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J. R. Welty

Summaries of FY 1986 Engineering Research

November 1986

U.S. Department of Energy
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Office of Basic Energy Sciences
Division of Engineering and Geosciences

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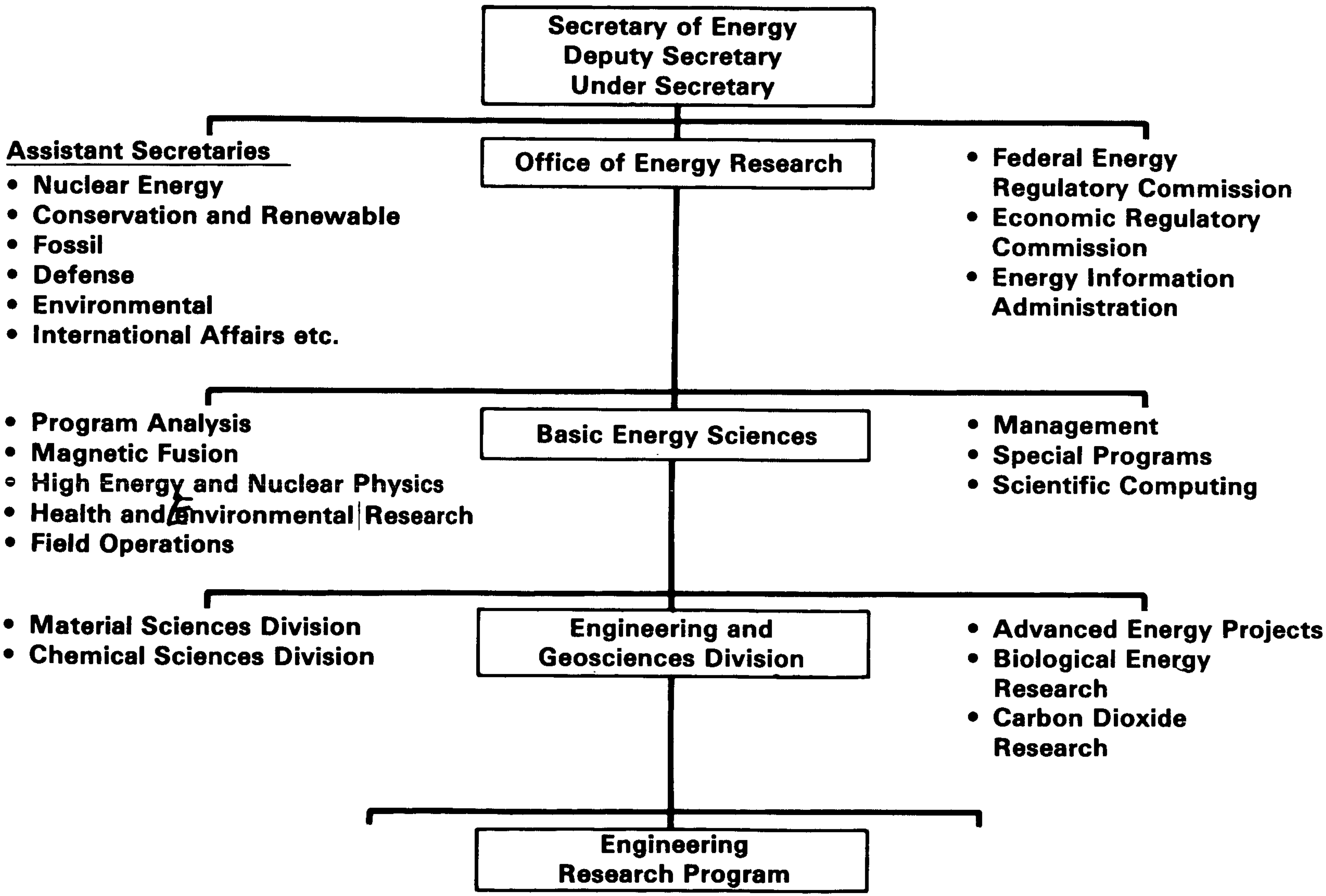
Washington, D.C. 20545

FOREWORD

This report documents the BES Engineering Research program for fiscal year 1986; it provides a summary for each of the program projects in addition to a brief program overview. The report is intended to provide staff of Congressional committees, other executive departments, and other DOE offices with substantive program information so as to facilitate governmental overview and coordination of Federal research programs. Of equal importance, its availability facilitates communication of program information to interested research engineers and scientists. The organizational chart for the DOE Office of Energy Research (OER) on the next page delineates the six Divisions within the OER Office of Basic Energy Sciences (BES). Each BES Division administers basic, mission oriented research programs in the area indicated by its title. The BES Engineering Research program is one such program; it is administered by the Engineering, and Geosciences Division of BES. Dr. Oscar P. Manley is technical manager of the Engineering Research program; inquiries concerning the program may be addressed to him, in writing or by phone at (301) 353-5822.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1986. The summaries received have been edited as necessary, but the press for timely publication made it impractical to have the investigators review and approve the summaries prior to publication. For more information about a given project, it is suggested that the investigators be contacted directly.

Engineering Research Program within DOE



INTRODUCTION

The individual project summaries follow the program overview. The summaries are ordered alphabetically by name of institution and so the table of contents lists all of the institutions at which projects were sponsored in fiscal year 1986.

The projects are numbered sequentially for individual identification in the indexes. Each project entry begins with a centered, institutional-departmental heading. The project number precedes the capitalized project title. The names of the investigators are listed immediately below the title. The funding level for fiscal year 1986 appears to the right of title; it is followed by the budget activity number (e.g., 01-A). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The year in which the project began and the anticipated duration in years are indicated respectively by the first two and last digits of the sequence directly below the budget activity number (e.g., 84-2). The summary description of the project completes the entry.

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PROGRAM REVIEW

BES ENGINEERING RESEARCH

The BES Engineering Research program is one of the component research programs which collectively constitute the DOE Basic Energy Sciences program. The DOE Basic Energy Sciences program supports energy related research in the physical and biological sciences, and in engineering. The chief purpose of the DOE Basic Energy Sciences program is to provide the fundamental scientific base on which identification and development of future, national energy options will depend. The major product of the program becomes part of the body of data and knowledge upon which the applied energy technologies are founded; the product is knowledge relevant to energy exploration, production, conversion and use.

The BES Engineering Research program was started 1979 to help resolve the numerous serious engineering issues arising from efforts to meet U.S. energy needs. The program supports fundamental research on broad, generic topics in energy related engineering--topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology. During the first year several workshops were sponsored for the purpose of identifying energy related engineering research needs and initial priorities. Representatives from industry, academic institutions, national laboratories, and leading members of professional organizations (Engineering Societies Commission on Energy, American Society of Mechanical Engineers, Society of Automotive Engineers, and Joint Automation and Control Committee) participated in the workshops. In addition to the participants in the workshops, staff representatives from the DOE technology programs and other leading U.S. energy engineering experts made significant contributions to the setting of program priorities. There resulted from this process a strong confirmation of the need for a long-range, fundamental engineering research program with two major goals. The broad goals that were established by this process for the BES Engineering Research program are:

1) To extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and

2) To broaden the technical and conceptual base for solving future engineering problems in the energy technologies.

In this process, it was further established that to achieve these goals, the BES Engineering Research program should address the following topics identified as essential to the progress of many energy technologies:

1) Advanced industrial Technology -- improvement of energy conversion and utilization, opening new technological possibilities, and improvement of energy systems.

2) Fluid Dynamics and Thermal Processes -- broadening of understanding of heat transfer in non-steady flows, methodology for reducing vibrations and noise in heat exchangers, and engineering aspects of combustion.

3) Solid Mechanics -- continuum mechanics and crack propagation in structures.

4) Dynamics and Control of Processes and Systems -- development and use of information describing system behavior (system models), performance criteria, and theories of control optimization to achieve the best possible system performance subject to known constraints.

A Scoping Workshop held in December, 1986 confirmed the continued needs for research in these topical areas. Because of budgetary limitations, the implemented BES Engineering Research program is somewhat less broad than the program envisioned above. at present, equal emphasis is being placed on three carefully selected, high priority research areas; namely,

1) Mechanical Sciences -- including tribology (basic nature of friction reduction phenomena), heat transfer, and solid mechanics (continuum mechanics and crack propagation).

2) System Sciences--including process control and instrumentation.

3) Engineering Analysis -- including non-linear dynamics, data bases for thermophysical properties of fluids, and modeling of combustion processes for engineering application.

These areas contain the most critical elements of the four topics enumerated above; as such they are of importance to energy technologies both in the short and long term, and therefore of immediate programmatic interest. It should be noted that other areas of basic research important to engineering are monitored elsewhere in BES. For instance, separation sciences and research on thermophysical properties, are among the responsibilities of the Chemical Sciences

Division, while microscopic aspects of fracture mechanics are in the domain of the Material Sciences Division. As resources permit, other high priority areas are being added to the Engineering Research program. Thus as a result of some growth in the program budget an important development has taken place in the Engineering Research Program: two major concentrations of research were initiated. First, a new program was organized at Oak Ridge National Lab dealing with intelligent machines in unstructured environment. It is expected that some resources will be available for coordinated, more narrowly focussed related, high quality research at universities and other research centers.

All such activities will be supported and administered directly by the Engineering Research Program, but some coordination of efforts with the ORNL program may prove useful. The research opportunities in this area of interest to the DOE - Engineering Research Program have been identified in a workshop held in November, 1983. Proceeding of the workshop entitled "Research Needs in Intelligent Machines" are available from the Center for Engineering Advanced Systems Research, Oak Ridge National Lab., Post Office Box X, Oak Ridge, TN, 37830.

Secondly in FY 1985 there has started a collaborative research effort between MIT and Idaho National Engineering Lab. At present, the collaboration is in four distinct areas: Plasma Process Engineering, Automated Welding, Fracture Mechanics, and Advanced Engineering Methods and Analysis.

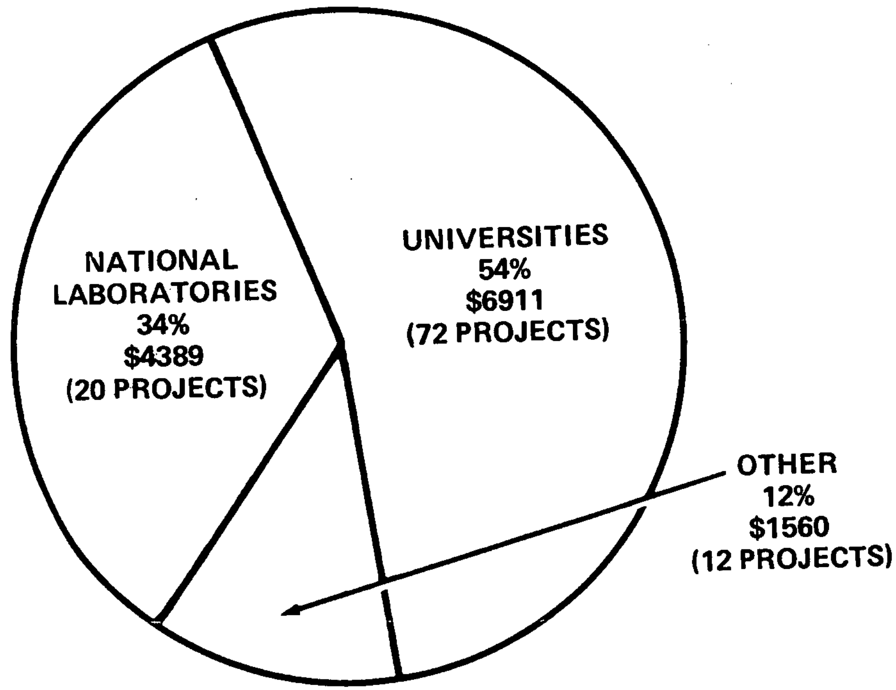
Colateral, high-quality research efforts at other institutions are supported by the Engineering Research program.

Finally, in the expectation of a future modest growth of this Program, an International Workshop on Two-Phase Flow Fundamentals was held in September 1985. This meeting was used to identify basic research needs in the field of two-phase flow and heat transfer; a summary report of the workshop is available from the Program Office. The full proceedings will be published as a volume in the series "Advances in Heat and Mass Transfer (Hemisphere Publishing Company).

It should be mentioned too, that some very limited support is available for research on large scale systems. A report of a Workshop on Needs, Opportunities, and Options in this field is available from Professor G. L. Thompson, Graduate School of Industrial Administration, Carnegie-Mellon University, Pittsburgh, PA, 15213.

Research projects sponsored by the BES Engineering Research program are currently underway at universities, private sector laboratories, and DOE national laboratories. In fiscal year 1986 the program operating funds available amounted to about $13 million. The distribution of these funds among various institutions and by topical areas is illustrated on the next page. Project funding levels are mostly in the range of $50,000 to $150,000 per year. Typical duration of a project is three to four years, with some projects expected to last as long as ten years or more. The BES Engineering Research projects stem almost without expection from unsolicited proposals for competitive grants. Proposals which anticipate definite results in less than two years are usually referred to the appropriate DOE technology program for consideration. Anyone interested in submitting a proposal is encouraged to discuss his ideas with the technical program manager prior to submission of a formal proposal. Such discussion helps to establish whether or not a potential project has a reasonable chance of being funded. The primary considerations for possible support are the technical quality of the proposal and the professional standing of the principal investigators and staff. An effort is made to attract first rate, younger research engineers and energy oriented applied scientists. A high technical caliber of research is maintained by requiring that the projects supported have potential for a significant contribution to energy-related engineering science, or for an initial contribution to a new energy relevant technology. Sponsored projects are selected primarily for their relevance to DOE mission requirements; the contribution to energy related higher education is an important but secondary consideration. Thus projects sponsored at universities are essentially limited to advanced studies both theoretical and experimental usually performed by faculty members, staff research scientists, and doctoral candidates.

ENGINEERING RESEARCH PROGRAM
FY '86 BUDGET ($000's) BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '86 BUDGET BY TECHNICAL AREAS

	($000 s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	3223	25	38
SYSTEMS SCIENCES	4723	37	34
ENGINEERING ANALYSIS	4955	38	32

AMES LABORATORY
Iowa State University
Ames, IA 50011

01. MULTIVIEWING TRANSDUCER SYSTEM $241,000
D. O. Thompson 03-B
81-7

The objective of this project is to demonstrate a composite, multiviewing ultrasonic transducer system suitable for detecting, characterizing, and reconstructing flaws in structural materials for various applications and for the evaluation of inverse algorithms for flaw sizing. Development of this transducer utilizes a combination of recent advances in ultrasonic scattering and inversion theories with new concepts in transducer configurations and excitation methods. Automated data acquisition has been developed using seven transducer elements multiplexed for both pulse-echo and pitch-catch modes. The reconstruction protocol fits the acquired data to an "equivalent" ellipsoid of general shape (3 axes, 3 angles), a shape that is compatible with a fracture mechanics description of growing flaws and thus suitable for failure prediction. In the effort to improve the reconstruction reliability with a limited aperture, a multi-angle signal amplitude contour technique was developed which instructed the automated system to acquire data with the most favorable angular configuration. This technique has dramatically improved the reconstruction reliability for flaws oriented at a difficult tilt angle for the reconstruction. In addition, artificial intelligence may be incorporated to determine the shape and angular configuration of the flaw from the signal amplitude contours and the full reconstruction may be constrained by such predetermined information for greater stability and reliability. New technqiues have also been developed for generating unipolar stress pulses in both pulse-echo and pitch-catch modes. These pulses show significantly broader bandwidths than do the usual ultrasonic pulses, a feature that is necessary in the application of inversion algorithms for flaw sizing. They are also important in the measurement of gradients of material properties. A new transducer system has also been designed using these advances that will extend reconstruction capabilities to include 2-D computed tomographic and 3-D ultrasonic reconstructions.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, IL 60439

02. THEORETICAL/EXPERIMENTAL STUDY OF STABILITY CONTROL $123,000
01-C
86-3

E. L. Reiss (Northwestern University), T. M. Mulcahy, S. P. Vanka, M. Wambsganns

Theoretical and experimental studies are aimed at enhancing the understanding of stability phenomena involving fluids, solids, and their coupling. The objective is to develop methods of controlling, delaying, and/or avoiding instability.

To develop mathematical techniques and gain physical insight into nonlinear instability phenomena, oscillator problems are studied. Application of periodic forces opposing unstable motion was identified and experimentally verified to control the instability of a pipe conveying fluid. Periodic forces will be investigated as a means to initiate secondary bifurcations; sometimes more desirable (acceptable) bifurcations, initiated below the critical conditions for primary bifurcation, will receive special attention. Also "internal" or parametric excitation, such as variation of governing dimensions, will be investigated as a method of active control.

Fluidelastic instabilities with laminar flow leaking in narrow constricted channels between closely spaced bodies, numerical will be studied. In particular, the slope joint region of telescoping tubes conveying fluids will be investigated. Model problems will be analyzed to help interpret the different instabilities experimentally observed and the flow damping correlations being developed.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, IL 60439

03. BOUNDS ON DYNAMIC PLASTIC DEFORMATION $123,000
C. K. Youngdahl 01-A
84-3

In many applications where load is transmitted to the structure through a fluid, details of the load history and spatial distribution affect significantly the final plastic deformation. The objective of this project is to devise load correlation parameters based on various weighted integrals of the time-space load distributions which can be used to characterize the effects of the load without resorting to detailed numerical analysis. These load correlation parameters have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events. The dynamic plastic deformation of some basic structural configurations will be analyzed for loadings which vary both in magnitude and region of application with time. Load correlation parameters will be hypothesized and their usefulness in predicting final plastic deformation will be determined. The analyses will be based initially on a rigid, perfectly plastic material model, but will be extended to include strain hardening and elastic effects if the work to determine load parameters is successful.

BOSTON UNIVERSITY
Department of Chemistry
Boston, MA 02215

04. DIFFUSION, FLUID FLOW, AND SOUND PROPAGATION IN DISORDERED MEDIA — $65,000
Thomas Keyes — 06-C, 86-3

The basic transport processes, of which those mentioned in the title are important examples, become extremely complicated in the presence of large amounts of disorder. For example, the effect of a low density of fixed scatterers upon diffusion is easy to calculate; at high density, diffusion may cease altogether and the problem becomes difficult. Lattice vibrations on an ordered lattice are described by perfect sound waves, but disorder-perhaps some broken bonds- can cause the vibrations to be "localized" with no ordinary long-wavelength sound at all (localization is thought to occur with an infinitesimal amount of disorder in two dimensions). Of course, large disorder is the rule in nature, as in the interior of a porous rock.

The aim of this project is to apply modern methods of nonequilibrium statistical mechanics to transport with large disorder. Those methods are the "Repeated Ring" kinetic equation, an extension of Boltzmann's equation to complicated systems, the Renormalization Group, and computer simulation. Transport coefficients and correlation functions will be calculated. The project has only just begun, but a molecular dynamics simulation of lattice vibrations (sound) on disordered lattices is running. While the program was being tested, almost accidentally, a clear manifestation of the unusual localization phenomenon in two dimensions was discovered and is now being analyzed; this phenomenon is most interesting theoretically. Lattice vibrations in several disordered systems, and the other transport problems listed, will be investigated as the project develops.

BROWN UNIVERSITY
Division of Engineering
Providence, RI 02912

05. GEOMETRIC ANALYSIS OF THE ENSEMBLE OF SOLUTIONS IN TWO-PHASE FLOWS AND COMPLETE RESOLUTION OF THE PROBLEM OF CHOKING — $ 83,000 / 06-C / 84-3
J. Kestin

The project studies a mathematical formalism for the qualitative analysis of the geometric-topological structure of all trajectories (solutions) of a two-phase model in a space formed with the state-velocity variables and physical distance. Such an analysis supplements the study of numerical solutions produced by an appropriate computer code. It serves to answer a number of questions of physics without actually solving the equations of the model, to establish a set of initial conditions for which the problem is well-posed, as well as that set for which no physically meaningful solutions exist. The most important advantage in carrying out such an analysis in detail is the fact that it provides us with a complete resolution of the problem of choking.

An analysis of a general form of the problem makes it possible to adapt the powerful analytic tools used in the study of dynamical systems to problems in two-phase flow. The most important discovery is based on the applicability of the center manifold theorem which reduces the study of the singular points of the nonlinear system to that of a locally linearized system.

The most important special result asserts that the state velocity which exists at a choked section depends only on the conservation equations used in the model and is independent of the closure conditions. The latter do, however, determine the location of the choked cross-section (together with the sufficient condition of choking) when it is located inside the channel.

A general theory makes it possible to relate the state-velocity vector at choking to the velocity of propagation of small disturbances and the characteristics of the wider, time-dependent model of two-phase flow.

Following one specific idea, we have made a contribution to the study of transition from bubble to slug to froth flow.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Department of Chemical Engineering
Pasadena, California

06. THE DEVELOPMENT OF PROCESS DESIGN AND CONTROL STRATEGIES FOR ENHANCED ENERGY EFFICIENCY IN THE PROCESS INDUSTRIES — $ 50,200 — 03-A — 84-2

M. Morari

The process industries are a major consumer of energy and the improvement of energy efficiency is an important goal. Process modifications aiming at a reduction of energy consumption tend to make a plant more integrated and thus more difficult to operate. In practice, the primary objective is not only steady state energy efficiency but that the plant is flexible, operable and controllable, i.e. resilient. The research goals are to develop design strategies for resilient processes and operating policies for highly integrated plants. The particular subtasks are: 1) Synthesis of resilient energy management network, 2) Development of control strategies for integrated distillation columns, and 3) Development of control and optimization procedures for systems with high parametric sensitivity (chemical reactors). The latter two tasks involve an intensive experimental verification phase. The development of interactive user-friendly CAD packages incorporating the fundamental theoretical developments are under way. This work is carried out in collaboration with the University of Wisconsin.

UNIVERSITY OF CALIFORNIA, BERKELEY
Department of Mechanical Engineering
Berkeley, CA 94720

07. INVESTIGATION OF SECONDARY MOTIONS AND TRANSITION TO TURBULENCE IN BUOYANCY-DRIVEN ENCLOSURE FLOWS WITH STREAMLINE CURVATURE — $ 67,000; 01-C; 85-3

J.A.C. Humphrey, R. Greif

A study is underway to clarify the role of secondary motions and transition to turbulence in buoyancy driven enclosure flows. Four flow modes will be investigated experimentally. The modes are determined by the boundary conditions imposed along the side walls of the enclosure. In three cases they include the unsteady two-dimensional collision of buoyancy driven, opposed, vertical boundary layer flows. The fourth case corresponds to the "classical" recirculating flow configuration with one side wall heated and the opposite wall cooled.

Preliminary experimentation suggests that centrifugal instabilities produced by steamline curvature may be expected to induce "Taylor-Gortler-Like" (TGL) vortex structures in the flows. The conditions for which the instabilities occur, and the characteristics of the flows before and after their appearance, are subjects for research.

The results of this work are expected to contribute directly to the basic understanding of transition to turbulence and turbulent flow, and the ability to model these flows mathematically.

UNIVERSITY OF CALIFORNIA
Department of Mechanical Engineering
Davis, CA 95616

08. STABILITY AND STABILIZATION OF PREMIXED FLAMES — $ 90,000
C. K. Law — 06-B — 86-3

The program aims to investigate effects of heat loss, aerodynamic stretching, and preferential diffusion on the limits and mechanisms for flame propagation and the generation, suppression, and sustenance of flame-front corrugations; to identify the influence of these phenomena on flame stabilization, and to explore possibilities of widening the stabilization limits. Experiments are being conducted by using a variety of laboratory-scale burners to systematically isolate and identify the importance of the various system parameters on the phenomena of interest. Theoretical analyses using large-activation-energy asymptotics are performed for the various experimental flame configurations to provide guidance and confirmation.

UNIVERSITY OF CALIFORNIA, LOS ANGELES
Department of Mechanical Aeropsace and Nuclear Engineering
School of Engineering and Applied Science
Los Angeles, CA 90024

09. BASIC STUDIES OF TRANSPORT PROCESSES IN POROUS MEDIA — $145,000 — 01-C — 82-6
Ivan Catton

The research covers two broad areas: 1) single-phase convection in porous media and 2) two-phase convection in porous media. The objective of this study is to develop physical understanding of the governing phenomena and models for prediction of transport processes by theoretical and experimental means.

On the basis of a phenomenological stochastic model for single-phase flow through packed beds of random structure, a more refined formulation of the problem of mass and heat transport through porous media was obtained. The Forchheimer momentum equation was justified and an expression for the "effective" conduction coefficient was obtained. The latter accounts for (hydrodynamic) dispersive effects which are shown to lower the mean heat transport even for the low velocities encountered in natural convection through porous media.

Two-phase flow through uniform and stratified porous media were studied. Pressure drop and void-fraction data were analyzed to establish microscopic flow equations. The resultant equations include models of capillary pressure, solid drag, and interfacial drag. Analyses of two-phase flow through stratified beds were performed to study the effects of medium stratification on the hydrodynamic behavior of flow. Experimental studies of counter-current flow of superheated steam and subcooled water in uniform beds are underway.

Transport phenomena associated with the heating of a stationary meniscus formed by an inclined partially submerged copper plate has been investigated experimentally and theoretically. For a near isothermal interline, the meniscus local heat transfer coefficient was evaluated using an integral method and compared against data obtained via laser holographic interferometry. The superheated interline led to a wavy profile. A two dimensional linear stability analysis has predicted the frequency of oscillation measured.

UNIVERSITY OF CALIFORNIA, LOS ANGELES
Department of Mechanical, Aerospace
and Nuclear Engienering
School of Engineering and Applied Science
Los Angeles, CA 90024

10. ENHANCEMENT OF CRITICAL HEAT FLUX IN TUBES USING STAGED TANGENTIAL FLOW INJECTION — $ 43,000
01-B
85-3

V. K. Dhir

The objective of this work is to study experimentally and analytically the staged swirl flow concept for enhancing subcooled critical heat flux in tubes. In the staged swirl flow concept part of the coolant is injected tangentially at discrete locations along the tube axis. This method of injection not only results in a significant increase in the critical heat flux (CHF) but can also be used to shift the location at which CHF occurs. The shift is made possible by adjustment of flow rate through the injectors. The present study is divided into two main tasks:

The first task deals with optimization of the enhancement in subcooled critical heat flux with respect to diameter of the injectors, the angle subtended by the injectors with the tube axis and superposition of swirl created at different injection locations along the tube axis. The experimental study will be complemented with models for the swirl flow CHF and the two phase pressure drop.

In the second task basic understanding of heat transfer and pressure drop in swirling single and two phase flows will be developed. This task will include development of models for bubble detachment and motion under centrifugal action and superposition and decay of swirl under single and two phase flow conditons.

Water and Freon-113 loops have been updated and are already operational. DC power supply rated at 2500 amps and 40 volts has been installed. Critical heat flux enhancement data with subcooled water at 2 atmospheres pressure have been obtained. Separate experiments to develop understanding of superposition and decay of swirl have been initiated. A semi-theoretical model for superposition of swirl has been developed.

UNIVERSITY OF CALIFORNIA, SAN DIEGO
Scripps Institution of Oceanography MC A-013
La Jolla, CA 92093

11. NONLINEAR DYNAMICS OF DISSIPATIVE SYSTEMS — $ 70,000
Henry D. I. Abarbanel — 06-C
84-2

This research involves investigating the mechanisms which make for efficient energy transfer from a slow, mean motion to a system characterized by high frequencies relative to the mean motion. The basic mechanism of viscosity in a fluid is an example of this. The goal is to learn how to quantitatively characterize the "effective" or "eddy" viscosities used in phenomenological studies of energy, momentum, and other transfers of a turbulent fluid. The work is proceeding by studying analytically and numerically the behavior of systems of a few degrees of freedom as a function of their coupling. The systems are known numerically and, in certain regimes using the Melnikov method, analytically to exhibit chaos. In regimes of parameter space where the motion is regular or laminar the energy transfers are weak; in regions of chaotic motion the rate of transfer can be given a quantitative interpretation in terms of phase space correlation functions. The exponential decay of these functions on a rapid time scale, possibly related to the nontrivial Liapunov exponents of the chaotic motion of the rapidly evolving system, gives an additional rapid rate scale for the transfer of energy to the coupled slow system. Applications to energy problems include all those setups where "friction" or dissipation of a slowly evolving flow are the result of its interaction with a higher frequency system.

UNIVERSITY OF CALIFORNIA, SAN DIEGO
Department of Applied Mechanics
and Engineering Sciences
La Jolla, CA 92093

12. CHAOTIC ADVECTION AND EFFICIENT MIXING BY DETERMINISTIC FLOWS — $ 56,000
Hassan Aref — 01-C, 85-3

This project is concerned with the kinematics of regions of fluid and/or individual particles being swept along by a flow. The focus is on those aspects of the flow that tend to enhance stirring and mixing quality, and the ultimate goal is to arrive at quantitative criteria that can be helpful in the design of devices where stirring and mixing are important. The research is of relevance to several aspects of chemical and mechanical engineering.

It has been known for some time that the kinematics of particles advected passively by a flow is formally a problem closely related to the phase space description used in the study of dynamical systems. This formal correspondence leads to the notion of "Lagrangian turbulence," a situation in which the trajectories of advected particles is extremely complicated although the advecting flow is relatively simple in the usual Eulerian description. Particle motions can be "chaotic," in the technical sense of the word, and such motions lead to highly efficient stirring. The main thrust of the research is to understand the applicability of chaotic dynamics to advection and to investigate certain model flows in detail using numerical simulation techniques.

The main novel insights produced so far pertain to time-dependent two-dimensional flows. The efficient stirring of very viscous fluids via the mechanisms mentioned is being investigated. Model flows pertaining to stirring in devices without moving parts and the rate at which material interfaces can be stretched are issues slated for investigation during the coming year.

UNIVERSITY OF CALIFORNIA, SAN DIEGO
Institute for Nonlinear Science, B-003
La Jolla, CA 92093

13. THE STOCHASTIC TRAJECTORY ANALYSIS TECHNIQUE (STAT) APPLIED TO CHEMICAL, MECHANICAL, AND QUANTUM SYSTEMS — $ 85,000
06-C
86-3
Bruce J. West

The understanding of a number of important physical, chemical, and systems problems has been limited by the dearth of analytic tools to deal with non-Markovian processes. We have formulated a new technique that we propose to further develop in directions dictated by a number of important applications. Each application requires a different kind of extension of the theory. The applications we propose to consider include chemical reactions in fluids, wave propagation in random media, the survival probabilities of randomly loaded systems, and quantum mechanical energy propagation in polymers.

UNIVERSITY OF CALIFORNIA, SANTA BARBARA
Department of Chemical and Nuclear Engineering
Santa Barbara, CA 93106

14. INVESTIGATION OF FLUID DYNAMIC PHENOMENA NEAR GAS-LIQUID INTERFACES — $ 90,000 — 01-C — 85-3
S. Banerjee, H. Fenech

The purpose of this project is to study the fluid dynamic phenomena near the interface of cocurrent and countercurrent gas-liquid stratified streams. Interfacial configuration, wave characteristics and turbulence structure are measured experimentally using two different techniques. Oxygen bubble tracers in water and long exposure photography are used to follow the path of individual bubbles and obtain a statistical distribution of the turbulent velocity components and Reynolds stress at several distances from the interface in a region of fully developed flow. The alternative method consists of capturing, photographically, the evolution of dye streaks in an organic liquid seeded with a photochromic dye which is activated in streaks by a UV laser. Two separate experimental facilities have been constructed and tests are being conducted using each method. The results obtained from the oxygen bubble technique at Reynolds numbers of 5,000 and 10,000 both show that, near the free surface, the motions into the free surface are damped while the streamwise motions are promoted.

CARNEGIE-MELLON UNIVERSITY
Chemical Engineering Department and
Graduate School of Industrial Administration
Pittsburgh, PA 15213

15. STRATEGIES FOR OPTIMAL REDESIGN IN A CHANGING ENVIRONMENT — $144,000 — 03-A — 85-4

L. T. Biegler, I. E. Grossmann,
G. L. Thompson, A. W. Westerberg

As the chemical industry matures it is important to consider the redesign of existing processes to accommodate changes in the environment. Redesign problems tend to be harder to solve than "grassroots" problems because constraints dealing with the existing process need to be considered. Therefore, determination of optimal modifications in an existing plant generally will be quite different from optimal solutions for a new plant. This project addresses the optimal redesign problem through the following areas:

(1) Optimization and heat integration strategies for existing flowsheets - process simulation or flowsheeting plays an important role in evaluating redesigns. Here, advanced optimization strategies are applied to rigorous and complex simulation models. In addition, simultaneous optimization and heat integration strategies have been developed to guide improved designs.

(2) Primal/dual linear (LP) and quadratic programming (QP) algorithms- these algorithms form the heart of many advanced nonlinear programming strategies. However, existing methods generally do not perform well for highly constrained problems. This project deals with the development of new LP and QP algorithms based on relaxation of primal and dual constraints. Preliminary results indicate that this strategy is about 10 times faster than current methods for large linear programs. A code for quadratic programming has also been developed and is currently being tested on both randomly generated problems and chemical engineering examples.

(3) Redesign for flexibility and controllability - based on recently developed strategies for evaluation of process operability, mixed integer nonlinear programming strategies are being developed for improving operability through structural modifications. Specialized to linear applications, these strategies are straightforward to apply and yield very useful information about the trade-off between cost and improved process operability. Also, problems are addressed for improving the dynamic behavior of a process by introducing minor structural changes.

CARNEGIE MELLON UNIVERSITY
Mechanical Engineering Department
Pittsburgh, PA 15213

16. EXPERIMENTAL AND THEORETICAL STUDIES OF VERTICAL ANNULAR LIQUID JETS — $ 95,000
N. Chigier, J. I. Ramos — 06-C, 86-3

The objective of this study is to determine the dynamics and convergence length of vertical annular jets as a function of the inlet inner radius, inlet thickness, inlet velocity, inlet flow angle, surface tension, and turbulence. Another objective is to study the start-up and stability of annular liquid jets. The experimental part of the program will be performed with different liquids in order to determine the effects of the Froude, Reynolds, and Weber numbers and geometry on the convergence and stability of annular jets. The theoretical part of the research program will deal with the development of an implicit finite-difference scheme for studying the dynamics and stability of annular liquid jets. These theoretical studies will be based on the solution of the time-dependent axisymmetric form of the Navier-Stokes equations and will account for surface tension and for the adverse axial pressure gradient which occurs near the annular liquid jet convergence. Simplified models based on a parabolic approximation in which the axial pressure gradient is neglected, and on an extension of the Boussinesq equations will also be developed. The results of these models will be compared with each other and with experimental data to be obtained at Carnegie Mellon University and at the Westinghouse R&D Center.

UNIVERSITY OF CHICAGO
Department of Chemistry
Chicago, IL 60637

17. TOPICS IN FINITE-TIME THERMODYNAMICS $ 75,000
R. Stephen Berry 06-C
86-3

The objective of this research is the analysis in thermodynamic terms of the performance of systems and processes subject to time or rate constraints. Part of the research deals with developing methods for conducting analyses, such as emerged from the introduction of a suitable metric in the space of thermodynamic variables and the evaluation of path lengths with that metric. The lengths so obtained have been shown to be directly related to the dissipation associated with the path. Another piece of recent work at this basic level just completed under this project is an attempt to introduce a variational formulation of irreversible heat transfer and diffusion, which is intended to apply in nonlinear as well as linear situations.

The other aspect of this research is the application of the general methods to the analysis of specific systems of current interest. During the initial period of this project, the stopping of a beam of atoms by absorption and re emission of laser light was analyzed and the entropy changes in the process were evaluated. The reduction in entropy of the atomic beam due to cooling and stopping is compensated a thousandfold over by the increases in the entropy of the light due to randomization of the phase, the polarization and especially the propagation direction.

UNIVERSITY OF CHICAGO
Enrico Fermi Institute
Chicago, IL 60637

18. FUNDAMENTALS AND TECHNIQUES OF NONIMAGING OPTICS FOR SOLAR ENERGY CONCENTRATION — $140,000 — 06-C — 81-6

R. Winston, J. J. O'Gallagher

Nonimaging optics departs from the methods of traditional optical design to develop instead techniques for maximizing the collecting power of concentrating elements and systems. Designs which exceed the concentration attainable with focusing techniques by factors of four or more and approach the theoretical limit are possible. This is accomplished by applying the concepts of Hamiltonian optics, phase space conservation, thermodynamic arguments, and radiative transfer methods. In the early nonimaging designs the mighty edifice of aberration theory was dismantled and replaced by a single key idea. According to this, maximum concentration is achieved by ensuring that rays collected at the extreme angle for which the concentrator is designed are redirected, after at most one reflection, to form a caustic on the absorber. This principle proved sufficiently elastic to accommodate most boundary conditions in two dimensions (i.e., linear geometry). Ideal solutions in three dimensions have also been formulated. Our work on vector flux has led to a reexamination of the foundations of radiometry with emphasis on observable effects. Experiments to detect these effects are being planned.

CLARKSON UNIVERSITY
Department of Chemical Engineering
Potsdam, NY 13676

19. NUMERICAL STUDIES OF COHERENT EDDIES IN WALL-BOUNDED FLOWS — $ 56,000
J. McLaughlin — 01-C, 82-6

The objectives of the work are to obtain information about the origin of the "coherent" wall eddies which are responsible for the formation of "streaks" in the viscous wall region of turbulent shear flows and to obtain information about their importance in transport. The work involves pseudospectral simulations of channel flow and a three dimensional model of the viscous wall region. The unique feature of the studies lies in the choice of computer experiments which are employed in order to obtain information about the coherent eddies. These experiments can be divided into three groups (1) "wave break-up" experiments in which, after integrating sufficiently far in time to achieve statistical steady-state, certain spatial Fourier components of the velocity field are set to zero and then allowed to recover their energy by time-evolving the velocity field using the modified field as an initial condition; (2) studies in which steady, spanwise-modulated transpiration is applied at the walls in an attempt to modify streak spacings and to determine what effect such a modification has on the transport of energy and momentum; and (3) studies of the breakdown from transitional to turbulent flow with emphasis on the formation of coherent wall eddies.

CORNELL UNIVERSITY
School of Electrical Engineering
School of Mechanical and Aerospace Engineering
Ithaca, NY 14853

20. COMBUSTION CONTROL WITH SMART SENSORS — $ 0
G. J. Wolga, F. C. Gouldin — 01-C
82-6

The objective of this project is to develop and demonstrate a "smart" spectroscopic sensor suitable for monitoring gaseous combustion products by differential infrared absorption spectroscopy. The sensor is a computer controlled tunable acoustooptic infrared filter with sufficient resolution to resolve individual vibration-rotation absorption lines in the 5-6.5 micron spectral region. It will be self calibrating with respect to temperature changes and thus the sensor can operate unattended indefinitely. A tunable CO laser has been used to develop an accurate tuning curve for the filter in the 5 to 6.5 micron spectral region. Differential absorption spectra from CO and CO_2 spectra are incompletely resolved due to the smaller rotational constant and overlapping hot bands. Thus, we use the CO spectrum to obtain the gas (rotational) temperature. Comparison of the observed spectrum with a synthesized spectrum permits a temperature determination which compares very favorably with thermocouple measurements within the exhaust plenum. Data analysis procedures for handling absorption integrated over a path length have been developed for conditions of cylindrical spatial symmetry and relatively small absorption. Current efforts concern: developing methods for determining gas concentration with resolved and unresolved spectra; introducing combustion particulates into the flow to determine the effects on signal to noise and consequently on the accuracy and precision of our measurements; modeling combustion exhaust gas flow in a power plant to select the best location for our sensor.

DARTMOUTH COLLEGE
Thayer School of Engineering
Hanover, NH 03755

21. SUBCOOLED SPRAYS IN A VAPOR ENVIRONMENT-TESTS OF THE TWO-FLUID MODEL FOR TWO-PHASE FLOW — $155,000 — 01-C — 86-3
G. B. Wallis, H. J. Richter

The "separated" or "two-fluid" model for two-phase flow is being used to describe the behavior of a subcooled spray in a vapor environment. Detailed measurements will be used to determine viable forms of the "interaction" terms describing mass, energy and momentum transfer between the phases. The overall purpose is to advance the state-of-the-art of basic analytical and computational tools for describing two-phase multidimensional flow.

In the two-fluid model each phase satisfies the usual set of equations of conservations of mass, momentum and energy with the influence of one phase on the other appearing as "interaction terms" that couple the two sets. While much effort has been devoted to writing down various forms of equations and discussing how they can be obtained by averaging the basic conservation laws for each phase, few workers have actually applied them to specific situations. It is likely that useful and reasonable simple expressions can be devised to represent coupling effects when the flow pattern is clearly defined: for instance, a dispersion of one phase in the other. Previously, physically-based formulations have been applied to a one-dimensonal representation of fluidized beds, sedimentation, and "mist-lift" processes or the two- and three-dimensional modeling of sprays in gases and particles interacting with a fluid.

This project concerns a dispersed flow regime in which heat and mass transfer play leading roles: the condensation of vapor on a subcooled spray of droplets. Analysis of this regime requires the inclusion of significant interaction terms in all of the conservation laws, thus providing a comprehensive test of the theory. Complementary analytical and experimental work are planned. The experiments are intended to build up to realistic complexity (e.g., a drop size spectrum in the spray, variations in spray flux as a function of angle) while keeping the flow pattern sufficiently well-defined to be amenable to theoretical representation.

ELECTROCHEMICAL TECHNOLOGY CORP.
1601 Dexter Ave. N.
Seattle, WA 98109

22. ELECTROCHEMICAL WEAR MECHANISM AND DEPOSIT FORMATION IN LUBRICATED SYSTEMS — $ 0, 01-D, 82-3

T. R. Beck

The objective of this research is to measure and determine the importance of electrokinetic or zeta corrosion and deposit formation in lubricating rolling and sliding systems. Zeta corrosion is a phenomenon identified and modeled in 1968 for hydraulic servo control valves in commercial jet airplanes. This corrosive wear problem has now been solved by appropriate additives based on the theory. The approach of the present research is to compare measurements of wear for rolling and sliding lubricated systems to calculated zeta corrosion rates based on extensions of the valve wear model. Extensive electrokinetic and wear experiments have been carried out with nylon filaments or cloth rubbing on steel with lubricants of micron-filtered water or salt solutions. This system eliminates abrasive and adhesive wear. Use of aqueous solutions allows comparison to phenomena in the extensive corrosion literature for iron. Waveform of electrokinetic currents measured with an iron microelectrode rubbing transversely on a nylon filament on a shaft were in agreement with predictions of a model derived from hydrodynamics and electrical double layer theory. The measured currents were sufficient to account by Faraday's law for weight losses by wear of thin steel disks rubbing on aqueous lubricated nylon cloth. This wear is independent of oxygen partial pressure from 5 ppm to 5000 ppm, indicating a wear component not driven by oxygen reduction. The wear can be eliminated by cathodic protection and by well-known corrosion inhibitors, indicating that it is electrochemical in nature. The various measurements all indicate that zeta corrosion is responsible for the wear results.

FLOW INDUSTRIES, INC.
21414 68th Avenue South
Kent, WA 98032

23. DIRECT NUMERICAL SIMULATIONS OF TURBULENT HEAT TRANSFER — $115,000
R. Metcalfe — 01-B
84-3

The purpose of this research is to apply the technique of direct numerical simulation to the study of turbulent heat transfer. Direct numerical simulation techniques have been applied successfully to such problems as the testing of turbulence theories, an examination of second order closure modeling assumptions, and addressing questions about the basic physics of the evolution of turbulent flows. In this work, direct numerical simulations of turbulent convection in the presence of background shear have been performed. The basic effect of the shear is to reduce the randomness of the convection and introduce anisotropy by aligning large scale structures in the direction of the mean flow. The presence of shear tends to decrease both the total heat transfer and the departures from the linear profiles of mean temperature and velocity. The simulations show that the pressure diffusion term plays an important role in the energy balance equation and should not be neglected in turbulence models.

GA TECHNOLOGIES INC.
10955 John Jay Hopkins Drive
San Diego, CA 92121

24. FLUID MECHANICS OF ACOUSTIC RESONANCE IN HEAT EXCHANGER TUBE BUNDLES — $ 0, 01-C, 82-4
R. D. Blevins

The purpose of this study is to develop a predictive fluid mechanics model for acoustic resonance in shell and tube heat exchangers. Acoustic resonance in heat exchangers is the result of acoustic oscillations of gas in sympathy with periodic fluctuations in the flow over tubes. In the experimental phase of the program, a simulated tube bundle is being constructed which will be tested in air flow. Direct measurements of the onset of resonance, intensity and mode of acoustic pressure will made with microphones, and measurements of the exciting fluid dynamic fluctuations about the tube will be made with hot wire anemometers. Results will be processed on-line using fast Fourier transforms. In the theoretical phase of the program, a linear acoustic model for the phenomenon will be developed using acoustic source and dissipation terms and a calculated acoustic mode shape. The experimental results will then be used to refine the acoustic source and dissipation terms, and develop a fundamental understanding of the fluid dynamic and acoustic interaction. A nonlinear model for the self-excitation will then be developed using Lighthill's formulation for aerodynamic sound in interaction with the coherent structures in the flow due to vortex shedding from the tubes.

GA TECHNOLOGIES INC.
P.O. Box 85608
San Diego, CA 92138

25. HIGHER DIMENSIONAL NONLINEAR DYNAMICS $ 0
John M. Greene and Jin-Soo Kim 06-C
85-3

The goal of this project is to explore how the methods of nonlinear dynamics can be applied to ever more complex systems.

The modern theory of nonlinear dynamics is, to a large extent, the understanding of the way in which computational results can be used to gain insight into the nature of chaotic and turbulent systems. A property of such systems is that two different orbits that are crudely indistinguishable are generally quite different in their detailed behavior. Thus a single orbit, or realization, contains a confusing mixture of uninteresting detailed information, and usefully generalizable information. The most easily obtained, additional, exact information that computers can provide comes from the solution of equations linearized around a given orbit. The objective of our program is a thorough understanding of the information available through linearization.

This information mostly falls under the key words of Lyapunov exponents and directions. That is, we will study the information available in the rates and directions of separation of nearby orbits, or realizations. The first phase will be a thorough analysis of some ordinary differential equations. Then we will undertake the study of some partial differential equations.

GEO-CHEM RESEARCH ASSOCIATES
400 East Third Street
Bloomington, IN 47401

26. PREDICTIVE MODELING OF URANIUM ROLL TYPE DEPOSITS — $ 80,000
P. J. Ortoleva — 06-A
83-4

Oxidizing meteoric waters percolating through a reduced sandstone aquifer can cause the accumulation of uranium and other ores at the redox interface. The oxidation of pyrite to hematite or geothite can lead to several instabilities underlying observed ore body properties. The existence (and in some cases non-uniqueness) of propagating redox fronts in ore-reductant systems (such as pyrite) was demonstrated and a general exact value for its speed was obtained for the lossless aquifer. The nonexistence of constant velocity redox fronts in multireductant systems was proven analytically and shown numerically to correspond to an accumulation of one mineral at the front of the other - the essential trapping process leading to redox deposits.

A class of instabilities was found when reaction-induced porosity variations were allowed to interact with the percolation flow through the porosity-dependent permeability of Darcy's law. The planar front of dissolution of soluble components in a sandstone aquifer (as pyrite in oxidizing inflow waters) was found analytically to be unstable to the formation of bumps. The range of wavelengths of the most rapidly growing array of bumps brackets the observed wavelengths in roll front deposits when geologically reasonable flow and porosity values were used in our expressions. Numerical simulations of the full nonlinear problem confirmed the linear analysis, and showed that, interestingly, a single bump (in the shape of the surface on which porosity changes) can branch into two fingers. Even very small changes in porosity across the redox front can lead to this fingering.

Nonlinear transport/reaction interactions underly the genesis of uranium roll-front deposits and directly control their geometry and quality. These insights are potentially very useful for exploration.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Technology Group
Idaho Falls, ID 83415

27. ELASTIC-PLASTIC FRACTURE ANALYSIS — $365,000
EMPHASIS ON SURFACE FLAWS — 01-A
W. G. Reuter — 81-6

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluation guiding the direction of experimental testing. Tests are being conducted on a material (a modified ASTM A-710) exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength. As test temperature increases, the specimen configuration-fracture toughness relationship complies initially with requirements for linear elastic-fracture mechanics and extends beyond the range of a J-controlled field. Presently, compact tension and bend specimens are being used to develop state-of-the-art fracture mechanics data on the lower shelf (K_{IC}), transition zone (J_{IC}, J-R curves, etc.) and on the upper shelf (J_{IC}, J-R. curves, etc.). Results from the lower shelf and transition region are being used to predict failure conditions for specimens containing surface flaws. Predictions are then compared with experimental test data. These tests have been supplemented by data generated from Ti-15-3 heat treated to develop a plastic zone size of nominally 0.1 mm. These comparisons are presently underway for 6.4 and 12.7 mm thick surface-flawed specimens. Metallographic techniques are being used to measure crack tip opening displacement and remaining ligament size for comparison with analytical models. Laser interferometry techniques are being used to evaluate and quantify the deformation in the crack region.

IDAHO NATIONAL ENGINEERING LABORATORY
Sensors and Diagnostics Group
Idaho Falls, ID 83415

28. IN-FLIGHT MEASUREMENT OF THE TEMPERATURE OF SMALL, HIGH VELOCITY PARTICLES — $ 90,000
J. R. Fincke — 06-A, 85-3

Knowledge of in-flight particle temperature is fundamental to understanding particle/plasma interactions in the physical and/or chemical processing of fine powders. The measurement of in-flight particle temperature is based on a coincidence technique. A small measurement volume is defined by two independent lens/sensing systems. When a particle is present in the measurement volume, a signal will be observed and recorded simultaneously by each sensing system. Once a signal is recorded, the particle temperature may be deduced. The uncertainty in this temperature determination will be due to lack of information concerning the particle size, shape, and emissivity; and due to the presence of an emitting, absorbing, and scattering medium.

The program consists of three phases. In Phase 1 (FY 85) individual particles were electrodynamically suspended, then heated by a laser beam. The particle temperatures and emissivities were measured. Results to date indicate that optical property data for the parent material are adequate for estimation of particle emissivity. In Phase II (FY 86) the in-flight coincidence technique was developed. This effort included the development of both analog and digital signal processing techniques. Phase III will apply, and modify as necessary, these techniques to measure particle temperatures in a high temperature plasma. This phase of the program will address the problems associated with the presence of an emitting, absorbing, and scattering atmosphere.

This project is one of six projects comprising a collaborative research program with the Massachusetts Institute of Technology.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Technology Group
Idaho Falls, ID 83415

29. EXPERIMENTAL MEASUREMENT OF THE PLASMA/PARTICLE INTERACTION — $328,000 — 06-A — 85-3
M. E. McIlwain, C. B. Shaw, S. C. Snyder, L. D. Reynolds

The objective of this research is to quantitatively describe the heat mass, and momentum transfer associated with metallic or oxide particles immersed in thermal plasma environments. In order to characterize the interaction between plasma constituents and particles, the development of new methods to determine plasma flow velocity and species compositions are being developed. Holographic interferometry is currently being considered for plasma flow velocity determination and planar laser induced fluorescence is being considered for compositional measurements adjacent to particle surfaces. Using these advanced techniques, temporal and spatially resolved distributions of the chemical and physical properties of the plasma/particle environment will be determined. Since this research is performed in collaboration with research at Massachusetts Institute of Technology, the resulting experimental data will be used to validate and correct theoretical models used for thermal plasma processing and for predictions relating to optimal torch and fixture design criteria. Experiments are currently being performed in two plasma torch designs, a constricted nozzle torch and an expanding nozzle torch. Input power dissipation levels ranging from 5 to 180 kW are being studied. These torch designs produce a representative plasma characteristic of those employed for industrial plasma processing.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Technology Group
Idaho Falls, ID 83415

30. INTEGRATED SENSOR/MODEL DEVELOPMENT FOR AUTOMATED WELDING — $496,000 — 03-A
H. B. Smartt, J. A. Johnson, J. O. Bolstad — 85-3

The objectives of this research are (1) to develop a model of the gas metal arc welding process suitable for real-time process control, (2) to develop an optical sensing capability to provide critical weld bead geometry data, and (3) to develop an ultrasonic sensing capability to directly sense weld bead side-wall fusion and penetration. This project is part of a collaborative research program with the Massachusetts Institute of Technology.

A fundamental model of the gas metal arc welding process has been developed which considers wire melting and heat and mass transfer to the base metal. Although iterative numerical solution techniques are required, finite difference/finite element methods are not used. A computer controlled welding machine has been built and used to demonstrate the ability to independently control the heat and mass input to the weld, using the above model in combination with an adaptive feedback control scheme. This work is being extended to allow real-time, optimized control of pulsed current welding to be achieved.

A pulsed laser enhanced, gated electro-optical sensor has been developed which suppresses most of the welding arc light, providing an image of the electrode wire, weld pool, and surrounding base metal which is suitable for image processing. Image processing techniques are being developed to obtain quantitative information from the above images regarding the weld pool geometry and position.

Direct sensing of the weld pool solid/liquid interface location is being developed using conventional pulse-echo ultrasonic transducers. Signal analysis/pattern recognition techniques are being developed for automated measurements. Signal generation by use of laser pulses directed on the weld pool surface is also being studied.

IDAHO NATIONAL ENGINEERING LABORATORY
Advanced Methods Projects Group
Idaho Falls, ID 83415

31. EXPERT SYSTEM AIDS FOR ANALYSIS CODES $246,000
V. H. Ransom, R. K. Fink 06-C
R. A. Callow, T. K. Larson 85-3

The objectives of this research are to establish the impact that expert systems will have on the architecture of engineerng analysis codes and to assess the potential benefits that expert systems can produce when used as aids to engineering analysis tasks. The tasks of physical system abstraction and modeling, input model preparation, output analysis, and code execution have been identified as profitable applications for expert systems. Programming language compatibilities and inter-computer communications have been identified as potential problems in implementation of such systems. These problems have been avoided in the present research by using a XEROX 1108 AI workstation for the expert system research and communicating with the engineering analysis computer via a local area network. In this way InterLISP D and LOOPS, an AI language and expert system building tool, can be used yet communication with a FORTRAN based analysis code.

A prototype modeling and input expert system has been built for the ATHENA code, a general purpose thermal hydraulic system transient simulation code. The input system is designed to provide an intelligent environment to assist the analyst in developing a model of a thermal hydraulic system. The intelligent environment provides input conviniences such as engineering units conversion as well as higher level assistance in the model abstraction process that embodies rules for correct use of the code and the heuristic knowledge that has evolved from successful application of the code to physical problems. Present research is focusing on the human-computer interface and means for facilitating the analytical model abstraction of the physical system. Future research will include experimentation with the use of expert system methods for output interpretation and to more effectively control the execution phase of the analysis code.

IDAHO NATIONAL ENGINEERING LABORATORY
Sensors and Diagnostics Group
Idaho Falls, ID 83415

32. NONDESTRUCTIVE CHARACTERIZATION OF FRACTURE DYNAMICS AND CRACK GROWTH — $193,000 — 03-B — 83-5

J. A. Johnson, B. A. Barna, R. A. Allemeir

The purpose of this research is to develop instrumentaiton and models to measure and predict the emission and interaction of ultrasound from growing cracks in engineerng materials, and to investigate methods of sensing the properties of growing cracks.

Models of the ultrasonic field/crack interaction are based on a numerical ray-tracing algorithm and on a numerical (finite difference) solution to the partial differential equations (PDE) describing the system. In the ray-tracing model, an ultrasonic transducer, operating in the pulse-echo mode is assumed to be equivalent to a large number of spherical sources spread uniformly over the face of the transducer. The total field in the region of a crack is calculated as the sum of the fields from all these sources. The reflected and diffracted fields from the crack are calculated from the incident field from the transducer and a model of the field-crack interaction. These fields are then traced back to the transducer face and the integrated field across the face is determined.

In the finite difference model, a source of acoustic emission (AE) is modeled by changing boundary conditions and the ultrasonic fields that propagate from the source to a receiver are calculated. All mode conversions are automatically included in the numerical solution to the PDE with the boundary conditions of the system.

The dynamic crack growth measurements have used ultrasonics techniques to measure the properties of a growing crack. An advanced AE detection system is being developed which will be capable of detecting and digitizing AE signals at much higher frequencies than in conventional systems. This will allow improved resolution in detecting the locations of the sources of emissions and in discriminating between types of sources.

This program is coordinated with the Elastic-Plastic Fracture Analysis program at INEL and the Modeling and Analysis of Surface Cracks at Massachusetts Institute of Technology.

UNIVERSITY OF ILLINOIS
Department of Chemical Engineering
Urbana, IL 61801

33. GAS-LIQUID FLOW IN PIPELINES $102,000
Thomas J. Hanratty 01-C
86-3

Research is being conducted to obtain a better understanding of gas-liquid flow in horizontal and vertical pipelines. The goals are (1) to develop methods to predict the initiation of slugs in horizontal gas-liquid flows, and (2) to obtain a better understanding of the interfacial wave patterns in stratified gas-liquid flows, (3) to obtain improved predictive models for horizontal and vertical annular flows, (4) to obtain an improved predictive model for stratified flows. Experiments are being conducted in two facilities which allow for studies with three different pipe diameters and a range of liquid viscosities.

A linear theory has been developed that describes the initiation of slugs at low gas velocities. This is being tested by examining the effect of liquid viscosity. The reason for the inapplicability of this theory at high gas velocities is being explored. The main feature of the model for stratified flow is that it incorporates the effect of waves on the interfacial stress. The principal problem in modeling annular flow is the prediction of the fraction of the liquid entrained. Correlations for this quantity are being developed from measured rates of atomization and deposition.

UNIVERSITY OF ILLINOIS AT CHICAGO
Energy Resources Center
Chicago, IL 60680

34. BOILING OF AQUEOUS POLYMER SOLUTIONS — $ 67,000
J. P. Hartnett — 06-A
85-2

The goal of this research is to study the pool boiling behavior of aqueous polymer solutions, both purely viscous and viscoelastic with the objective of providing accurate boiling measurements using well-defined fluids. Detailed measurements of the transport and rheological properties of the test fluids are being carried out prior to and following the experiments. It has been determined that the chemistry (i.e. changes in the polymer structure as a result of increases in operating temperature level, interactions with the materials of the test section, etc.) plays a major role. Consequently, careful monitoring of the rheology is critical if the boiling results are to be meaningful. The direct measurements of the boiling heat flux and surface and fluid temperatures will be supplemented by photographic studies to provide additional insight into the boiling process.

Measurements of free convection heat transfer from horizontal platinum wires to surrounding purely viscous and viscoelastic non-Newtonian fluids have been carried out prior to the boiling studies. For free convection to purely viscous non-Newtonian fluids at Rayleigh numbers of the order of 10^{-2} to 1 it is found that the Nusselt number decreases with decreasing power law index whereas at high Rayleigh number $Ra \gg 1$, the Nusselt number increases with decreasing power law index. In the case of free convection to viscoelastic fluids the heat transfer measurements are in agreement with values predicted for Newtonian fluids provided that the zero shear rate viscosity is used for the viscoelastic fluid viscosity.

UNIVERSITY OF ILLINOIS AT CHICAGO
Department of Civil Engineering,
Mechanics, and Metallurgy
Chicago, IL 60680

35. CONTINUOUS DAMAGE THEORY — $ 44,000
Dusan Krajcinovic — 01-A
83-4

The research conducted during the past year was focused on two seemingly disparate tasks; establishment of a common mathematical basis for the phenomenological models and formulation of a micromechanically based continuum damage model. As it turned out the two tasks had a lot in common. Using the effective field approximation it was possible to derive the compliance tensor for an elastic solid weakened by an ensemble of microcracks.

Once the essential structure of the analytical model was established it was possible to demonstrate that the so called scalar, second and fourth order tensor models are only the truncations of the general model. Moreover, the phenomenological model developed during the work on this project proves to be directly related to the micromechanical one. In other words, the proposed phenomenological model also contains the scalar, second and fourth order tensor models as special cases.

The so called Taylor approximation was used to simplify the analyses using the micromechanical model. The results in replicating the experimental trends are very encouraging.

The current plans are to further develop the formulated models with an ultimate objective of the combined brittle-ductile phenomena.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Chemical Engineering
Chicago, IL 60616

36. METHOD OF VIBRATIONAL CONTROL IN THE PROBLEM OF STABILIZATION OF CHEMICAL REACTORS — $ 54,000 — 03-A — 84-3

Ali Cinar

The objective of this project is to develop the vibrational control technique for complex nonlinear dynamic systems with multiple steady states and limit cycles. From the mathematical standpoint, the goal of this research is to analyze the effects of fast parametric oscillations on the dynamics of the systems studied. During the third period of the project the tasks were:

1. To study the effects of simultaneous vibrations in two input variables. The effect of frequency, amplitude and phase shift have been studied numerically and experimentally using a CSTR with homogeneous liquid phase exothermic reaction.

2. To complete the construction of a reaction system with a packed-bed CSTR and to conduct preliminary experiments for assessing the effect of vibrational operation on the selectivity of a parallel reaction. As a test reaction the oxidation of ethylene over supported silver catalysts to ethylene oxide and to carbon dioxide is used.

3. To study the effect of vibrational control on distributed parameter systems. A tubular packed-bed reactor system is used. Detailed and reduced-order models of a packed-bed tubular reactor system have been formulated. To determine the ranges of input variables for stable operation, steady state bifurcation diagrams based on the detailed reactor model as well as short-cut techniques for stability analysis have been developed.

The models developed in tasks 2 and 3 are being used by the research group at the University of Michigan (S. M. Meerkov, Principal Investigator) for theoretical studies in vibrational control.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Mechanical and
Aerospace Engineering
Chicago, IL 60616

37. INTERFEROMETRIC MEASURMENTS IN DOUBLE-DIFFUSIVE SYSTEMS — $ 80,000
William M. Worek, Zalman Lavan — 03-B, 84-3

The objective of the project is to develop a nonintrusive experimental technique to simultaneously measure two scalar variables in double-diffusive or other two component systems. The experimental technique utilizes a dual-frequency (i.e., dual-source) Mach-Zehnder Interferometer to simultaneously measure the variation of refractive index within the test system at two disparate wavelengths. Two interferograms, simultaneously acquired at the two wavelengths, are then analyzed using refractive index data, which are temperature, concentration and wavelength dependent, to resolve the temperature and concentration fields in the test system.

The variation of refractive index with temperature, concentration and wavelength in a saline water solution was not thoroughly documented previously. The first part of the experimental program was expanded to acquire this data. This data is then used in subsequent experimental tests in a laboratory scaled double-diffusive system. Also, the experimental program will be integrated with an analytical approach in an attempt to identify and assess the potential application of such a technique and the impact on stability studies in double-diffusive systems.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

38. BASIC DATA FOR THE DEVELOPEMENT OF MOLECULES AS THRESHOLD ELECTRON DETECTORS — $ 0 — 03-B

A. Chutjian, S. Alajajian — 82-3

Measurements are being made of, at ultralow electron energies and at high electron energy resolution, lineshapes and cross sections for attachment of thermal electrons to a number of perfluorinated and chlorohalocarbon compounds. These molecules have been shown to be viable candidates for use as molecular detectors of extremely low-energy (0-20 millielectron volt) electrons. In particular, the molecules c-C_5F_8 (perfluorocyclopentene) have been shown to have extremely large cross sections, and narrow wings, and are well-suited to use as electron detectors in an appropriate collision geometry. In parallel, theoretical calculations are carried out to understand observations in terms of the molecular potential energy surfaces involved, and to explain temperature dependencies of the attachment phenomena.

LAWRENCE BERKELEY LABORATORY
Physics Division and
Accelerator and Fusion Division
University of California
Berkeley, CA 94720

39. STUDIES IN NONLINEAR DYNAMICS $150,000
Allan N. Kaufman, Robert G. Littlejohn 06-C
80-6

This project involves studies of fundamental properties of nonlinear dynamical systems which arise in physical situations of important to energy research. Four subjects are being explored. First, theoretical studies to generalize the WKB representation of wave phenomena are in progress. The main theme of this work is the use of phase space methods to represent wave fields and evolution operators. These are most conveniently implemented in terms of wave packets, and lead to results which are uniform, representation-independent, and free of caustic singularities. Recent progress includes a general theory of quantization with wave packets. Second, a new formulation of conservative dissipative processes is being explored, in which the entropy and energy functionals jointly generate the time-evolution of the system. Third, action principles are being used to imbed single-particle Lie-transform perturbation methods in collective models, such as Vlasov-Maxwell systems. Nonlinear phenomena (e.g., ponderomotive forces) are thus dealt with self-consistently. Fourth, we have initiated a study of adiabatic variation of parameters in non-ergodic, non-integrable Hamiltonian systems.

LAWRENCE BERKELEY LABORATORY
Energy and Environment Division
University of California
Berkeley, CA 94720

40. CONTROLLED COMBUSTION $190,00
A. K. Oppenheim 06-B
79-8

The principal objective of this study is to provide scientific background for the development of controlled combustion systems, i.e. prime movers whose combustors are not only sources of power, as they are according to current technology, but also operate as chemical reactors at a modern high tech level, so that the evolution of exothermic energy is properly monitored to eliminate combustion instabilities and minimize the formation of pollutants. For I.C. engines this offers the prospect of efficient and clean combustion associated with relatively low exhaust temperatures, devoid of such problems as knock and cycle-to-cycle variation, leading thus to the annihilation of major technological constraints imposed upon the automotive industry: the octane standard and the catalytic converter. Means to accomplish this involve an exploitation of active radicals obtainable from plasma and flame jets as well as from product recirculation. Major laboratory apparatus consists of a molecular beam mass spetrometer and a shock tube associated with an assortment of laser-powered optical apparatus including systems for megacycle-frequency schlieren cinematography and laser induced fluorescence imagery. The experimental program is supplemented by a significant effort in numerical modeling of the fluid mechanic, thermodynamic, and chemical kinetic aspects of the processes under study.

LOS ALAMOS NATIONAL LABORATORY
Electronics Division
Los Alamos, NM 87545

41. DEVELOPMENT OF THERMIONIC INTEGRATED CIRCUITS (TICs) — $ 96,000, 03-B, 82-6

B. McCormick, D. Wilde, R. Lemons, M. MacRoberts, D. Lynn, R. Dooley, D. Brown

The object of this project is to develop electronics that are capable of operating in both high-temperature and high-radiation environments while maintaining levels of circuit sophistication, integration, and reliability demanded of modern electronics. The approach taken for these active electronic-gain devices has been to use the intrinsically high-temperature phenomenon of thermionic emission in conjunction with the thin-film technology of integrated circuits to produce microminiature vacuum triodes. High-temperature tests have been conducted at 500°C with no degradation in device characteristics. Current research is focused on improving cathode lifetime, emission, and geometry to ensure the reliability and functionality of TIC technology in high-temperature and high radiation environments.

UNIVERSITY OF MARYLAND
Department of Mechanical Engineering
College Park, MD 20742

42. NUMERICAL MODELLING ENERGY RELATED FLOWS $ 0
B.S. Berger 01-C
85-1

The objective of the current study is the numerical determination of the motion of elastic tubes oscillating in a crossflow. A computer program has been written and fully tested which calculates the transient two dimensional motion of an unconstrained circular cylinder which is restrained by a spring and damper. The fully coupled Navier Stokes rigid body equations are solved. Extensive numerical tests have been performed for Re=400 which are in agreement with experimental results. Solutions for the static case have been found for Re=1000 and 2000.

The model of the vibrating tube as a rigid circular cylinder restrained by a spring and damper has been replaced in a second computer simulation by a continuous model. The linear partial differential equations describing the motion of a slender beam have been coupled with the two dimensional Navier Stokes equations. This approximation is currently under test for Re=400. It is anticipated that higher values of Reynold's number will be attained.

THE UNIVERSITY OF MARYLAND
Department of Mechanical Engineering
College Park, MD 20742

43. AN INVESTIGATION OF THE ENERGY AND VORTICITY DYNAMICS OF TURBULENT SHEAR FLOWS — $ 30,000 / 01-C / 85-3

Peter S. Bernard

A description of the dynamics of the vorticity field is central to an understanding of the physics of turbulent shear flows. This follows both from the ubiquitous presence of coherent vortical structures in turbulent flows as well as from the role played by vortex stretching in energy transference and the establishment of local dissipation rates. The MVC (Mean Vorticity and Covariance) closure allows for a connection to be made between phenomenological events occurring in shear flows and the overall balance of the vorticity field. The objective of this research effort is to use these properties of the MVC theory to formulate a complete model of the energy and vorticity dynamics of turbulent shear flows. This is to be carried out by seeking numerical solutions to the closure equations in the context of channel and zero pressure gradient turbulent boundary layer flows. To aid in the analysis of the boundary layer as well as for comparison purposes, experimental measurements of terms in the vorticity and energy equations taken by a nine-sensor vorticity probe are also being obtained.

UNIVERSITY OF MARYLAND
Department of Electrical Engineering
College Park, MD 20742

44. STUDY OF MAGNETOSTATIC PROBLEMS IN NONLINEAR MEDIA WITH HYSTERESIS — $ 62,000 / 06-C / 83-4

I. C. Mayergoyz

This project has two main research objectives: (1) to develop boundary Galerkin's approach and its quasi-finite-element realization in order to circumvent the difficulties which are related to the unbounded regions of field distribution, and (2) to investigate mathematical models of hysteresis and develop the methods for the calculation of magnetostatic problems in media with hysteresis.

As far as the first objective is concerned, the calculation of magnetic fields in unbounded regions will be reduced to coupled boundary/volume Galerkin's forms and a new quasi-finite-element projection technique will be developed on this basis. The problems concerning convergence of the quasi-finite-element methods, existence and uniqueness of the solution of simultaneous nonlinear quasi-finite-element equations and global iterative methods of the calculation of the solution of these equations will be the focus of this research.

For the second objective, mathematical models of hysteresis as continuous superposition of rectangular hysteresis nonlinearities will be investigated. Special attention will be paid to the solution of identification problems and to the generalization of these models for the case of vector hysteresis. The application of continuation methods to the calculation of magnetostatic fields in media with hysteresis will be studied.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, MA 02139

45. TURBULENT PREMIXED FLAME STUDY $ 0
Wai Cheng, James Keck, 06-B
Steve Pope (Cornell University) 83-3

This program is a combined experimental and theoretical study of premixed turbulent flames. The primary aim of the experiment is to study the growth behavior and some detailed properties of statistically spherical flames. The theoretical part of the program centers on the description of the flame behavior using the pdf formulation. Techniques using a thin sheet laser light to illuminate the flame ball have been developed to look at the relationship between the flame structure and the burn rate. The illuminated flow will be recorded on high speed movies and the image will be digitized. Then the topology and dynamics of the flame structures will be analyzed statistically. Experiments to examine the effect of pressure gradient on the flame propagation characteristics is planned. The development of a pdf description of the turbulent flame behavior follows the experiment closely. The approach is to model the topology of the flame surface by studying their kinematics and dynamics. Initially the reaction zone will be modelled as a simple regular propagating surface which propagates at the laminar flame speed. Then the effects of curvature and stretching on the flame speed will be added and local breakdown on the regular surface due to self-intersection and the formation of cusps will be examined. The experimental and theoretical efforts will lead to a comprehensive description of the turbulent premixed flames.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Energy Laboratory
Cambridge, MA 02139

46. A PARITY SIMULATOR FOR NUCLEAR POWER PLANT DYNAMICS — $1,386,000
06-C
K.F. Hansen — 85-3

The simulation of the behavior of dynamic systems is an important part of the computer field. The great advances in digital electronics are such that most simulation is done digitally. However, problems unique to the use of digital computers, such as computer languages, numerical algorithms, and computer/user interfaces have made simulation of engineering systems difficult and/or awkward. This is particularly true with regard to transient analysis of nuclear power plants.

One area of analog simulation that has remained in widespread use is that of "breadboard" circuits to simulate electric electronic networks. Recent developments have led to a very flexible and convenient breadboard technique called parity simulation, where individual integrated circuits in the simulator behave as individual circuit elements. The system is also user friendly in that the analyst communicates in his own engineering language.

It is well-known that electric analogs can be constructed to other physical systems such as mechanical, thermal, fluid, magnetic, or acoustic systems. Research in this project is aimed at developing integrated circuit analogs to plant components, such as pipes, reactor cores, heat exchangers, pumps, etc. The IC elements will solve the conservation equations of mass, energy, and momentum. Thus far elements have been developed for single phase compressible and incompressible flow.

This is one of several projects carried out in cooperation with Idaho National Engineering Laboratory/EG&G.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Materials Science and Engineering
Cambridge, MA 02139

47. PLASMA REDUCTION OF METALLIC OXIDE PARTICLES — $ 76,000 — 06-A — 85-3
J. F. Elliott, J.Szekely, R. E. Spjut

The objective of this research is to characterize the reduction to metal of oxide particles injected into the tail flame of an arc plasma. At the present time, it is not known if a significant degree of reaction occurs in flight, or if such reduction processes require a molten bath and, hence, a transferred arc plasma. The experimental method involves injecting mixtures of carbon and metallic oxide particles, in the size range of 20 to 100 microns, into an arc plasma just beyond the point of initial generation and sampling downstream at various distances with a simple, water-cooled suction cup. The particles thus removed from the plasma may be examined by microscopy and electron microanalysis to determine the extent of reduction.

Another important aspect of this work is to determine the rate of heat transfer between the plasma and injected solid particles. In a preliminary set of experiments, solid particles of varying thermophysical properties will be injected into the plasma and then collected. By sectioning and analyzing these particles it will be possible to establish the extent to which melting has in fact occurred. These experimental measurements will be critically compared with the theoretical predictions.

The new 50ks furnace has been installed and placed in operation. It can be operated in either the non-transferred arc or transferred arc mode. The system is equipped with automatically controlled devices for feeding powders into the plasma flame. Initial work has been begun on the physical and chemical modification of simple oxide particles and composite carbon-oxide particles that have passed through the plasma flame.

This work is closely coordinated with the plasma modelling and gas-particle studies in progress at MIT, and with measurements of particle trajectories and temperatures of particles passing through plasma flames that are in progress at the Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Plasma Program
Cambridge, MA 02139

48. HIGH TEMPERATURE GAS-PARTICLE REACTIONS — $230,000
J. F. Elliot, R. E. Spjut, P. P. Bolsaitis — 06-A
85-3

The objective of the research program is to examine the physicochemical behavior of individual inorganic particles in conditions simulating those to which particles are exposed in arc plasmas. In the experimental arrangement, a particle is suspended by the field in an electrostatic balance and it is heated in a laser beam. Manipulation of the charge on the particle and precise measurement of the strength of the field permits determination of the weight of the particle before and after its exposure to the laser beam, and under some conditions, during the heating and cooling of the particle in the experiment. The composition of the gas in the reaction chamber is controlled, and the temperature of the particle can be measured and controlled with a time resolution as short as one or two milliseconds.

Experiments are in progress to determine the rate of volatilization of alumina and silica particles in various gas compositions, and the kinetics of reactions in composite carbon-alumina and carbon-silica particles.

This work is closely coordinated with the other plasma processing programs in the Department of Materials Science and Engineering at MIT and with the experimental program on plasma processing at the Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Materials Science and Engineering
Cambridge, MA 02139

49. MATHEMATICAL MODELLING OF TRANSPORT PHENOMENA IN PLASMA SYSTEMS — $102,000
J. Szekely — 06-A
85-3

The purpose of this investigation is to develop a comprehensive mathematical representation of the electromagnetic force field, the velocity field, temperature field and chemical composition of plasma flames, together with their interaction with solid particles.

To date, computed results have been obtained describing the flow field, the temperatures and the composition of a non-transferred arc with swirl, with annular and sideways injected gas streams.

It has been shown that swirl plays a profound effect in modifying both the flow and the entrainment of the secondary and tertiary streams. These calculations should form the basis of the rational design of plasma reactors.

The theoretical predictions are being compared to measurements conducted at the Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, MA 02139

50. ENERGETICS OF COMMINUTION $148,000
Carl Peterson 06-C
85-3

This program is central to a broader program of comminution research that includes basic studies on the behavior of single particles, particulate beds, and the design and testing of a novel coal crushing concept.

Single particle work has progressed the furthest. A very rigid miniature compression testing device has been fabricated and data generation has just begun. Behavior of the device is satisfactory and computer data acquisition is being installed to permit routine testing of a statistically significant number of particles. This device will provide information on force and energy requirements for particle fracture as a function of particle size and material properties. A new theory of comminution has been proposed which seems to explain the shift in energies required for failure as size decreases for uniform materials. More complex materials such as particles with voids and composite materials will be examined next. The increased difficulty to fracture a particle of smaller size has a practical significance in the crushing behavior of particulate beds.

Particulated bed work will include both analytical and experimental studies, seeking the combination of bed stress and strain required to cause individual particle fracture within some zones of the bed. These studies will ultimately tie back to the individual particle failure studies when computer simulations are used to predict particle movements and forces acting on the particles.

A novel comminution mill has been designed which uses particle-to-particle shear to cause particle failure.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Ocean Engineering
Cambridge, MA 02139

51. IN-PROCESS CONTROL OF RESIDUAL STRESSES AND DISTORTION IN AUTOMATIC WELDING — $ 87,000
03-A
85-3

Koichi Masubuchi

The objective of this research program is to develop the technology of in-process control of residual stresses and distortion in automatic welding. The program consists of the following three phases:

Phase 1: In-process control of residual stresses and distortion in some weldments.

Phase 2: Development of technologies for minizing and eliminating, if possible, tack welds.

Phase 3: Plans for future advancement of the technology of in-process control of residual stresses and distortion.

The effort thus far covers primarily Phases 1 and 2. The program has been carried out smoothly as originally proposed.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, MA 02139

52. INVESTIGATION OF VISIBLE AND NEAR VISIBLE LIGHT EMISSIONS AS SENSORS FOR CONTROL OF ARC WELDING PROCESSES — $ 75,000 — 03-B — 85-3
Thomas W. Eagar

The present research is part of a cooperative program among faculty at MIT and staff at Idaho National Engineering Laboratory to develop sensing and control methods which can be used to automate the gas metal arc welding processes.

Recent research has mapped the light emissions spatially, temporally, and spectrally, from gas tungsten welding arcs. The experimental method makes use of a somewhat unique subtractive double monochromator, which provides a two dimensional image of the arc while filtering out all but a specific range of light wavenumbers. Thus it is possible to photograph the distribution of relatively weak elements in the arc without the disturbance of the strong argon or helium background spectra. By studying the emission of Mn or Cr on stainless steels, it is possible to see clearly the anode spot on the weld surface. Video movies of the spot movement are being made and will be analyzed to determine the true heat distribution on the weld surface. Spectra from arcs on several different materials have been measured to determine regions in the frequency spectrum which are relatively free of light. It is hoped that such regions will identify windows where it will be best to utilize the laser weld pool sensor being developed by INEL.

Additional work has begun on modelling of the mechanism of metal transfer in gas metal arcs. Experimentally, a laser back lit viewing system has been developed which permits viewing of anode and cathode jet phenomena, thus helping to determine the effect of these gas flows on metal transfer. An image intensifier has been added to the subtractive double monochromator described above with the intent of studying the metal vapors produced during GMAW welding. This work interfaces with the experimental GMAW control system being developed at INEL.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Laboratory for Manufacturing and Productivity
Cambridge, MA 02139

53. MULTIVARIABLE CONTROL OF THE GAS-METAL ARC WELDING PROCESS — $102,000
David E. Hardt — 03-B, 85-3

The process of Gas Metal Arc Welding (GMAW) involves many process control variables such as arc voltage, current, travel speed, wire feed rate, and voltage pulsing profile. These multiple inputs to the weld cause changes in multiple outputs such as weld width, depth, reinforcement height and thermal effects in the weldment. All existing work in closed-loop control of welding, however, has treated this highly coupled, multiple input-multiple output system as a single variable control problem, concentrating, for example, on controlling just the weld width or depth.

The objective of this work is to cast the GMAW control problem in its most general sense and then examine the use of advanced mutlivariable control methods. We have begun this work at two extremes, one starting from a specific two-variable problem in GMAW for which models and measurements exist, and the other from a more basic, but idealized perspective. The former will allow us to quickly identify where gaps in our knowledge of the process and the characterization of the measurements exist, and allow us to perform initial experiments within the first year of the project. The latter will begin building a comprehensive framework for the solution of the complete control problem, defined as independent regulation of all relevant outputs while rejecting a significant range of system disturbances.

This project is coordinated with the experimental work at Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Energy Laboratory
Cambridge, MA 02139

54. MODELING OF GMA WELD POOL GEOMETRY AND METAL TRANSFER — $ 88,000
William Unkel — 03-B
85-3

Realtime control of weld parameters such as weld pool geometry can reduce welding flaws and therefore increase the productivity of producing welded structures. One important component to achieving online control is a physically-based model of the welding process. For a complex process such as welding, models play several roles including:

a) interpreting noisy and often indirect measurement data;

b) identifying process modifications that make multivariable control easier; and,

c) providing a component of the actual control algorithm.

Previous modeling efforts have concentrated on the Gas Tungsten Arc Welding (GTAW) process and have laid the groundwork for the present work on the Gas Metal Arc Welding (GMAW) process.

The principal goal of the present work is to develop physically based, but computationally simple models for the GMAW situation and to use these models to identify process modifications to allow a more effective multivariable control system to be implemented. Those models will be confirmed by comparison with experimental data and will also be considered for use in online interpretation of sensor data.

This research is coordinated with the experimental work at Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Mechanical Engineering
Cambridge, MA 02139

55. MODELING AND ANALYSIS OF SURFACE CRACKS — $200,000 — 01-A — 85-3

David M. Parks
Frank A. McClintock

This research focuses on the analysis of ductile crack initiation, growth and instability in part-through surface-cracked plates and shells. The overall approach consists of determining parametric limits of applicability of the "dominant singularity" formalism at nonlinear fracture mechanics in these crack configurations as they are influenced (principally) by material strain hardening, load biaxiality, and crack geometry. When such single-parameter dominance is obtained, correlations of crack response with J-integral or related measures may be justified. The analysis requires detailed finite element computations which are too costly for routine applications, so further development of simplified analytical models such as the so-called "line-spring" model is underway. Exploratory experiments are also being undertaken to probe effects of asymmetry of loading, prior plastic strain history, and other factors on subsequent ductile fracture. Load biaxiality effects have been simulated for axial tension and internal pressure loading on pipes containing a circumferential crack. Accepted solutions for J derived for tension alone can underestimate fully plastic biaxial J-values by up to an order of magnitude.

Recent developments have resulted in marked improvement in agreement between calculations and experimental data obtained in a parallel effort at INEL.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Energy Laboratory
Cambridge, MA 02139

56. DEVELOPMENT OF AN EXPERT SYSTEM TO SYNTHESIZE HEAT AND WORK INTEGRATION SYSTEMS FOR PROCESS PLANTS — $ 62,000 — 06-C — 85-3
L. B. Evans

The goal of this research is to develop a prototype expert system for the synthesis of heat and work integration systems in process plants. This is an important problem in the design of new plants and the retrofitting of existing plants for energy conservation.

The expert system will assist the process engineer in designing heat and work integration systems. A scientific approach to the design of such systems based upon sound thermodynamic principles has emerged within the past decade, so there is now an accepted set of design rules or heuristics that is a prerequisite for an expert system.

The development of a prototype system seeks to answer many open questions, such as: What is the appropriate architecture for the system? How should the knowledge base be represented? What is the best strategy for generating and evaluating alternative solutions? Are standard tools of artificial intelligence suitable for this problem or must we develop specialized procedures? Is an expert system useful either as an aid or alternative to the solution of the problem by a human designer?

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, MA 02139

57. PISTON RING FRICTION AND VEHICLE FUEL ECONOMY — $115,000
D. P. Hoult — 01-D
80-6

A novel method, using laser fluorescence, has been used to measure oil film thickness on the piston skirt, liner, and piston lands for the first time. Preliminary results shows that although the oil film thickness between the rings and liner is in good agreement with theory, the thickness of lubricant on the piston lands is nearly 5-10 times larger than theory predicts.

The method is accurate to a fraction of a micron, and is self calibrating in a running engine. A study is underway to make a detailed survey of the oil film thickness on the piston lands and skirt.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Mechanical Engineering
Cambridge, MA 02139

58. THE DEVELOPMENT OF A FRICTION MODEL PREDICTING THE SLIDING BEHAVIOR OF MATERIAL PAIRS, ESPECIALLY AT LOW TEMPERATURES — $ 65,000, 01-D, 85-2
Yukikazu Iwasa

The principal objectives of this research program are 1) to develop a friction model which predicts correctly whether a system sliding at low speeds will give steady or unsteady sliding behavior and 2) to advance basic understanding of the friction process.

The program consists of experimental and analytical studies. Experimental work includes collection of data on creep properties of the two contacting materials, namely bulk creep behavior in tension and interface creep data in shear. The interface creep takes place when one material is pressed against the other by a constant force and a shear force insufficient to produce gross sliding is applied. The extent to which the bulk creep properties determine the interfacial creep behavior both at room temperature and at cryogenic temperatures will be determined, and this knowledge should lead to better models of the friction process. In turn, such knowlege will contribute to a more reliable operation of superconducting magnets.

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, MA 01003

59. A DESIGN AND SYNTHESIS PROCEDURE FOR HOMOGENEOUS AND HETEROGENEOUS AZEOTROPIC DISTILLATIONS — $ 35,000 — 06-A — 85-3

M. F. Doherty

New techniques are being developed to aid in the design and synthesis of multicomponent, nonideal and azeotropic separation systems. The synthesis problem is a difficult one for it not only entails choosing the optimal column configuration and processing conditions, but also involves choosing the optimal entrainer. The problem is compounded by the presence of distillation boundaries in azeotropic mixtures which put severe constraints on the feasible class of column sequences. At present there is no systematic method available in the literature for solving this synthesis problem.

The technique being developed is based on the concept of a residue curve map. These maps represent the fundamental phase-equilibrium behavior of the mixture in a way which is uniquely suited for separation-system studies. The maps provide information for discriminating between feasible and infeasible column sequences. New design tools have also been developed for calculating such quantities as minimum reflux ratios for azeotropic mixtures. The ultimate aim of this research program is to develop a comprehensive body of theory which will result in automatic computer procedures for synthesising optimal separation sequences for multicomponent azeotropic mixtures.

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, MA 01003-0011

60. A HIERARCHICAL PROCEDURE FOR FLOWSHEET, CONTROL SYSTEM, AND RETROFIT DESIGN FOR CHEMICAL PROCESSES — $130,000 — 03-B — 83-6

J. M. Douglas, M. F. Malone

The objectives of the research were to develop new tools that could be used to develop conceptual process designs, to quickly screen retrofit opportunities, and to assess potential control problems at the conceptual stage of a process design. An interactive computer program for conceptual design has almost been completed. This code contains both a qualitative knowledge base (including many new design heuristics that we have developed) and a quantitative knowledge base (including many new short-cut design procedures that we have developed). The code proceeds through a hierarchy of decisions, so that projects with poor prospects can be terminated early. However, in its present form, it is limited to vapor-liquid processes. The short-cut design procedures for complex distillation columns, which were developed with funding from this grant, are currently being added to the code.

A code for process retrofits has just been started. The models for complex columns will also be included in this code. Again, a systematic procedure for screening retrofits will be used as the basis for the code. We have developed a systematic approach for synthesizing steady-state control systems that are close to optimal, but we are still working on a procedure to extend the results to dynamic systems.

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, MA 01003-0011

61. MIXING: STRETCHING, BREAKUP, AND CHAOTIC MOTION OF IMMISCIBLE LIQUIDS — $ 53,000
J. M. Ottino — 01-C
85-3

In spite of its universality and practical implications, mixing of fluids is largely an empirical art. The goal of our research focuses on two aspects of the problem with long range objective of establishing a sound background for the analysis of such processes:

(i) experimental investigation of the conditions that determine the onset of chaos in deterministic two dimensional flows.

(ii) studies of the dynamics of stretching and breakup of small droplets in such flows.

Thus, (i) focuses on a global scale whereas (ii) is a local analysis--deformation and breakup in a Lagrangian (linear) time dependent flow. This brief report highlights primarily point (i). During the past year we established experimentally that a periodically operated two dimensional cavity flow is capable of chaotic behavior. Since this implies exponential separation of initial conditions (fluid filaments) this finding has also practical significance. Our investigation centered primarily on the detection of horseshoe functions and in contrasting the behavior of periodically operated flows with steady flows, investigation of the influence of the period of the oscillation, and the geometry of the cavity. We determined that there is an optimum period to accomplish the best mixing (in a qualitative sense) in a given time. Similar studies are being conducted in a newly developed eccentric journal bearing flow. So far, most of our work was conducted using only one fluid (Newtonian) but we are now starting experiments involving two different fluids, for example a blob of a Newtonian fluid immersed in a viscoelastic one. Finally, in (ii) we developed models to study the stretching of slender low-viscosity breakup in linear flows. Our long-range goal is to be able to connect these studies with those developed in (i).

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, MA 01003

62. MULTIVARIABLE AND DISTRIBUTED CONTROL OF NON-LINEAR SYSTEMS — $ 57,000
E. Ydstie — 03-B
85-3

The objective of this work is to develop a methodology for nonlinear, adaptive control of chemical and petroleum processes. The algorithm we investigate is suited for implementation in a distributed network of computers and it is amenable for complete plant control and optimization. The approach is motivated by the many recent successful applications of linear adaptive control theory, however our approach relies on physically based process models and the maximum use of prior information about system characteristics. Our investigation will include:

- algorithmic development and stability analysis,
- application to a distributed control of pilot process,
- simulation and optimization of a complete plant.

UNIVERSITY OF MICHIGAN
Department of Mechanical Engineering and Applied Mechanics
Ann Arbor, MI 48109

63. LOSS CHARACTERISTICS OF CORD-RUBBER COMPOSITES — $ 73,000
S. K. Clark — 01-D
83-3

The research to be carried out under this contract is divided roughly into two phases. The first is the completion of data acquisition on the loss characteristics of cord-rubber composites under both uniaxial and multiaxial stress states. This effort will utilize information currently available as well as measurements made here. The effects of prestrain, frequency, strain amplitude and temperature will be included in the assessment of the viscoelastic properties of these materials.

The major activity during the latter part of the work will be analysis and measurement of the rolling loss of a relatively simple pneumatic tire. The tire geometry will be essentially cylindrical in form, similar to the type of tire used in vehicles traversing soft or marshy terrain. These are essentially cylindrical rollers, but with end closures making it possible to inflate them. Analysis will be carried out using the viscoelastic material properties previously obtained, as well as finite element codes suitable for this type of problem. Comparison of calculated and measured rolling resistance values will give valuable insight into the types of finite element models best suited for this computation, and should give confidence to the tire industry in its efforts to apply finite element techniques to the calculation of tire operating properties.

Since tire rolling resistance represents a major component in the vehicular fuel consumption, minimization of it represents an important part of the overall national energy consumption effort.

UNIVERSITY OF MICHIGAN
Department of Electrical Engineering
and Computer Science
Ann Arbor, MI 48109

64. METHOD OF VIBRATIONAL CONTROL IN THE PROBLEM OF STABILIZATION OF CHEMICAL REACTORS — $ 97,000
Semyon M. Meerkov — 03-B — 85-2

The objective of this research project is to develop a new control technique, referred to as vibrational control, and apply it to systems where traditional approaches, based on the feedback or feedforward principles, are not applicable. From the mathematical standpoint, the goal of the project is to analyze the effects of fast parametric oscillations on the dynamics of nonlinear systems with multiple steady states and limit cycles. The approach used in the research is based on asymptotic analysis (averaging theory) of deterministic and stochastic, ordinary and partial differential equations. The results obtained or being currently developed include: (i) theory of vibrational control for nonlinear systems; (ii) theory of vibrational-feedback control; (iii) vibrational control of distributed parameter systems; (iv) vibrational control of stochastic systems. The main application considered is in the area of exothermic and catalytic CSTR's and tubular reactors. The obtained theoretical results and their implementation in terms of chemical reactors have been utilized by the research group at the Illinois Institute of Technology (A. Cinar, Principal Investigator) in experimental studies on vibrational control.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, MN 55455

65. FLOW AND HEAT TRANSFER WITH IMPINGING JETS AND WALL JETS — $120,000
R. J. Goldstein — 01-B, 81-6

This program consists of a number of interrelated projects on heat and mass transfer, as well as flow distribution in impinging jets, wall jets and separated flows. The research on impinging jets includes a study of the influence of angle of inclination, between the jet and surface, on heat transfer and another study on heat transfer in a three temperature problem when the surface, jet and ambient are at different temperatures. The latter study requires further consideration of adiabatic or recovery wall temperatures, as occur in other problems with mixing fluid streams. When the spacing between the origin of the jet and the wall is relatively small, there appears to be a thermal or enthalpy separation due to the large curvature of the flow.

In a wall jet, measurements are made of detailed turbulence properties determined from a specially designed laser-Doppler system and newly developed software to determine velocity fluctuations from measurements at two different orientations. Results, including profiles of shear stress, are being compared to predictions for turbulent transport, which have been developed in other studies.

The separated flow research includes mass transfer measurements, over two dimensional cavities, as well as flow around two and three dimensional roughness elements. With flow around small or large circular cylinders protruding from the surface, a horseshoe vortex and a series of smaller vortices within the horseshoe vortex are inferred from mass transfer measurements. At some locations transport coefficients are an order of magnitude greater than those observed along the cylinder far from the plate surface.

In these studies, special measurement techniques are being developed. One is the use of liquid crystals with a special constant temperature bath to reduce heat losses as well as prevent overheating of the surface; another is a microprobe to measure local heat flow; a third in an automated profilometer to measure changes in a subliming surface.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, MN 55455

66. THERMAL PLASMA PROCESSING OF MATERIALS $142,000
E. Pfender 06-A
85-3

A combined analytical/experimental program is carried out directed towards a better understanding of the interaction of particulate matter with thermal plasmas. One of the major objectives of the work is the development and diagnosis of a new plasma reactor which should solve the problems of particle injection, particle confinement, and particle dwell time in the plasma. Finally, it is intended to use this reactor for materials studies involving superconducting alloys.

The modeling work is primarily concerned with a detailed assessment of the relative importance of the numerous effects which determine heat, momentum, and mass transfer to and from particles injected into thermal plasmas. Diagnostic methods for the plasma include emission spectroscopy, laser Doppler anemometry, current, voltage, and calorimetric heat transfer measurements. Product powders will be analyzed using scanning and transmission electron microscopy, x-ray and electron diffraction, and measurements of the transition temperature for superconducting compounds.

NATIONAL BUREAU OF STANDARDS
Tribology Group
Institute for Materials Science & Engineering
Gaithersburg, MD 20899

67. A STUDY OF THE CHEMICAL MECHANISM IN LUBRICATION $ 86,000
S. M. Hsu 01-D
84-4

The chemical mechanisms responsible for lubrication in concentrated tribological contacts are not well understood. The project is examining systematically both the nature and extent of the influence of chemical reactions on friction and wear in the contact zone. Advances have been made in theoretical modeling of the temperature profiles in a four-ball contact; modeling of elastohydrodynamic film at concentrated contacts; analytical characterization of model structures; and the investigation of interactions between naturally occurring polar species and antiwear additives. Pure model structures are being used as lubricants to test the effects of chemical functional groups on friction and wear. Chemical kinetic studies on tribochemical reaction rates for various classes of compounds under wearing conditions will be compiled. The topography of worn surfaces will be characterized to predict oil film thickness under different speed and load combinations using the NBS six-microliter four-ball wear tester. Micro-asperity and contact zone temperatures will be studied and computations will be made using Archard-Jaeger equations as well as finite element analysis. A theoretical model linking elastohydrodynamic theories to tribochemical rate constants with material properties will be attempted to predict lubrication effectiveness a priori.

NATIONAL BUREAU OF STANDARDS
Thermophysics Division
Gaithersburg, MD 20899 and Boulder, CO 80303

68. THERMOPHYSICAL PROPERTY MEASUREMENTS IN FLUID MIXTURES — $520,000 — 03-B
N. A. Olien, J. M. H. Levelt Sengers — 84-3

The project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multiphase, fluid mixtures containing hydrocarbons. The research is being done jointly by two research groups within the Thermophysics Division of the NBS Center for Chemical Engineering. One group is located at the Gaithersburg, MD laboratories and the other at the Boulder, CO laboratories. The properties involved are PVT (pressure-volume-temperature), PVTx (pressure-volume-temperatures-composition), phase equilibria (liquid-vapor and liquid-liquid equilibria), phase behavior in interfaces, and transport properties (viscosity, thermal conductivity, and diffusion coefficient). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (800K) and high pressure (30 MPa and in some cases 70 MPa). Also under study are methods for evaluating supercritical solvent mixtures and related fluid mixtures.

CITY UNIVERSITY OF NEW YORK
The City College
Department of Chemical Engineering
New York, NY 10031

69. TOPICS IN PHYSICO-CHEMICAL HYDRODYNAMICS — $250,000, 06-A, 80-8
Benjamin G. Levich

This research comprises two main directions:

(i) Fully Developed Turbulence (FDT). We aim at the entirely novel understanding of the nature of FDT. We assert that the structure of FDT is determined by a foam-like topology of the vorticity field lines where the prime role is played by the hierarchy of helical fluctuations. The active production of turbulence in this picture proceeds outside of these fluctuations and concentrates in space of fractal dimensionality. Presently, we have extensive experimental data to support our view. Further experiments are underway.

(ii) *Interfacial Mechanics.*

(a) A mechanism for the development of the deformation patterns commonly observed on the surfaces of biological cell plasma membranes was suggested. In this mechanism, the membrane is treated as a viscoelastic continuum and a chemical reaction network on the surface of the membrane regulates the membrane elasticity.

(b) Hydrodynamic waves induced by chemical reactivity waves were studied. Results indicate that a wave of chemical reactivity derived from a multistable chemical reaction on the surface of a thin liquid film is able to induce a hydrodynamic wave in the film through the Marangoni tractions due to the reactivity wave.

(c) The classical linear capillary instability of a thin fluid filament surrounded by a bulk fluid was investigated for the case in which the filament is in steady shear flow. Results indicate that a nonlinear interaction between the shear flow and the capillary forces can, under certain conditions, stabilize the developing linear instability.

NORTH CAROLINA STATE UNIVERSITY
Department of Mechanical and Aerospace Engineering
Raleigh, NC 27695-7910

70. TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA FROM THE MICROSTRUCTURE — $ 90,000 — 01-C — 86-3
S. Torquato

This research program is concerned with the quantitative relationship between certain transport properties of a disordered porous medium that arise in various energy-related problems (e.g., thermal (and electrical) conductivity and the fluid permeability) and its microstructure. In particular, we shall focus our attention on studying the effect of: porosity, spatial distribution of the phase elements, interfacial surface statistics, phase conductivity, and size distribution of the phase elements, on the conductivity and permeability of models of both unconsolidated media (e.g., soils and packed beds of discrete particles) and consolidated media (e.g., sandstones and sintered materials).

The program has been broken down into four basic tasks: (1) the development of theoretical expressions for the bulk properties which depend upon the microstructure through various sets of statistical correlation functions, (2) the evaluation of these and other correlation functions that have arisen in the literature for nontrivial models of porous media, using results and methods of statistical mechanics, (3) the calculation of transport-property expressions which involve this statistical formulation, and (4) the comparison of theoretical results to experimental measurements of the conductivity and permeability of porous media. We are in the process of computing microstructure-sensitive property relations for models of porous media with heretofore unattained accuracy.

NORTHWESTERN UNIVERSITY
Department of Civil Engineering
Evanston, IL 60201

71. EFFECTS OF CRACK GEOMETRY AND NEAR-CRACK MATERIAL BEHAVIOR ON SCATTERING OF ULTRASONIC WAVES FOR QNDE APPLICATIONS — $ 65,000 / 03-B / 83-3
J. D. Achenbach

Among the methods of quantitative non-destructive evaluation of structural elements, the method based on scattering of ultrasonic (elastic) waves by flaws is particularly useful. The work on this project is concerned with applications of the scattered field approach to the detection and characterization of cracklike flaws. The work is both analytical and numerical in nature. Several forward solutions to model problems have proven to be very helpful in the design of experimental configurations. They have also provided invaluable aid in the interpretation of scattering data for the inverse problem. In recent work, numerical results have been obtained by the finite difference method (flaws near surfaces) and by the boundary element method (distributions of voids). The usual mathematical modeling of ultrasonic wave scattering by cracks is being extended to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks. Work is in progress on scattering by a cloud of microcracks and/or a plastic zone, which surrounds a crack tip. Further parametric studies are expected to display the masking of characteristic "crack-like" features of the scattered field by a spectrum of signals due to deviations from idealized crack geometries and idealized material behavior.

NORTHWESTERN UNIVERSITY
Department of Chemical Engineering
2145 Sheridan Road
Evanston, IL 60201

72. THINNING AND RUPTURE OF A THIN LIQUID FILM ON A HORIZONTAL HEATED SOLID SURFACE — $334,000 — 01-C — 86-3

S. G. Bankoff

The proposed work aims at studying the non-isothermal rupture of a thin liquid film under controlled conditions. The program consists of experiments on a horizontal film on a plate containing a heater strip and theoretical analyses of such systems. The experiments will monitor the film profile and observe the critical heat fluxes for film rupture and for rewetting. The theory will account for thermocapillarity and evaporation during an initial phase of the process. It will be augmented by disjoining pressures due to van der Waals attractions during the final phase of rupture.

OAK RIDGE NATIONAL LABORATORY
Engineering Physics and Mathematics Division
Oak Ridge, TN 37831

73. CENTER FOR ENGINEERING SYSTEMS ADVANCED RESEARCH (CESAR) — $965,000
C. R. Weisbin — 03-C, 84-10

The Center for Engineering Systems Advanced Research (CESAR) conducts interdisciplinary long-range research and concept demonstration related to intelligent machines. CESAR provides a framework for merging concepts from the fields of artificial and machine intelligence with advanced control theory. There are two primary themes: robotic systems for identification, navigation, and manipulation in unstructured environments; and multi-purpose plant management and maintenance.

Specific FY 86 research initiatives resulting in publications included: (1) development of methods for real-time planning with sensor feedback, (2) determination of concurrent algorithms for optimal implementation on advanced parallel computers, (3) formulation of a learning theory for enhanced knowledge acquisition and interpretation, (4) modelling the dynamics of flexible structures, (5) generation of automated sensitivity analysis methods for model simplification and parameter identification (6) generation of a machine vision system based on principles of human vision, and (7) inclusion of (1)-(6) within a systems integration framework encompassing concept demonstration and feasibility.

PHYSICAL SCIENCES INC.
Research Park, P.O. Box 3100
Andover, MA 01810

74. EXPERIMENTAL AND THEORETICAL STUDIES OF CONDENSATION IN MULTICOMPONENT SYSTEMS — $114,000, 06-A, 84-4
M. B. Frish, G. Wilemski

This research program comprises experimental and theoretical studies of nucleation and condensation in multicomponent gas mixtures. The program goals are: 1) to improve basic understanding of binary nucleation and droplet growth, 2) to stringently test theories of binary nucleation at high nucleation rates and under nonisothermal conditions, 3) to develop improved theories where needed, 4) to enlarge the data base for systems of both fundamental and practical interest, and 5) to provide reliable means for predicting the behavior of mixtures used in practical applications such as turbo-machinery. Experimentally, gas mixtures will be cooled in a supersonic nozzle to obtain much higher binary nucleation rates than have previously been studied. The nozzle is designed to insure that steady state nucleation occurs and to give satisfactory spatial resolution of the temperature profile. Laser light scattering is the primary means of detecting nuclei as small as 10A in radius and of monitoring droplet growth. Interferometry is used to diagnose the temperature profile within the nozzle. By varying the amount of insert carrier gas used, both isothermal and nonisothermal nucleation will be studied. Construction of the flow and optical systems is complete, and data collection has begun. A new thermodynamic theory of binary cluster composition has been developed. Calculations with this theory have established the feasibility of using bulk liquid mixture surface tensions to compute nucleation onset (for small rates) in aqueous alcohol and acetone mixtures, thus removing a severe deficiency of classical binary nucleation theory.

PURDUE UNIVERSITY
School of Mechanical Engineering
West Lafayette, IN 47907

75. HEATING AND EVAPORATION OF TURBULENT LIQUID FILMS — $110,000
Issam Mudawwar — 01-B — 85-4

The purpose of this project is to investigate turbulent activity in freely-falling films. During the first two years of the project, emphasis will be placed on obtaining heat transfer data for turbulent falling films subjected to sensible heating or to surface evaporation. General correlations of the data will be developed, and attempts will be made to predict the results in terms of an empirical turbulence model. Special efforts will be made to cover the widest possible ranges of Reynolds, Prandtl, and Kapitza numbers. During the later stages of the project, the eddy-viscosity profile across freely-falling films will be correlated experimentally using a Laser-Doppler Velocimeter (LDV) system. Simultaneous measurements of the instantaneous longitudinal and transverse velocity components, and of the film thickness will be used to correlate the turbulent shear stress in the presence of surface waves. Based on these results, a new empirical turbulence model will be developed. Predictions based on this model will be compared to heat transfer results obtained during earlier stages of the project.

The final outcome of the proposed project will be a new turbulence model which accounts for the effects of waves and surface tension damping forces on the free interface of freely-falling films.

RENSSELAER POLYTECHNIC INSTITUTE
Department of Mechanical Engineering
and Aeronautical Engineering and Mechanics
Troy, NY 12180-3590

76. INELASTIC DEFORMATION AND DAMAGE AT HIGH TEMPERATURE — $120,000
Erhard Krempl — 01-A, 86-3

A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of AISI Type 304 Stainless Steel under low-cycle fatigue conditions at elevated temperature. The purpose is to characterize the material behavior in mathematical equations which are ultimately intended for use in inelastic stress analysis and life prediction. Creep-fatigue interaction and ratcheting are of special concern. The long-term goal is the development of a finite element program that can directly calculate the life-to-crack initiation of a component under a given load history.

The previously-developed viscoplasticity theory based on overstress which uses neither a yield surface nor loading and unloading conditions will be augmented to include the effects of recovery and aging. This constitutive equation will be combined with an incremental damage accumulation law. It exists in uniaxial form and will be reviewed and extended to multiaxial, isotropic conditions. The theory will be checked against companion experiments.

For the experiments an MTS servohydraulic axial torsion test system is available together with an MTS Data/Control Processor. Induction heating (10 KHz frequency), MTS biaxial grips and an MTS biaxial extensometer will be used for the first time in this study of biaxial deformation and failure behavior.

At the temperature of interest (presumably 550°C or 600°C) tests will be conducted to ascertain whether aging and recovery are significant. Exploratory experiments and tests intended for identifying material functions of the theory will be performed. They include biaxial, high temperature low-cycle fatigue and ratcheting experiments. These test results and data from the literature are needed to find material constants and functions of the theory. Test results not used in determining the material properties provide for a check of the predictive capability of the theory.

RENSSELAER POLYTECHNIC INSTITUTE
Department of Nuclear Engineering and Science
Troy, NY 12180-3590

77. AN ANALYSIS OF THE CLOSURE CONDITIONS FOR TWO FLUID MODELS OF TWO-PHASE FLOW — $ 98,000, 06-C, 86-3
R. T. Lahey, Jr., D. A. Drew

The objective of the analytical study being conducted is to investigate the constraints imposed on the closure conditions of two fluid models of two-phase flow by:

(1) The postulate of continuum mechanics.

(2) The second law of thermodynamics.

(3) Mathematical well-posedness.

(4) Stability considerations.

In particular, we plan to develop an analytical basis on which unacceptable interfacial transfer laws and parameters can be filtered out. We have now begun work on investigating some of the existing closure laws which are commonly used in two fluid models. Formulation for the Basset force and the Reynolds stress are now being investigated. In addition, numerically-based algebraic manipulations are being employed to investigate the eigenvalues of current-generation two-fluid models. It is felt that the results of this research should significantly advance the state-of-the-art in the two fluid modeling of two-phase flows such that, in the future, well-posed models can be developed which only exhibit instabilities of physical origin.

ROCKEFELLER UNIVERSITY
Department of Physics and Mathematics
1230 York Avenue
New York, NY 10021

78. SOME BASIC RESEARCH PROBLEMS RELATED TO ENERGY — $ 97,000
Kenneth M. Case, E.G.D. Cohen — 06-C, 81-6

This project is concerned with investigations of three specific areas: 1) the prediction and evaluation of thermophysical data of fluids and fluid mixtures, and 2) a study of the applications of nonlinear evolution equations. Work is underway to construct a model which can give a first approximation to the transport properties of fluid mixtures in their dependence on size and mass of the constituent particles. The nonlinear evolution equations being investigated describe a very large number of energy related processes. One such equation, the so-called Sine-Gordon equation, has been under study and a number of previously unknown results for the equation have been found.

SANDIA NATIONAL LABORATORIES
Device Research Division
Albuquerque, NM 87185

79. HIGH-TEMPERATURE ELECTRONICS — $115,000
P. S. Peercy, L. R. Dawson, — 03-B
D. R. Myers, T. E. Zipperian — 80-7

The project addresses fundamental engineering questions relevant to the development of high-temperature (up to 500^{o}C) electronics for energy technologies. Included are sensors, passive components, and active semiconductor devices which provide electronic gain or control. The FY-85 work has concentrated on electronic devices formed from heterojunctions of gallium arsenide and aluminum gallium arsenide, and heterojunctions formed from gallium phosphide and aluminum gallium phosphide. Mesa-isolated, liquid-phase epitaxial heterojunction bipolar transistors and heterojunction, semiconductor controlled rectifiers have been fabricated. High-temperature evaluation of these devices is currently in progress. Future studies include optimization of these structures for high-temperature service as well as development of stable metallization systems for these devices. An ultimate goal is the development of a viable high-temperature integrated circuit technology.

SANDIA NATIONAL LABORATORIES
Combustion Research Facility
Thermofluids Division
Livermore, CA 94550

80. DYNAMICAL PERCOLATION PROCESSES AND APPLICATIONS — $130,000
A. R. Kerstein, B. F. Edwards — 06-C, 85-3

The technical goal of this project is to develop a unified framework for predicting and interpreting phenomena in combustion and fracture mechanics which are strongly influenced by underlying spatial random processes. The underlying processes for coal combustion are those determining macromolecular chemical structure and pore morphology. For combustion of heterogeneous propellants or fracture of heterogeneous solids, the underlying process determines the spatial distribution of phases or structural defects within the material. For these applications and others, explicit models of the underlying spatial random processes will be formulated and their observable consequences will be predicted by means of computer simulations and anlytical methods. Special emphasis will be placed on "percolation threshold" effects associated with loss of global connectedness.

SANDIA NATIONAL LABORATORIES
Combustion Research Facility
Thermofluids Division
Livermore, CA 94550

81. DYNAMICS OF MULTICOMPONENT LIQUID FUEL DROPLETS — $130,000
B. R. Sanders, H. A. Dwyer — 06-B, 81-7

Theoverall objective of this program is the development of a comprehensive model of multicomponent liquid fueldroplet vaporizationandcombustion. Inparticular, we will numerically solve for the two-dimensional, unsteady behavior ofmulticomponentliquid fuel droplets in a strong convective environment representative of typicalcombustion systems. Experimental evidence has shown that multicomponent liquid fuels can undergo disruptivebehavior and micro-explosive combustion;however, there is no detailed model available to explain such dynamic events. Disruptive behavior and microexplosion phenomena are of intense practical interest as secondary atomization methods to provide rapid fuel dropletdisintegration,vaporization and combustion.

SCIENCE APPLICATIONS, INC.
1200 Prospect Street, P. O. Box 2351
La Jolla, California 91038

82. ASPECTS OF TURBULENCE IN NONLINEAR SYSTEMS $119,336
E. Frieman, William Hagan 06-C
84-3

The basic goal of this program is to advance the understanding of flow and transport in turbulent systems. A central strategy is to exploit the distinct sets of temporal and spatial scales exhibited by most physical systems. The plasma system is chosen as a specific example in which to develop and demonstrate these methods.

The program has been broken down into five tasks: (1) The first task is to understand the relation between the various gyroradius kinetic theories. (2) The second task is to derive these gyrokinetic equations from the viewpoint of contemporary Hamiltonian dynamics. The relation between divergencies in the generating functions (for Lie transform theory) and resonances in the solutions to the nonlinear perturbative equations of motion will also be explored in this task. (3) The third task involves application of modern procedures to the resulting nonlinear systems arrived at in the first two tasks. Field theoretic techniques will lead to expansions which might be parameterized in terms of the linearization amplitude and ratio of Larmor theory. (4) The fourth task involves the investigation of applying renormalization group theories to these equations to yield nonperturbative relations among correlation functions. The nature and distinction between intrinsic and extrinsic stochasticity will also be examined. (5) Lastly, application of the concepts and lessons learned to a broader class of turbulent systems will be considered.

SCIENTIFIC SYSTEMS, INC.
54 Ringe Avenue Extension
Cambridge, MA 02140

83. CHAOTIC DYNAMICS IN FEEDBACK SYSTEMS $ 0
J. Baillieul, R. W. Brockett 03-A
N. Kopell 82-4

The objective of this research effort is to study chaotic motions occuring in certain classes of dynamical systems which arise in the study of feedback control systems, electric power conversion circuitry and various other engineering applications. Part of the effort is focused on a simple class of differential equations whose coefficients depend piecewise linearly on the state. Because this is a simpler class of dynamical systems than others which have been widely studied recently, it is possible to obtain especially accurate simulations of system trajectories. On the other hand, numerical simulations that have been carried out indicate very interesting qualitative features of the dynamics of such systems, and there is evidence of a strange attractor in a very simple third order system. Specific research is aimed at these and other classes of models in three areas: (i) the use of singular perturbation techniques to analyze first return maps, (ii) the use of difference equations to study the qualitative behavior of "chaotic" differential equations, and (iii) the use of input/output analysis (particularly various control theoretic techniques involving Nyquist plots, describing functions, etc.) to study the qualitative behavior of feedback models.

SKF TRIBONETICS
1100 First Avenue
King of Prussia, PA 19406-1352

84. MECHANICAL INTERACTIONS OF ROUGH SURFACES — $ 135,294
J. I. McCool — 01-D, 82-5

This program is aimed at developing fundamental information and resolving a number of issues that impact the design of mechanical systems in which surface microtopography per se or events which occur on the microgeometric scale play critical roles.

The work is organized into two distinct tasks:

In Task I, a rig designed and built by SKF is being used to provide optical interferograms of the lubricated contact of rough surfaces along with measurements of the traction transmitted under conditions of combined rolling, sliding, and spinning. These tests serve to explore the limitations of predictive models of film thickness, traction, and the frequency of asperity contact interactions and micropitting in the so-called partial EHD regime wherein the thickness of the lubricant film separating the bodies is of the same order as the surface roughness amplitudes.

The objective of Task II is to develop guidelines and techniques for the digital processing of surface roughness data generated in analog form by a stylus profile instrument.

Results to date include i) application of microcontact models to microfracture in ceramics, ii) methodology enabling the use of stylus instrument output for computation of microcontact conditions, iii) a comprehensive comparison of extant microcontact models, iv) an evaluation of the predictive ability of an isothermal elastic/plastic traction model in the presence of lateral sliding and spin and v) the determination via simulation of the distribution of contact area, pressure, load and flash temperature at asperity sites under the Greenwood-Williamson microcontact model.

SOLAR ENERGY RESEARCH INSTITUTE
Thermal Sciences Research Branch
1617 Cole Blvd.
Golden, CO 80401

85. SHEAR-INDUCED INSTABILITIES IN A DOUBLE-DIFFUSIVE PARTIALLY STRATIFIED FLUID — $ 91,000 — 01-C — 85-3

F. Zangrando

This basic experimental study concentrates on mixing mechanisms in a double-diffusive, stratified fluid subjected to the combined effects of bottom heating and horizontal flow. The fluid contains two components (in this case, heat and salt) that contribute in an opposing manner to the fluid density and have significantly different diffusivities (ratio of order 100). The tasks proposed emphasize qualitative and quantitative observation of the behavior of the interfacial layer between a double-diffusive stratification and an initially well mixed region, both of arbitrary thickness, in the presence of buoyancy driven convection due to bottom heating and of shear flow imposed on the mixed region. The effect of each destabilizing component, including line jet discharge and flow into a sink, will be first studied separately and compared with results obtained with single-component stratifications. The combined effect of buoyancy driven convection with a superposed lateral flow (recirculation) will then be studied in order to compare the various mixing mechanisms under similar experimental conditions and to determine the entrainment at the interfacial boundary layer.

STANFORD UNIVERSITY
Department of Chemical Engineering
Stanford, CA 94305

86. TRANSPORT CHARACTERISTICS OF CONCENTRATED SLURRIES — $ 70,000
Andreas Acrivos — 01-C, 85-3

The aim of this research is to study the flow behavior of concentrated suspensions from a fundamental point of view. The work to date has uncovered a host of seemingly unrelated phenomena pertaining to the rheology of concentrated suspensions, to which explanations have been provided that have shed new light on the understanding of such systems. The principal phenomena in question are: a) the observed resuspension of a settled bed of particles in a viscous fluid upon being sheared, b) the existence of a shear-induced anisotropy in a concentrated suspension which manifests itself in measurable normal stresses; and c) the slow decay with time of the effective viscosity of a concentrated suspension, as measured in a Couette viscometer, together with a shear thinning behavior in such systems. Evidence has been provided that many of these phenomena arise as a result of the existence of a shear-induced diffusion mechanism which produces a flux of particles from regions of high particle concentration to low, or from regions of high shear to low.

The current research has the following aims: a) to study the resuspension mechanism in detail experimentally and to develop a reliable theory which would account for the experimental observations; b) to measure the shear-induced diffusion coefficient by a novel technique over a wide range of particle sizes, particle concentrations and degrees of polydispersity, and to construct a theory for determining this coefficient; c) to examine in depth the shear-induced anisotropy, as inferred from our normal stress measurements, and determine to what extent it can lead to a drift of particles in concentrated suspensions; and d) to identify the mechanism responsible for the observed shear thinning behavior in concentrated suspension, an experimental fact which at present is unexplained.

The overall goal of this combined experimental and theoretical program is to develop a theoretical framework, currently lacking, for modelling quantitatively the flow behavior of concentrated suspensions.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Stanford, CA 94305-3030

87. HEAT TRANSFER EFFECTS OF LONGITUDINAL VORTICES EMBEDDED IN A TURBULENT BOUNDARY LAYER — $ 60,000 — 01-B — 83-3

John Eaton

Embedded longitudinal vortices with length scales of the order of the boundary layer thickness, develop naturally in many flows and are purposely introduced in other cases. Such vortices can cause significant augmentation of the heat-transfer rate. The objectives of the present study are (i) to examine the effects of single vortices and vortex pairs independent of other interfering phenomena and (ii) to understand the physical mechanisms responsible for the heat transfer augmentation. The experiments are conducted in a two-dimensional boundary layer wind tunnel. The measurements include the spatially resolved heat transfer and skin friction coefficients, all components of the mean velocity vector and Reynolds stress tensor, and temperature profiles. The data and analysis of the single vortex cases are complete. The inner layers of the boundary layer behave as simple 2-D boundary layers for these weakly three-dimensional flows and simple analytical methods could be used to predict the heat transfer augmentation, but not the vortex decay. The work is now being extended to vortex pairs which impose a stronger three-dimensional perturbation and may reduce the Reynolds stresses. The mean velocity measurements show that appropriately chosen vortex pairs can produce a wide region of boundary layer thinning which should result in a sharply increased average heat transfer coefficient.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Division of Applied Mechanics
Stanford, CA 94305

88. ENERGY CHANGES IN TRANSFORMING SOLIDS $ 0
George Herrmann, David M. Barnett 01-A
82-4

A variety of processes occuring in stressed deformable solids, such as void formation, void growth, motion of dislocations and point defects, grain boundary sliding, etc., are accompanied by energy changes. It is these energy changes which give rise to the concept of generalized configurational (or material) forces and provide a most promising way to characterize state changes and the processes in question. During the past year we have examined material forces associated with solids containing a specified distribution of dislocations and disclinations. Furthermore, a remarkably simple formula has been derived for calculating the hoop stress distribution along the boundary of a circular cavity in an infinite sheet containing arbitrary sources of internal stresses; the calculation can be made without solving an elastic boundary value problem. As several specific examples show, this formula is most useful for calculating energy release rates. Work on generalizing this approach to cavities of arbitrary shape is currently in progress.

STANFORD UNIVERSITY
Department of Aeronautics/Astonautics
Stanford, CA 94305-2186

89. TOMOGRAPHIC OPTICAL DATA ACQUISITION SYSTEMS FOR COMBUSTION RESEARCH — $ 80,000
03-B
85-3

L. Hesselink

The objective of the research is to study a coflowing combusting jet using high speed optical tomography.

The approach involves development of a unique optical data acquisition system which incorporates holographic optical elements (HOE's) for making rapid holographic interferometry measurements from a large number of directions about the object (projections). Subsequent data anlysis allows 3-D reconstruction of the density or species concentration field. Algebraic reconstruction and convolution backprojection techniques have been evaluated for this application. All interferometry projections are recorded in 1 msec and after development the film is digitized for further processing. Nonlinear regression methods and Fourier techniques are studied for fringe readout.

Presently measurements of species concentration are being made in a cold coflowing jet and temperature distribution in a combusting jet.

STANFORD UNIVERSITY
W. W. Hansen Laboratories of Physics
Stanford, CA 94305

90. NONDESTRUCTIVE TESTING — $115,000
G. S. Kino — 03-B
81-6

The aim of this project is to arrive at techniques for contactless nondestructive testing and range sensing. Devices which can be rapidly scanned over a surface so as to detect flaws and measure their profiles are badly needed. The measurement of parameters such as surface roughness are also required. For this purpose, we are developing acoustic sensors operating in air and contactless photoacoustic techniques.

We have developed a new type of PZT ceramic acoustic transducer with a quarter wavelength matching layer of RTV rubber which operates in air in the frequency range of 1-8 MHz. The transducer itself has been used for range sensing and for photoacoustic measurements. As an example, it has enabled us to measure regions of high surface recombination rates on semiconductors by varying the number of injected carriers in a semiconductor, using a laser beam modulated at 2 MHz. We detect the rf term in the surface temperature due to recombination. Similar techniques have been used by us to measure film thicknesses and profiles.

We are now developing a new acoustic transducer operating in air which utilized a 1000 A thick pellicle of boron nitride as the detector of acoustic waves in the air. The deflection of the surface is measured by highly sensitive optical phase measurement of an optical beam reflected from the pellicle. The system is as sensitive as our previous acoustic transducer, but has the advantage that it can be operated over a bandwidth from a few Hz to several MHz.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Stanford, CA 94305

91. FLEXIBLE AUTOMATED OPTICAL SENSING SYSTEMS FOR THE STUDY AND CONTROL OF ENERGY CONVERSION PROCESSES — $192,000 — 03-B — 85-3

C. H. Kruger, G. Kychakoff

The integration of optical sensors with computers is needed for the study and control of energy conversion processes. The aim of this program is to develop systematic methods for combining the capabilities of optical sensors and computers, and to apply these methods to generate a family of advanced optical sensing systems.

The system architecture being investigated consists of light sources, an optical muliplexer, optical waveguides and transducers, hybrid optical/electronic signal analysis modules and a digital computer. The multiplexer directs light via an optical fiber from a source to one of a number of remotely located fiber-optic tranducers; the light is altered by interaction with the environment and returns via a demultiplexer to a hybrid optical/electronic signal analysis module. Here the light is analyzed and a digital representation is generated. The computer interprets the data, converting it to a form suitable for process control.

Optical waveguide transducers have many attractive features for our application, including ease of optical alignment, insensitivity to electrical interferences, durability and low cost. New transducers to sense parameters such as electric fields in low pressure plasma (using Stark-parity-mixing spectroscopy), chemical species in a liquid (using evanescent field absorption spectroscopy), solid body curvature (using reflectance measurements) and pattern misalignment (using LCDTVs as spatial light modulators) are being developed.

STANFORD UNIVERSITY
Department of Chemistry
Stanford, CA 94305

92. REDUCTION OF DISSIPATION IN COMBUSTION AND ENGINES — $105,000 — 06-C
J. Ross — 82-4

Research is concerned with the issue of the enhancement of power output in thermal and chemical engines by means of external perturbations of constraints coupled to nolinearities of the mechanism of the engine. The possibility has been shown of the increase in power output of the thermal engine driven by a chemical reaction by means of external periodic variations of pressure, temperature, and mass flux for the same average chemical throughput as the unperturbed (steady or periodic) state. Since the power output of an engine is necessarily accompanied by dissipation due to irreversible processes essential for power production, an increase in the power output by means of external perturbations is accompanied by a decrease in the rate of entropy production. There exist particular frequencies of external perturbations at which resonance effects lead to enhancement of power output. Full nonlinear analyses are being made on two systems: combustion of fuel with steady and oscillatory fuel input; and model reactions of a proton pump.

STANFORD UNIVERSITY
Department of Civil Engineering
Environmenal Fluid Mechanics Laboratory
Stanford, CA 94305-2179

93. MOMENTUM AND HEAT TRANSFER IN A COMPLEX, BUT WELL-DEFINED TURBULENT FLOW — $ 94,000 — 01-B — 84-3
R. L. Street, J. R. Koseff

A basic study of the heat and momentum transfers in three-dimensional variable density, recirculating flows is being conducted. Current objectives of the research are (1) to gain deeper insight into the characteristics of mixed (natural and forced) convection flows over a range of Archimedes numbers and flow geometries, (2) to complete development of our numerical simulation code, and (3) to carry out simulations of several significant natural and mixed convection flows. A unique experimental facility was constructed. It employs water as the working fluid and a moving lid to drive the flow in a cavity. In addition, a powerful numerical code, called REMIXCS, was constructed to simulate the three-dimensional unsteady motions and heat transfer. Measurements have included those obtained by laser-Doppler-anemometry, thermocouple-based temperature probes, and a new flow visualization technique employing liquid crystal microcapsules (which yield both particle tracks and temperature fields). The numerical code has successfully simulated the complex motions and heat transfers in natural, forced and mixed convection cases which were studied experimentally in the facility. The simulations led to the discovery of the key role of longitudinal (Taylor-Goertler-type) vortices in the that transfer and mixing processes in the forced or mixed convection modes. Both experiments in the facility and the simulation of natural and mixed convection cases are continuing.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Design Division
Stanford, CA 94305

94. GLOBAL OPTIMIZATION OF NON-POSYNOMIAL DESIGN MODELS — $ 83,000
Douglass J. Wilde — 03-C, 86-3

The overall goal is to develop rigorous, efficient ways to solve realistic design optimization problems lacking convexity, or even unimodality, by decomposing them into more easily solvable convex or unimodel subproblems. Two approaches are under study: (1) least-squares approximation and primal-dual methods based on posynomial Geometric Programming, and (2) convex decomposition of non-convex polyhedral sets.

Geometric Programming optimization problems can be solved by maximizing a dual function subject to linear constraints. This dual, although convex, is only poorly approximated by a homogeneous quadratic form, but allowing axis rotation gives a remarkably good fit by the method of least squares. The resulting quadratic program has a closed form matrix solution to be used iteratively. A primal-dual formulation for solving non-convex problems is also under study.

The only known convex decomposition scheme for three dimensional polyhedra fails in the presence of certain types of vertices. Now under study is a remedy for this degeneracy giving a decomposition scheme possibly extendable to non-convex polyhedra and curved objects in higher dimensions. Such a method may prove capable of decomposing multimodel optimization problems into unimodal subproblems.

STEVENS INSTITUTE OF TECHNOLOGY
Department of Physics and Engineering Physics
Hoboken, NJ 07030

95. INVESTIGATIONS OF TRANSITIONS FROM ORDER TO CHAOS IN DYNAMICAL SYSTEMS — $ 38,000 — 06-C — 83-3
George Schmidt

The transition from order to chaos in dynamical systems of few degrees of freedom are studied, using theory, numerical computation, and a laboratory experiment as tools of this investigation. The first phase of the program is now completed.

We have performed a laboratory experiment studying the orbit of a magnetic dipole in an oscillating magnetic field, with controlled dissipation. Period doubling bifurcation sequences leading to chaotic motion have been observed, as well as period three orbits. For sufficiently large dissipation, chaotic motion takes the form of a strange attractor.

While the transition to chaos in low dimensional Hamiltonian systems is by now well understood, there is not a comprehensive theory for dissipative systems. We established a basis for such a theory by studying the dissipative standard map numerically. It was found that all studied stable periodic orbits of the Hamiltonian map turn into attractors for all values of the dissipation parameter. As the dissipation parameter is reduced strange attractors are gradually wiped out so that none exists for the Hamiltonian system. These results are likely to apply to a large variety of dynamical systems.

The detailed study of the disappearance of strange attractors in several systems led to the following conclusions: As the dissipation is reduced the one piece strange attractor disappears first, then the two, four, eight etc. piece strange attractors. The dissipation parameter values where these transitions occur follow a universal geometric progression.

With this evidence from computer experiments we performed a renormalization calculation, that indeed proves universal behavior for strange attractors. It follows further that all aspects of the behavior of dissipative systems that belong to the class investigated are universal, e.g. Liapunov exponents, fractal dimensions, homoclinic and hetroclinic crisis etc. behave in a universal way. Thus the fundamental theory of dissipative dynamical systems, represented by two dimensional maps has been established.

UNIVERSITY OF TEXAS AT AUSTIN
Center for Studies in Statistical Mechanics
Austin, TX 78712

96. THE BEHAVIOR OF MATTER UNDER NONEQUILIBRIUM CONDITIONS: FUNDAMENTAL ASPECTS AND APPLICATION IN ENERGY-ORIENTED PROBLEMS — $ 40,000 — 06-C — 81-6
I. Prigogine

This research aims at new fundamental developments in the area of non-equilibrium phenomena, as well as at various applications to disciplines in which complex systems giving rise to instabilities and bifurcations are of current and primary concern. Special emphasis is being placed on three principal directions. First, the methods of nonlinear dynamical systems will be applied to investigate the transition phenomena occuring in physico-chemical problems such as atmospheric dynamics, the Belusov-Zhabotinski reaction and the oxidation of hydrocarbons in the gaseous phase. Both perturbative and global techniques will be applied, since current experimental evidence suggests that some of these transitions involve chaotic dynamics and homoclinic orbits. Second, problems arising in connection with selection of nonequilibrium states will be analyzed. In particular, the effect of extremely small influences in the selection of symmetry-breaking states -- which are realized in chemical, electronic, and other systems -- will be studied, taking both additive and multiplicative fluctuations into consideration. The implication of the results for the origin of biomolecular chirality will be assessed. Collaborative experiments are planned to substantiate the theoretical developments. Third, special attention will be focused on the problem of combustion. A fundamental analysis of this phenomenon, from both the standpoint of the theory of dynamical systems and the standpoint of stochastic theory, is still lacking. In the proposed research, the effect of stochastic perturbations, of inhomogeneities and of internal fluctuations during the process of ignition, in which the system is expected to present a high sensitivity, will be analyzed using Semenov's model for combustion as well as more realistic models. A fundamental theory of nucleation of flame fronts is expected to be one of the outcomes of these developments.

UNIVERSITY OF TEXAS AT AUSTIN
Department of Physics
Austin, TX 78712

97. PERTURBATION AND CHARACTERIZATION OF NONLINEAR PROCESSES — $125,000
Harry L. Swinney, J. Swift — 06-C, 83-4

In this study techniques are being developed to characterize regular and chaotic behavior in nonlinear systems. Although recent theoretical and experimental studies have shown that nonlinear nonequilibrium processes often exhibit nonperiodic behavior, it is difficult to relate these results to nolinear systems in industry and in nature because research thus far has concerned primarily deterministic systems with no perturbations, while noise is always present for real systems. Moreover, the observed nonperiodic behavior has not been well quantified, so experiments cannot be easily compared with one another and with theory. In this research we are addressing these problems by (1) conducting experimental studies of the instabilities and transition sequences in nonequilibrium chemical reactions in a well-stirred flow reactor, (2) examining the effect of periodic and nonperiodic perturbations on the system dynamics in nonequilibrium reactions, and (3) developing general methods for determining from laboratory data various dynamical invariants, including Lyapunov exponents, fractal dimension, mutual information, and the metric entropy.

TUFTS UNIVERSITY
Department of Mechanical Engineering
Medford, MA 02155

98. EFFECTIVE ELASTIC PROPERTIES OF CRACKED SOLIDS — $107,000
Mark Kachanov — 01-A, 86-2

Effective elastic properties of solids with cracks will be investigated on the basis of the new approach to many cracks problems developed recently by the author. The results will be sensitive to mutual positions of cracks within the representative volume and will be applicable up to quite high crack densities.

UNITED TECHNOLOGIES RESEARCH CENTER
Propulsion Science Laboratory
East Hartford, CT 06108

99. LASER DIAGNOSTICS OF PACVD PROCESSES | $180,000
W. C. Roman, J. H. Stufflebeam, | 06-A
F. A. Otter, A. C. Eckbreth | 86-3

The objectives of this research are to perform a comprehensive experimental investigation of the fundamental nonequilibirum reactive plasma mechanisms of the plasma assisted chemical vapor deposition (PACVD) process applicable to hard face coatings. Based on its superior erosion resistance, TiB_2 will be the initial hard face coating material. In the first task, novel non-intrusive laser diagnostic techniques (e.g., optical emission and absorption spectoscopy, Laser Induced Fluorescence (LIF), Coherent Anti-Stokes Raman Spectroscopy (CARS) and Frequency Modulation (FM) laser absorption spectoscopy) will be used to determine, in situ, the reactive plasma composition, temperature, and species concentrated and distribution in the gas phase. The second task includes use of Auger Electron Spectoscopy (AES), Ion Scattering Spectrometry (ISS), Secondary Ion Mass Spectrometry (SIMS), Rutherford Back Scattering (RBS), and Glancing Angle X-ray Diffraction Analysis for detailed coating characterization combined with physical measurement of coating surface smoothness, density, hardness, and adherence. These combined tasks will allow a correlation of the PACVD parameters with their required coating properties, thus providing a predictive capability that is severely lacking in the present science base of advanced coatings. Preparation of the experimental facility, including an oil-free high vacuum system, is underway. Characterization of reference (Ti-6Al-4V) substrates has been initiated together with a detailed assessment of the diagnostic technique.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
Departments of Engineering Science,
Mechanics, and Mechanical Engineering
Blacksburg, VA 24061

100. HEAT TRANSFER IN OSCILLATORY FLOW $ 0
D. P. Telionis, T. E. Diller 01-B
82-4

The objective has been to study the response of the velocity field and heat transfer of a single cylinder and bundles of cylinders to forced oscillations of the fluid crossflow. Experiments were conducted in a wind tunnel with an emphasis on the heat transfer, and a water tunnel where the flow was examined in detail via Laser-Doppler Velocimetry and Flow Visualization. Both tunnels were modified to provide a well-controlled pulsating flow. Analytical efforts were based on numerical integrations of boundary layer equations and special mathematical tools for modeling the flow and heat transfer in the wake of the cylinders.

WASHINGTON STATE UNIVERSITY
Department of Mechanical Engineering
Pullman, WA 99164-2920

101. PARTICLE DISPERSON BY ORDERED MOTION IN MIXING LAYERS — $ 65,000
T. R. Troutt — 01-B
86-3

This research program is directed towards understanding the role of quasi deterministic large scale vortices in the dispersions of particles by turbulent mixing layers. The primary objective of this experimental study, which has just been initiated, is to determine the influence and importance of these vortex structures on the particle dispersion process over a range of particle and flow parameters. It is hypothesized that if the time scale associated with the vortex motion and the particle relaxation time are of the same order, significantly enhanced particle dispersion may occur.

The experiments will employ high speed photographic methods to track the dispersing particles. The nature of the instantaneous vortex structures will be determined by simultaneously measuring the particle dispersions and the large scale flow features. Direct cause and effect relations between large vortices and the particle dispersion process can be ascertained in this way. Artificial forcing techniques will be used to control the vortex structures for aiding the interpretation of the experiments.

The primary anticipated result of this study is a new physical model for interpreting and predicting particle dispersion in unbounded turbulent shear flows. New techniques for controlling or modifying the dispersion of particles in turbulent flows are a possible outcome of the research program.

WESTINGHOUSE R&D CENTER
Advanced Chemical Research Department
1310 Beulah Road
Pittsburg, PA 15235

102. THE DESIGN OF A CYLINDRICAL FILM CHEMICAL REACTOR — $145,000
01-C
R. M. Roidt — 86-3

This research is to investigate the basic characteristics of a cylindrical film chemical reactor; i.e., a falling annulus of liquid within which gases and sprays may be injected to react chemically. The program is primarily experimental and will focus upon film stability and its relationship to fluid properties as well as geometry variables such as film thickness, annular eccentricity and diameter. Gas entrainment rates, the effect of spray injection and heat release will also be considered.

This work is closely coordinated with the Carnegie-Mellon University Combustion Laboratory.

UNIVERSITY OF WISCONSIN
Department of Chemical Engineering
Madison, WI 53706

103. THE DEVELOPMENT OF PROCESS DESIGN AND CONTROL STRATEGIES FOR ENERGY EFFICIENCY, HIGH PRODUCT QUALITY, AND IMPROVED PRODUCTIVITY IN THE PROCESS INDUSTRIES $106,000 03-A 80-6
W. Harmon Ray

The process industries are having great difficulty competing in the world market because of high energy costs, high labor rates, and old technology for many processes. This project is concerned with the development of process design and control strategies for improving energy efficiency, product quality, and productivity in the process industry. In particular, (i) the resilient design and control of chemical reactors, and (ii) the operation of complex processing systems, will be investigated. Major emphasis in part (i) will be on two important classes of chemical reactors: polymerization processes and packed bed reactors. In part (ii), the main focus will be on developing process identification and control procedures which allow the design of advanced control systems based on limited process information and which will work reliably when process parameters change in an unknown manner. Specific topics to be studies include new process identification procedures, nonlinear controller designs, adaptive control methods, and techniques for distributed parameter systems. Both fundamental and immediately applicable results are expected. The theoretical developments are being tested experimentally on pilot scale equipment in the laboratory. These experiments not only allow improvements in theoretical work, but also represent real life demonstrations of the effectiveness of the methods and of the feasibility of implementing them in an industrial environment. The new techniques developed in this project will be incorporated into computer-aided design packages and disseminated to industry. Therefore, it is expected that the work will have an impact on industrial practice.

BUDGET NUMBER INDEX

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