Executive Committee inherits a healthy CAST, with a large, growing membership that should reach 600 members this year and gain self-supporting status within AIChE. The Miami meeting was successful, both technically and socially, with an outstanding first Annual CAST Division Banquet. Plans are already underway for Banquet II in San Francisco - let us have your suggestions for Featured Speaker. High standards for the CAST Newsletter were established by Sig Lawrence during our first year, creating a challenge for Peter Hanik, our new editor, and his editorial board. All news of general interest to CAST members is welcome.

Apart from carrying-on the excellent precedents established last year, the 1979 Executive Committee faces several challenges. First, under Fred Stults, the Programming Board of CAST will consider new modes of programming, such as one week symposia, and respond to problems created when merging Areas 1d, 2L, and 5c into CAST. One new initiative is a one week International Conference on "Foundations of Computer-Aided Process Design" being scheduled for June, 1980 (news of this conference appears elsewhere in this newsletter). The merger-related problems concern the number of sessions allocated by the National Program Committee to Areas 15a, b, and c (formerly 1d, 2L, and 5c). In recent years, 15-20 sessions were allocated, with each area requesting sessions through its group. Now, with the three areas in Group 15, there is evidence of pressure to reduce the number of sessions and we plan to respond.

Another challenge is in organizing an awards structure. Mike Tayyabkhan and Bob Morris are cochairing an Awards Committee which includes the five Directors of CAST, Vern Sterba, Paul Gallier, and Bob Fisher. The committee will recommend to the Executive Committee what awards should be sponsored, including the naming of the awards and how the awards will be supported, and the mechanism for selecting the awardees. We have hopes for at least one award at the Division Banquet in San Francisco - with two pledges of support, totalling 1,000 dollars, already received.

In addition, CAST applauds the outstanding quarterly journal Computers and Chemical Engineering, edited by Dick Hughes, and published by Pergamon Press. We need to encourage more authors to submit articles for publication to CACE. There have been some delays due principally to the small number of articles that receive outstanding reviews. More articles of outstanding quality are needed to fill the "pipeline" and assure regular publication.

It is an exciting time to serve as Chairman of CAST and I welcome the opportunity. Let us have your comments concerning our plans and your suggestions. We look forward to an active year and to your participation in 1979.

W. D. Seider
January 22, 1979

HIGHLIGHTS OF EXECUTIVE COMMITTEE MEETING
NOVEMBER 13, 1978, MIAMI, FLORIDA

Bob Harris reported that our present membership is approximately 450 and a major increase is expected before the next meeting when National sends out the annual dues billing.

Lowell Fellingner reported that more new divisions are in the formation stage. Among these new divisions are Safety & Health, Marketing and Management.

Fred Stults reported that the overall emphasis and direction of the programming board will be toward more participation from the industrial sector, i.e., more applied areas. The programming committee for computers in management and information systems has been selected. The members are:

Mike Tayyabkhan, Herb Zellnick, Ted Peterson and Norm Rawson.

Norm Rawson reported that the Liason Committee has established contacts with the American Chemical Society and the American Production and Inventory Control Society.

Sig Lawrence reported that his resignation as chairman of the publications board had to become effective as soon as possible. A resolution was passed to commend Sig for the excellent job he has done over the past years: for not only establishing the newsletter but having it become a recognized standard for others.

Mike Tayyabkhan and Bob Morris requested volunteers for the Awards Committee. The Committee now consists of, in addition to Mike and Bob, Vern Sterba, Paul Gallier, Ted Peterson and Bob Fisher.

Mac Clarke agreed to prepare a walking guide to the Petro-Expo at the Houston meeting.

Dick Hughes reported that subscriptions to computers and chemical engineering are good but there is some difficulty in obtaining papers. The problem seems to be with

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Chairman.....	Warren D. Seider
1st Vice Chairman.....	Richard R. Hughes
2nd Vice Chairman.....	Brice Carrahan
Secretary/Treasurer.....	Robert E. Harris
Directors.....	Richard R. Hughes Robert L. Morris Theodore I. Peterson Michael I. Tayyabkhan Paul J. Horvath Norman E. Rawson
Publications Chairman.....	Peter P. Hanik
Editors.....	Edward Gordon Rodolphe L. Motard Edward C. Roche, Jr. Joseph F. Zemaitis, Jr.

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reviewers; more are necessary with better response.

Paul Gallier reported that Project Aspen is into the programming phase (design completed). The expected date for release will be the summer of 1979.

Ted Leninger will study the needs for a division directory.

A motion was passed appointing Pete Hanik as Chairman of the publications board.

*** ELECTION RESULTS ***

Officers & Directors for 1979 have been elected. The term for officers is one year; Directors serve for three years. CAST Division officers, Directors and Chairmen are listed below

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Membership Committee

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AREA 15a

SYSTEMS AND PROCESS DESIGN
HOUSTON SESSIONS

Please note two recent changes in Area 15a programs at the Houston meeting. The session "Optimal Allocation in Energy Networks" has been cancelled and the title of the session "Sparse Matrix Computational Methods" has been changed to "New Developments in Process Analysis". The schedule for Area 15a follows:

*****SESSION 30*****

New Developments in Process Analysis
Tuesday 3 April 1979
8:30-11:30 A.M.
Room 315

Richard S. H. Mah, Chairman
Northwestern University

Arthur W. Westerberg, Co-Chairman
Carnegie-Mellon University

SESSION 37

Simulation of Fossil Fuel Related Processes
Tuesday 3 April 1979
2:30-5:30 P.M.
Room 123

Lawrence B. Evans, Chairman
Massachusetts Institute of Technology

Larry M. Joseph, Co-Chairman
U.S. Department of Energy

WALKING GUIDE TO PETRO EXPO '79

Planning to be in Houston for the AIChE meeting during the first week of April? Don't forget to pick up your copy of CAST'S Walking Guide to Petro Expo '79 at the AIChE registration area.

The guide lists exhibits of special interest to CAST members. Further, it lists them in the order you will see them as you walk through the Expo.

If you plan to see every booth, use the Expo guide put out by the Expo management. But if your time is limited, CAST'S Walking Guide can help you use it efficiently.

This will be the second Walking Guide CAST is providing for its members.

REPORT ON LIASON ACTIVITIES

. In April 1979 the ACS/CSJ Chemical Congress will hold their meeting in Honolulu, Hawaii. The Division on Computers and Chemistry will hold a symposium on "Computer Assisted Drug Design".

. Information on the activities of the IEEE can be obtained from Alan Glueck, Chem Tech Consultants, P.O. Box 246, Lawrenceville, NJ 08648 (609-921-1900).

. Activities of the American Chemical Society can be gotten from Norm Rawson, IBM Corporation, Bethesda, Maryland 20034 (301-897-2399).

. The doings of the American Production and Inventory Control Society (APICS) can be gotten from Richard Heard, Philips Petroleum Bartlesville, OK 74004 (918-661-5419).

Bob Lackmeyer is liason committee chairman.

He can be reached at SOHIO, Midland Building, Cleveland, OH 44115 (216-575-5002)

DIPPR Alive and Well

At the Miami meeting, Council established the Design Institute for Physical Property Data (DIPPR). The committee was established to meet the needs of industry for more complete and accurate data for process and equipment design. John Prados, Vice-President for Academic Affairs at the University of Tennessee, was named committee chairman. The committee will be critically evaluating existing data and will try to fill in the gaps in existing data through sponsorship of projects to generate the missing data. The committee will begin by compiling data on pure components and will promote the collection and determination of property data on mixtures. The Institute will also produce a technical data book. There are presently about 35 member companies and individuals in the Institute. Participation and funding from sources other than chemical companies is being sought.

INTERNATIONAL CONFERENCE ON FOUNDATIONS OF COMPUTER-AIDED PROCESS DESIGN

As a project of CAST, Professors Richard S. H. Mah and Warren D. Seider are undertaking to broaden the scope of AIChE programming by introducing the first International Conference on Foundations of Computer-aided Process Design. A one week conference is being planned to be held in June, 1980. The conference will bring together engineers from universities, industry, and government laboratories for a week-long intensive assessment of the present status and future needs in computer-aided process design.

Eight sessions will cover key areas in our field, with each session featuring a "State-of-the-Art Review" by one of the leading experts and invited papers describing 3 or 4 recent advances. All reviews and papers will be published in a Conference Proceedings, along with session summaries to be prepared by Reporters who will place the contents of the sessions in perspective. The proceeding will be published within 6 months to a year following the conference.

The Engineering Foundation will work with

CAST to make arrangements for the conference. Professors Mah and Seider have completed a proposal to the National Science Foundation requesting funds to partially cover conference fees and travel expenses for participants from universities.

Many arrangements are being completed during the next four months and details will be reported in the next Newsletter.

AICHE TO SPONSOR 1979 JACC

The 1979 Joint Automatic Control Conference, to be held June 17-20, 1979, in Denver, Colorado, will be sponsored by the American Institute of Chemical Engineers. The conference has been held annually since 1959 and is sponsored on a rotating basis among the member societies of the American Automatic Control Council. The member societies include ASME, IEEE, ISA, and SME, in addition to AIChE. This inter-society conference allows the exchange of information among control scientists and engineers from a wide variety of disciplinary areas.

General Chairman for the 1979 JACC is Professor W. F. Ramirez of the Department of Chemical Engineering at the University of Colorado. Technical Program Chairman is Professor T. F. Edgar of the Department of Chemical Engineering at the University of Texas at Austin. Arrangements Chairman is Dr. Chuck Vestal of Marathon Oil Company, Littleton, Colorado. Program Representative for AIChE is Prof. George Stephanopoulos of the University of Minnesota.

The program for the 1979 JACC features seven theme areas, each of which will contain general survey papers as well as state-of-the-art contributors. The theme areas are automation in manufacturing, measurements and components, microprocessors in control applications, large scale systems, biomedical control applications, control of large aerospace structures, and nonlinear systems.

Other invited sessions will focus on such topics as chemical process control, distributed computer control, multivariable control techniques, communication, parameter and state estimation, digital signal processing, and control of electric power plants.

Finally, contributed papers dealing with various aspects of control theory and practice will be presented.

The program for the meeting will be mailed in April, 1979. Inquires about attendance at the conference should be directed to Mr. Joel Henry at AIChE headquarters.

SUMMER COMPUTER SIMULATION CONFERENCE

This year's conference will be held July 16-18, 1979 at the Sheraton Centre, Toronto, Ontario. The conference theme will be simulation in a rapidly changing computer world. Topical areas are simulation methodology, hybrid systems, chemical sciences, physical sciences, environmental sciences, biomedical systems, managerial and social sciences, simulation, credibility and validation, energy, system engineering and simulation for training. Conference sponsors are AMS, ISA, SCS and SHARE. The General Chairman is Arthur Schiewe, The Aerospace Corporation, P.O. Box 92957, Los Angeles, CA. 90009, 213-648-6120.

DATA BANK OF PROFESSOR REID AVAILABLE

Need a physical property data bank for 468 organic and inorganic chemicals at low cost? The ASPEN project at M.I.T. is making the data bank of Professor Reid available for CAST and the AIChE. The data bank may be ordered on tape for \$45 or on cards for \$60. Checks should be made payable to Massachusetts Institute of Technology.

This data bank is listed in the book, "The Properties of Gases and Liquids", Third Edition, by Robert C. Reid, John M. Prausnitz, and Thomas K. Sherwood, McGraw Hill, 1977. These data are from literature sources and industrial corporation files and have been reviewed for accuracy.

The format being made available is different from the book. Property values are in SI units. The Harlacher equation for vapor pressure has been converted into a more convenient form. This is a seven constant extended range Antoine equation form. The constants of this equation were regressed to fit the Harlacher equation and four other requirements such as the normal boiling point and conditions at the critical temperature and pressure.

Of the two versions available the tape version contains complete property constants for 6 components per page. The tape is in EBCDIC code, available in 800 or 1600 bpi and 25 lines per block. The card version contains 3 components per page. A printed listing is supplied with each.

You may place an order by writing to:

Ms. Jean Gerlock
IPS, Bldg. 39-427
Massachusetts Institute of Technology
77 Massachusetts Ave.
Cambridge, MA 02139

three times per year, hopefully about two weeks before each National meeting (God and the Post Office willing). If you are receiving your issue much later than this, please let me know and I will attempt to find out why. Also, should you wish to have an announcement listed in the Newsletter (e.g. call for papers, notice of seminar, recommendation of a good book or magazine article) the deadline is three (count 'em) months prior to each National meeting. Thus the deadline for this Newsletter was January 1 with the next National meeting being April 2.

A NOTE OF THANKS

At the Miami Meeting the executive committee of CAST voted to commend Sig Lawrence for the excellent job he has done over the past years as publications chairman. Sig not only established the CAST Newsletter but refined it to the point where it is now a standard for comparison. As the new publications chairman, I feel most fortunate to have a man such as Sig to call upon for advice. I would also like to take this opportunity to thank Ed Gordon, Rudy Motard and Joe Zemaitis for their continued cooperation and dedication. Thanks is likewise due to my employer, Northern Natural Gas Company, for supporting my activity as publications board chairman.

WELCOME ABOARD

I am pleased to announce that Ed Roche has joined the Newsletter staff as news editor. Ed has been instrumental in helping with preparation of this Newsletter and is a most valuable addition to the staff.

POTPOURI

On the new masthead please note that this issue of the Newsletter is designed as Volume 2, Number 1, March 1979. Previous newsletters were not numbered and were dated "Spring", "Midyear", and "Fall". I have grouped all unnumbered newsletters (both MCC and CAST) and called them Volume 1. In the future the number (1, 2, or 3) will correspond to the previous "Spring", "Midyear", and "Fall" notation. You should be receiving the Newsletter

OFFLINE REVIEWS
JOE ZEMAITIS

Having been involved recently in a major conversion of scientific software from one FORTRAN dialect to another as a result of a change in computers, I was amazed at the wide variety of programming practices exhibited in the programs to be converted. Most of the problems that arose during the conversion process were the result of the poor programming styles used by the many contributors to this particular software library, yours truly being one of the culprits. In addition, I was going to review a recent acquisition, namely, Vapor-Liquid Equilibria Using UNIFAC by Fredenslund, Gmehling, and Rasmussen, Elsevier Scientific Publishing Co., (1977). But again the question of programming style arose as we started to use their programs and adapt them for our inhouse use and ran into problems.

So, let's devote this column to programming style, and review two slim volumes, either of which if read, will help to improve programming style and proficiency. The books are: The Elements Of Programming Style by Kernighan and Plauger, McGraw-Hill(1974); and, Programming Proverbs For Fortran Programmers by H.F. Ledgard, Hayden Book Co. (1975).

Both books owe a lot to a classic guide for writers, The Elements of Style by W. Strunk and E.B. White, in that they both use a similar form and approach and attempt to concentrate on the essential practical aspects of style. Each principle or proverb is followed by a short discussion with examples of both good and bad code. Topics covered include: program structure, input and output, efficiency, common blunders, documentation, debugging techniques, etc.

An example of the types of comments to be found in Kernighan and Plauger concerning input:

_____ _____
Make input easy to prepare and output self-explanatory

_____ _____
Make input easy to proofread

How often though these principles are ignored! For instance, as input to the UNIFAC parameter estimation program the following numbers are read:
305.1511 0.0750 2.051620 0.9250 1.0055

The format statement for this line is:
101 FORMAT(F7.2,3(I2,2F7.4))

with the read statement being:
100 READ(NC,101) T(N), (NU(N,I),XXX(N,I),
GME(N,I), I=1,2)

Clearly, when proofreading the input, one would be unable to quickly see what variable is assigned what value. The input lines just above this, found on page 270 of Fredenslund ET AL., defy description and error-checking, so much so, that I found it impossible to have it typed correctly for this review.

Either of these two books should be read and reread before starting on any new major programming project. The proverbs they contain are little gems of truth which will help any person involved in computer programming upgrade their work. One final quote:

Proverb 25: Don't be afraid to start over

Except for some of the poor style in the codes that make up a large portion of the book by Fredenslund Et Al, Vapor-Liquid Equilibria Using UNIFAC provides an excellent source of information and readily adaptable code for the UNIFAC method of calculating phase equilibria. Contained in this book are the basic programs for the calculation of activity coefficients, predictions of liquid-liquid equilibria compositions, calculation of UNIQUAC or Wilson parameters from UNIFAC, parameter estimation programs, and distillation programs. A wealth of material that can be used on a standalone basis or interchanged into other systems is contained in this book.

COMPUTER AIDED INSTRUCTION IN CHEMICAL ENGINEERING
FEATURE ARTICLE
CHUCK ECKERT

At this time this appears to be the fastest growing area of computer applications in chemical engineering in terms of investment growth and numbers of students. This is primarily due to the growing momentum of the PLATO system. This medium has implications beyond university-level education since the system can support a variety of continuing education and other training programs for any age-level or experience.

The computer-based PLATO educational system provides interactive, self-paced instruction to large numbers of students. It has been widely used in physics, chemistry, and a variety of other fields and shown itself to be eminently successful. The PLATO system, for which both the hardware and software were developed at the University of Illinois, is the only large system with full-scale graphics capable of handling hundreds of terminals simultaneously. Currently there are approximately 1000 terminals all over the U.S. hooked up to the University of Illinois PLATO computer alone. The PLATO system has an extremely sophisticated set of software which makes possible the programming of complex interactive problems utilizing graphs, diagrams, animations, and even projected slides, in addition to all the usual computational abilities of a large computer. The programming language is such that it permits not only instant recognition of correct students responses (permitting if the instructor wishes, misspellings, various phrases, or an error tolerance on a numerical answer), but also permits the instructor to identify the most probable wrong answers and respond to each of these with comments or other questions pointing out their errors to the students.

The main computer for the PLATO system is the CDC-Cyber and the extensive memory available at the University of Illinois currently contains many thousands of hours of lessons in a wide variety of fields. The student PLATO terminal consists of a keyboard and screen about nine inches square, capable of displaying texts, diagrams, graphs, or even color photographs. Students using the system require no knowledge of computer language or computer

techniques. They need only to know how to use a typewriter keyboard with a few extra keys and the first lesson given is instruction in the use of these keys. Students complete this lesson in five or ten minutes and with this little instruction are able to utilize completely the student mode of the PLATO computer.

Professor Eckert and his colleagues have been developing PLATO lessons for approximately two years, the first effort was to set up a series of lessons for use in the first chemical engineering course, Ch E 261, "Introduction to Chemical Engineering". All of the lessons have been course tested. Three-quarters of these have now been course tested with in excess of 100 students, some with as many as 300 students.

The PLATO lessons have had a significant effect on student morale in that they have materially augmented interest and participation. Perhaps part of the credit for this ought to go to a grader lesson currently being used which displays to each student at his request, at any time during the course, all of his grades in the course to date including not only PLATO lessons but also quizzes, homework and tests taken and shows him the histogram of the class performance with an indication of his standing in class and his current grade.

However, in an even more documentable way, well-written lessons prove to be excellent motivators; students are quite eager to do all the lessons available. In the Fall of 1977, students in this course showed a lesson completion rate in excess of 97%. In the Spring of 1978, this figure reached an almost unbelievable 99.75%. Invariably, student performance on examinations improved; for example, on similar material balance problems given on examinations before and after the introduction of PLATO lessons, the average performance has increased from approximately 50% (based on examinations given ten years ago) to about 75% now.

The major effectiveness of the PLATO lessons is in permitting students to do a wider variety of problems in a short time with instantaneous interaction in a non-intimi-

dating manner. That is, a student can do in an hour the same number of homework problems that would take him four to six hours to do in a conventional manner and he need not wait a week to have his graded paper returned. His errors are corrected immediately just as though he were working directly with the professor but without the intimidation that such direct interaction would entail. Further much "hack" calculations can be eliminated so that more material may be covered. An example of this is an adiabatic flame temperature problem. Such a problem was formerly given (over a two-week period) as a Fortran assignment; now this is one of six problems in a one hour lesson. Not only does the student see instantly his errors in setting up the equations but he can visualize the effectiveness of his root-finding technique. Also in the same hour he can do five other related problems. Very simply, he is using his time better and we can teach the student more, better and newer problem-solving and design methods more effectively.

It should be noted that the PLATO programming is not being used to replace all regular homework or any lecture material. It is replacing some of the homework material but the students are also required to do conventional homework problems; they have lectures, quizzes and exams as usual and at the present time PLATO is never used for examination purposes. Most of the problems are set up with random number generators so that students redoing the problems will get a different problem each time. We find that the students spend approximately 2/3 of their time doing problems the first time and approximately 1/3 of their time on PLATO reviewing the problems they have already done for examinations.

Work is continuing on PLATO lessons for thermodynamics, unit operations, kinetics and reactor design courses at Illinois and at other sites.

In addition to the Illinois system, PLATO is offered through the Control Data Corporation and is available on several dedicated University systems: Alberta, Brussels, Delaware, Florida, Minnesota, Texas and Quebec. Each PLATO machine can handle 1024 terminals. The cost of terminals is \$5300 each but the price is decreasing. A computer port costs \$3280

but will support 4 terminals. One cannot run a PLATO course with one terminal; it requires a battery. For instance, the Chemistry Department at Illinois has over 40 terminals and the Chemical Engineering Department has 12.

BEING TOO COMPLICATED

ALGORITHM 1

```
IF(X .LT. Y) GO TO 30
IF (Y .LY. Z) GO TO 50
SMALL = Z
GO TO 70
30 IF (X .LT. Z) GO TO 60
SMALL = Z
GO TO 70
50 SMALL = Y
GO TO 70
60 SMALL = X
70
```

ALGORITHM 2

```
SMALL = X
IF( Y .LT. SMALL ) SMALL = Y
IF( Z .LT. SMALL ) SMALL = Z
```

ALGORITHM 3

```
SMALL = AMINI(X, Y, Z)
```

This interesting Fortran example is one of several well chosen examples in the article "Programming Style: Examples and Counterexamples" by Brian W. Kernighan and P. J. Plauger in ACM Computing Surveys, Volume 6, Number 4, December 1974. How much code like ALGORITHM 1 have you seen or perhaps

COMPUTING & SYSTEMS TECHNOLOGY DIVISION

AIChE

Membership Application.

I wish to join the newly formed C&ST Division of AIChE. My dues payment of \$3.00 is enclosed.

NAME _____

ADDRESS _____

EMPLOYER (IF NOT IN ADDRESS)

My two primary areas of professional interest are:

(NOTE: Sections devoted to specific professional areas of interest will be formed within the division.)

I am willing to work on a Division Committee:

- | | |
|---------------------------------------|--|
| <input type="checkbox"/> Programming | <input type="checkbox"/> Special Interest Sections |
| <input type="checkbox"/> Publications | <input type="checkbox"/> Awards |
| <input type="checkbox"/> Membership | <input type="checkbox"/> Other |

Complete the above form. Staple your check (made out to CAST Division, AIChE) to it, fold and mail it to the membership chairman:

R. E. Harris
SOHIO
Midland Bldg. - 206 CB
Cleveland, Ohio 44115