

Summaries of FY 1987 Engineering Research

November 1987



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

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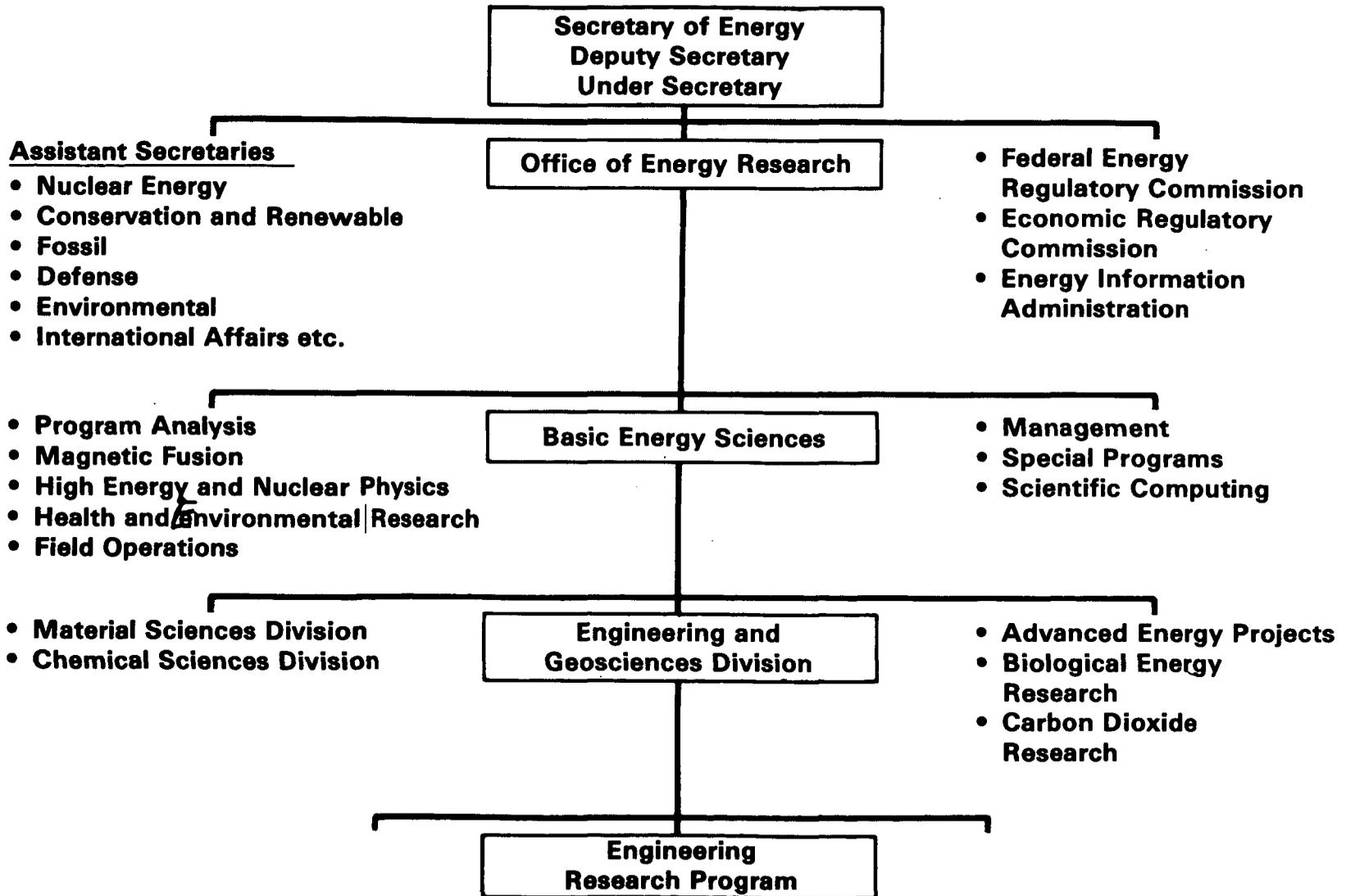
U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences
Washington, D.C. 20545

FOREWORD

This report documents the BES Engineering Research program for fiscal year 1987; 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 1987. 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 1987.

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 1987 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.

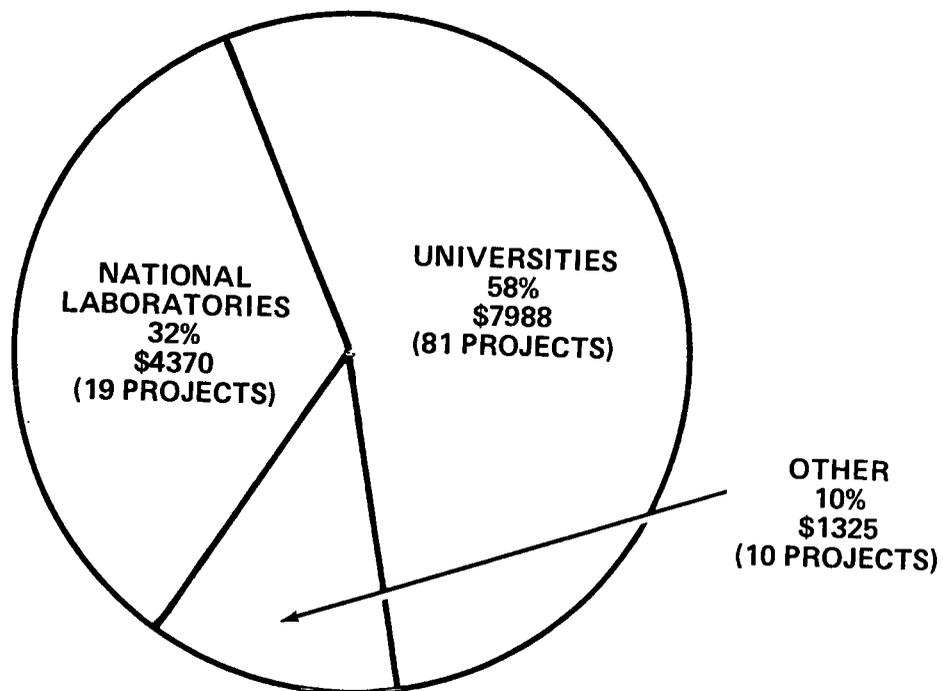
Finally, in the expectation of a future modest growth of this Program, two International Workshops on Two-Phase Flow Fundamentals were held one in September 1985 and the other in March 1987. The meetings were used to identify basic research needs in the field of two-phase flow and heat transfer; summary reports of the workshops are available from the Program Office. The full proceedings of the first workshop have been published as a volume in the series "Advances in Heat and Mass Transfer" (Hemisphere Publishing Company), while those of the second are in preparation for publication in the same series.

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 1987 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 exception 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. All those interested in submitting a proposal are encouraged to discuss their 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 '87 BUDGET (\$000's)
BY INSTITUTIONAL TYPE**



**ENGINEERING RESEARCH PROGRAM
FY '87 BUDGET
BY TECHNICAL AREAS**

	<u>(\$000 s)</u>	<u>%</u>	<u>NUMBER OF PROJECTS</u>
MECHANICAL SCIENCES	4122	30	40
SYSTEMS SCIENCES	4986	37	27
ENGINEERING ANALYSIS	4497	33	43

AMES LABORATORY
Iowa State University
Ames, IA 50011

01. MULTIVIEWING TRANSDUCER SYSTEM \$250,000
D. O. Thompson and D. K. Hsu 03-B
81-7

The objective of this project is to develop a multiviewing ultrasonic technology for detecting, characterizing and reconstructing flaws in structural materials for component reliability assessment. The method makes use of recent advances in ultrasonic inverse scattering theories and flaw sizing algorithms, combined with new concepts in transducer configurations and excitation techniques. An automated multiviewing system consisting of a six-element composite transducer and the associated data acquisition and signal processing software has been completed. The reconstruction protocol fits the data acquired through electronically multiplexed pulse-echo and pitch-catch combinations to an equivalent general ellipsoid. This shape is compatible with fracture mechanics model of flaw growth and failure prediction. The reconstruction reliability with a limited aperture has been dramatically improved with a multi-angle signal amplitude contour technique which instructs the automated system to acquire data using the most favorable aperture configuration for the particular flaw encountered. The versatility of the transducer system (with a total of 22 translational and angular degrees of freedom) has made the amplitude contour technique possible. The new transducer system will extend reconstruction capabilities to include 2-D computed tomographic and 3-D ultrasonic reconstructions. New techniques have also been developed for generating unipolar stress pulses in both pulse-echo and pitch-catch modes. These pulses have significantly broader frequency bandwidths, a feature that is necessary for characterizing flaws over a wider size range. This feature will also be utilized in the measurement and characterization of material property gradients and interfaces.

ARGONNE NATIONAL LABORATORY
Materials and Components Technology Division
Argonne, IL 60439

02. THEORETICAL/EXPERIMENTAL STUDY OF STABILITY CONTROL \$125,000
T. M. Mulcahy, E. L. Reiss (Northwestern University), S. P. Vanka 01-C
86-3

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 in engineering components. Currently fluidelastic instabilities caused by flow leaking between closely spaced bodies are being investigated.

To interpret and present the experimentally observed fluid-structure interaction at the slip-joint region of telescoping tubes conveying fluids, a mathematical model of the unsteady, one-dimensional flow in a narrow, finite length channel, which includes a piecewise linear variation in channel width and several sharp-edged constrictions, has been solved for harmonic perturbations in the channel width. Model problem parameter variations are being investigated to identify spatial distributions of flow resistance which produce negative flow-damping and dynamic instabilities for the fundamental vibration mode of the tubes. Observed phenomena not explainable using one-dimensional flow models will be investigated using computational fluid mechanics techniques.

Another model problem, consisting of two different, infinitely long, uniform, and parallel flow channels that interact through a common wall, has been formulated to study linear and nonlinear responses and to develop mathematical techniques. In particular, spatially periodic bifurcation and secondary bifurcation solutions for the three channel walls, modeled using nonlinear von Karman plate theory, are being investigated for steady, one-dimensional viscous flow modeled by Darcy's law. Also sought is justification for the use of Darcy's law as an approximation to the Navier Stokes equations.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, IL 60439

03. BOUNDS ON DYNAMIC PLASTIC DEFORMATION
C. K. Youngdahl

\$125,000

01-A

84-3

6149

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.

ARIZONA STATE UNIVERSITY
Department of Mechanical and Aerospace Engineering
Tempe, AZ 85287-6106

04. COMBUSTION AND HEAT TRANSFER IN POROUS MEDIA \$ 60,000
R. E. Peck, T. W. Tong 01-B
87-3

A study of combustion and heat transfer of premixed, gaseous fuel-air mixtures in inert porous media is underway. The objective is to generate fundamental information about flame propagation and heat release behavior in porous materials.

A theoretical model for predicting the combustion and heat transfer characteristics in planar porous media as a function of the relevant factors is being developed. The model includes finite-rate reaction kinetics and the equation of transfer for describing radiative heat transfer in porous media. A preliminary heat transfer analysis has been performed indicating the influence of the optical properties of the porous media and the location of the heat generation zone on the radiant output.

Experimental measurements will be conducted to validate the theoretical model. A laboratory-scale burner is being assembled to obtain flame speed, product species concentration and temperature profiles, and energy output data under various operating conditions for comparison to theoretical predictions. In addition, the limits for free-flame, stable interstitial combustion, and flashback will be determined.

The findings will be useful for applying the relatively unexploited technology of porous radiant burners to industrial heating systems, yielding potentially large savings in energy consumption and operating costs for the industrial sector. The results will also provide a scientific basis for understanding combustion and heat transfer in other energy technologies including catalytic combustors and combustion in packed beds and geological systems.

BOSTON UNIVERSITY
Department of Chemistry
Boston, MA 02215

05. DIFFUSION, FLUID FLOW, AND SOUND \$ 68,000
PROPAGATION IN DISORDERED MEDIA 06-C
Thomas Keyes 86-3

The goal of this project is a unified theoretical attack on transport processes-prime examples being those mentioned in the project title-in highly disordered, or inhomogeneous, materials. We are especially interested in materials with percolation thresholds, at which the disorder is so large that transport is blocked altogether, and in those with aspects of fractal structure. Since the theoretical methods needed to treat one problem can usually be applied to others the presence of large disorder is more important than the particular process to be studied. In the past year, we have obtained results in several areas.

In "hydrodynamic dispersion," a pinch of material injected into a flowing fluid spreads out with time. We studied this dispersion for flow through a material composed of randomly placed scatterers with a percolation threshold. As the threshold is approached we calculated how the dispersion diverges, and many other properties.

We also considered chemical reaction and diffusion where the reaction takes place on the surface of randomly placed catalysts. We showed that this system shows qualitatively different macroscopic behavior as a function of the magnitude of the diffusion constant, "reaction controlled" at large D and "diffusion controlled" at small D , and we worked out many details of the crossover and of the different regimes.

Light scattering has been used in attempts to probe, or establish, the fractal structure of disordered materials. We derived the consequences for Raman scattering of lattice vibrations on fractals, and we studied the consequences for multiple scattering of a fractal structure.

BROWN UNIVERSITY
Division of Engineering
Providence, RI 02912

06. TWO STUDIES OF NONLINEAR PROCESSES IN IRREVERSIBLE THERMODYNAMICS \$120,000
J. Kestin 06-C
84-3

The project studies two potentially productive lines of research into two well-defined problems, both linked in that they fall into the broad field of irreversible thermodynamics.

The first task studies a mathematical formalism for the qualitative analysis of the geometric-topological structure of all trajectories (solutions) of a mathematical model of two-phase flow conducted in a phase space formed with the thermodynamics state variables, the velocities of the two fluid phases and the space variable.

The most important result of the analysis is a complete resolution of the problem of choking. The theory leads to a classification of points in phase space into: (a) regular points; (b) turning points; and (c) singular points. Points (a) are not descriptive of choking, and through them there passes one and only one trajectory. Points (b) describe choking at the end of the channel, and points (c) describe choking inside the channel. The analysis is applicable to a wide class of mathematical models of two-phase flow now employed in industry and makes use of the powerful tools of the mathematical discipline of dynamical systems.

The second task seeks to apply the methods of classical ("conservative") thermodynamics to self-consistent formulations of constitutive laws descriptive of inelastic deformations, damage and fracture, with special emphasis on plastic deformation. The identification of the internal variables and their associated intensive affinities is essential for the calculation of entropy and for the derivation of explicit formulae which are descriptive of the local rate of entropy production in each system.

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

08. INVESTIGATION OF SECONDARY MOTIONS AND TRANSITION TO TURBULENCE IN BUOYANCY-DRIVEN ENCLOSURE FLOWS WITH STREAMLINE CURVATURE \$ 70,000
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 buoyance driven enclosure flows. The primary flow of interest is determined by the boundary conditions imposed along the side walls of the enclosure. The conditions induce the unsteady collision of two buoyancy driven, opposed, vertical boundary layers.

Experiments are underway with the objective to map 2 - and 3-D unsteady flow structures as a function of the Rayleigh number. The measurements consist of simultaneous determinations of temperature at two points as a function of the distance between them and time. Autocorrelations, power spectra, length and time scales are being derived from the time histories. These observations will be interpreted with the help of corresponding flow visualization experiments.

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. In this regard, a direct numerical simulation has been undertaken that models a simplified aspect of the experiental flow configuration. Predictions to date confirm the limited experimental evidence pointing to a dependence of the 3-D instability wavelength on the Richardson number.

UNIVERSITY OF CALIFORNIA, BERKELEY
Department of Electrical Engineering and Computer Sciences
Berkeley, CA 94720

09. SELF-GENERATED STOCHASTIC HEATING IN AN RF DISCHARGE \$ 97,000
A. J. Lichtenberg and M. A. Lieberman 06-C
87-3

The purpose of this project is to study electron heating mechanisms in plane parallel, radio frequency (r.f.) discharge. These discharges are used extensively by industry for surface modification of electronic and mechanical materials. The energy deposition in these discharges is not well understood. In addition to the usual r.f. ohmic heating in the plasma interior, stochastic heating at the plasma surface is believed to play a major role.

The stochastic electron heating arises from successive decorrelated reflections of electrons with the oscillating sheath near the surface of the discharge. By examining the dynamics of the electron collisions with the sheath, a mapping is derived that describes the electron motion. For high frequency, low pressure discharges (frequency above 50 MHz, pressure below 1 mTorr) the electron motion is found to be stochastic rather than adiabatic and heating occurs. After combining these dynamics with collisional effects in the bulk plasma, numerical studies show that the electron motion lies on the surface of a strange attractor in the position-velocity phase space. A simulation model of the discharge is developed using self-consistent physical constraints, in which features of the strange attractor persist. Averaging over phases, a Fokker-Planck equation is used to calculate the electron energy distribution, which is shown to be non-Maxwellian. An experiment is being designed in order to characterize the properties of discharges for the predicted conditions of stochastic heating.

UNIVERSITY OF CALIFORNIA, BERKELEY
Energy and Environment Division
Berkeley, CA 94720

10. CONTROLLED COMBUSTION	\$155,000
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 today, but operate also as modern, high-tech chemical reactors, so that the evolution of exothermic energy is carried out under proper fluid mechanical and thermo-chemical conditions to eliminate all sorts of combustion instabilities and minimize the formation of pollutants. For automobile engines this offers the prospect of efficient and clean combustion associated with relatively low exhaust temperature, devoid of the problems of 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 the exploitation of active radicals obtainable from plasma and flame jets as well as from recirculated products. Major laboratory apparatus for our studies consists of a shock tube and molecular beam mass spectrometer, associated with an assortment of laser-powered optical instruments, including apparatus for megacycle-frequency schlieren cinematography and laser induced fluorescence imagery. The experimental program is associated with a significant effort in numerical modeling of the fluid mechanical, thermodynamic, and chemical kinetic processes influencing the control of ignition and combustion in engines.

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

11. RADIATION IN PARTICULATE SYSTEMS \$ 81,000
C. L. Tien 01-B
87-3

The aim of this study is to investigate, analytically and experimentally, the effect of inter-particle interactions on the scattering and absorption of radiation in densely packed systems. Inter-particle or dependent effects may be important in packed and fluidized bed combustors, deposited soot layers, soot conglomerates and microsphere insulation.

A wide spectrum of particle sizes that range from very small particles in the Rayleigh scattering regime to very large geometric scatters are considered. The dependent effects of scattering and absorption are analytically predicted using classical electromagnetic theory. Experiments on dependent scattering have been used to verify these theoretical predictions and those on dependent absorption are in progress.

Flow of fluid has appreciable influence on transport of energy in systems such as fluidized beds, furnaces and solar collectors. The interaction of radiation and convection in particulate systems is being studied. In combustion systems, such as furnaces, soot layers are deposited on the walls and mixtures of particles and participating gases are generated. The effect of radiation in these systems will be investigated.

UNIVERSITY OF CALIFORNIA, DAVIS
Department of Mechanical Engineering
Davis, CA 95616

12. STRUCTURE AND STABILIZATION OF PREMIXED AND DIFFUSION FLAMES \$ 94,000
C. K. Law 06-B
86-3

The program aims to gain fundamental understanding on the structure and stabilization of premixed and diffusion flames. The program involves both theoretical and experimental phases, and consists of three components, namely (1) Studies of the stabilization mechanisms of both premixed and diffusion flames in mixing-layer-type flows, with emphasis on the basically elliptic structure of the leading edge of the flame which controls flame holding and propagation; (2) Studies of the dynamics of stretched flames due to flame curvature and flow nonuniformity, with emphases on the extinction behavior and on synthesizing existing experimental and theoretical results from a unified viewpoint; and (3) Studies of the properties of thermal-diffusional flame-front instabilities, with emphases on the spinning and secondary bifurcation of polyhedral flames.

During the reporting period the stabilization and stability of flat flames over porous-plate burners were analytically studied. The steady-state results reveal the existence of two flame speeds for a given heat loss rate, and of two flame speeds for a given flamefront standoff distance. Stability analysis shows that there exist situations under which both flames are stable. These results therefore substantiate the experimental observations of Spalding and of Ferguson and Keck on the existence of two flame speeds.

An integral analysis has been performed for the structure and propagation of stretched premixed flames with preferential diffusion. Specific flame configurations studied include the one-dimensional steadily-propagating planar flame, the steady curved flame in nonuniform flow, and the outwardly/inwardly propagating spherical flame. Results agree with those obtained from asymptotic analysis in the linearized limit of small stretch, and yield enhanced insight into the dominant and coupled physical-processes governing these complex flame phenomena.

UNIVERSITY OF CALIFORNIA, LOS ANGELES
Mechanical, Aerospace and Nuclear Engineering Dept.
School of Engineering and Applied Science
Los Angeles, CA 90024-1597

13. BASIC STUDIES OF TRANSPORT PROCESSES IN POROUS MEDIA \$ 80,000
Ivan Catton 01-C
82-6

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.

The validity of stochastic models for single-phase flow through randomly packed beds was established by demonstrating that the predicted dispersive enhancement of the axial "effective" transport coefficient agrees with measurements found in the literature of both heat and mass transfer. The role of this dispersive component on the heat transfer was considered in the porous Benard problem. Numerical predictions along with corroborative experimental evidence demonstrated that dispersion enhances the net heat transport through the layer, while inertia diminishes it. If the packed bed is very shallow (low layer thickness to bed diameter ratio), both effects decrease the Nusselt number. Dispersion dominates inertia unless the porous Prandtl number is order 0.001 or less.

Steam injection in a porous channel is being studied experimentally and theoretically. In the experimental studies the qualitative behavior of a steam-water interface in a porous channel will be analyzed through high speed movies of the two phase flow and interface movement. The principal parameters of interest include the frequency of the interface movement, the shape of two phase region and flow patterns. The pressure and temperature distributions will be measured along with flow rates of steam and water. The physical mechanisms causing the observed rapid oscillation of the interface between the two phase region and the subcooled water are being delineated. A stability analysis will be carried out. Numerical modeling will include mechanisms that are important.

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

14. ENHANCEMENT OF CRITICAL HEAT FLUX IN TUBES USING STAGED TANGENTIAL FLOW INJECTION \$ 44,000
V. K. Dhir 01-B
85-3

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, LOS ANGELES
Department of Physics
Los Angeles, CA 90024

15. WAVE TURBULENCE AND SELF-LOCALIZATION IN CONTINUOUS MEDIA \$ 75,000
Seth Putterman 06-C
87-3

The goal of this project is to advance our understanding of the response of nonlinear elastic media driven far from equilibrium. Research efforts are focused on the competition between turbulence and localization and how these processes affect the fate of energy which is injected, into a continuous medium, in the form of wave motion.

Regarding turbulence in propagating waves an attempt is being made to determine the distribution function for the higher order correlations. Particular aims are to describe the build-up of cross-correlations between different modes, and to generate a workable description of the role of mechanical noise in activation processes. Recent research also indicates that the wave turbulent state possesses structure in that it can support new propagating modes. This elasticity of turbulence is a classical analogue of second sound. Currently this effect is being calculated for wind waves in a stormy sea.

In one and two dimensional systems high amplitude wave motion can self-focus into long lived structures. These soliton-like properties are being studied as regards possible applications to flexing plates and shells. Of special interest are the thermal properties of the solitons, the role of damping in the formation of the solitary wave, and possible consequences for metal fatigue as regards the recently discovered non-propagating soliton.

UNIVERSITY OF CALIFORNIA, SAN DIEGO
Scripps Institution of Oceanography
La Jolla, CA 92093

16. NONLINEAR DYNAMICS OF DISSIPATIVE SYSTEMS \$ 73,000
Henry D. I. Abarbanel 06-C
86-2

This work is directed toward the understanding of the dynamics and nonlinear stability of multi-phase flows from a Hamiltonian point of view. The Hamiltonian formulation of multiphase flow problems will be the first part of the research. As a second part the conservation laws, in addition to energy, for these flows will be investigated using methods originated by Sophus Lie and further developed in the past decade by several mathematicians. With the conserved quantities respected by these flows in hand, the nonlinear stability of particular flows can be investigated using the Liapunov method of Arnol'd and others. The result of this work will be a set of criteria for the stability of free boundary flows--material surfaces separating phases--under finite perturbations. Several examples of gravity driven flows will be studied.

The dissipative or viscous versions of these flows will build on the dynamical description of these results. A variational principle arising from the consideration of the evolution of the energy plus all conserved quantities will be used to provide ranges for the absolute stability of viscous multiphase flows. This extends the older energy methods often employed in this kind of analysis. The addition of other conserved quantities allows the exploration of a larger part of the allowed phase space for the deviations from a chosen flow whose stability one wishes to investigate.

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

17. CHAOTIC ADVECTION AND EFFICIENT MIXING BY \$ 58,000
DETERMINISTIC FLOWS 01-C
Hassan Aref 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.

Two examples investigated are the model flow problem consisting of a pulsed source and sink in two dimensions, and the transverse stirring produced by the secondary flow pattern in a twisted pipe, a steady three-dimensional flow. Diagnostics include computer graphic images of particle paths, Poincare sections, Lyapunov exponents and other measures of regular and chaotic regions.

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

18. FUEL DROPLETS SUBJECT TO STRAINING FLOW \$ 93,000
Paul A. Libby and K. Seshadri 06-B
87-3

This research which has only been underway for several months involves a theoretical and experimental investigation of fuel droplets in a well-defined straining flow, that associated with a nonpremixed flame established in counterflowing streams of gaseous fuel and oxidizer. The initial purpose of this effort is to determine the validity of current theories of droplet burning under dynamically changing velocity and ambient conditions. Existing theories are based on highly idealized models of such burning and have been evaluated only under conditions closely approximating those assumed in the theory. The question arises as to their applicability to conditions which prevail in applications, typically in turbulent flows involving fluctuations in velocity and composition. Follow-on studies will be concerned with improved theories of droplet burning if called for and with droplet loadings sufficiently large so that a significant interaction between the droplets and the flame occurs. The experimental effort is complemented by appropriate theoretical investigations. Thus the trajectories and histories of the droplets in the initial experiments will be compared with calculations based on a series of descriptions of increasing completeness in order to establish which if any of the theories predicts the observed behavior. Subsequent theoretical work will involve application to the counterflowing configuration of the spray equation which contains more of the aerothermochemical details of droplet behavior than the equations of coexisting continua.

The initial effort will study the behavior of individual droplets of hexane injected on the fuel side of a methane-air flame. An appropriate counterflow burner and droplet injection system have been designed and constructed. The photographic system which involves a camera and stroboscopic light of high repetition rate and intensity is being assembled. The complementary theoretical effort concerned with the calculation of droplet trajectories and histories in a methane-air flame is underway.

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

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| 19. PARAMETERIZATION OF INTERMITTENT TURBULENCE | \$ 78,000 |
| AND THE VORTON METHOD | 01-C |
| E. A. Novikov | 87-3 |

This research project involves the study of a new type of parameterization of small-scale turbulence, which recognizes the important phenomena of intermittency. The parameterization is based on the theory of intermittent relative motion of fluid particles, which may be of independent interest. The method of three-dimensional vortex singularities (vortons) is used for the calculations of elementary events in the intermittent turbulence (breakdown, reconnection and double reconnection of vortex filaments). The vorton method may also have applications to some problems in aeronautics. Some vorton calculations, including Crow instability of two perturbed antiparallel vortex filaments and merging and subsequent splitting of vortex rings, have been presented at IUTAM Symposium of Fundamental Aspects of Vortex Motion (September, 1987, Tokyo, Japan).

UNIVERSITY OF CALIFORNIA, SAN DIEGO
Institute for Nonlinear Science, R-002
La Jolla, CA 92093

20. THE STOCHASTIC TRAJECTORY ANALYSIS TECHNIQUE (STAT) \$ 88,000
APPLIED TO CHEMICAL, MECHANICAL AND QUANTUM SYSTEMS 06-C
Bruce J. West, Katja Lindenberg 86-3

A number of important physical problems are described by dynamical equations containing fluctuating parameters. In dealing with such systems one has until recently been forced to assume that the fluctuations are delta-correlated, i.e. that their spectrum is white, thus restricting the scales of the spatial and/or temporal inhomogeneities to be much shorter than the response scales of the system. This assumption is often known to be quite unphysical, especially in nonlinear systems in which all scales are present. Of particular interest in this program are applications involving chemical reactions in fluids in which the rate coefficients fluctuate due to spatial inhomogeneities and thermal effects, dynamical processes in solid materials in which fluctuations arise due to spatial disorder and thermal effects, and wave propagation in random media in a geophysical context.

A number of methods to deal with the problem of correlated fluctuations have been developed under this program. One of these involves an explicit construction of trajectories (STAT). This procedure is particularly useful when the noise has simple statistics and can be used to deal with highly correlated noise. The approach has been applied to linear systems driven by dichotomous noise, multivalued noise, and shot noise. Another class of methods relies on perturbative approximations around the white noise limit. These methods can be applied most fruitfully to systems driven by weak Gaussian slightly colored noise, and have been used to calculate rates of transitions in bistable systems driven by colored noise.

UNIVERSITY OF CALIFORNIA, SANTA BARBARA
Department of Physics
Santa Barbara, CA 93106

21. BIFURCATIONS AND PATTERNS IN NONLINEAR SYSTEMS \$124,000
G. Ahlers, D. S. Cannell 06-C
87-3

This project consists of experimental investigations of non-linear non-equilibrium fluid-mechanical systems, with an emphasis on heat transport, pattern formation, and bifurcation phenomena. These issues are being studied in Rayleigh-Bénard convection, using both pure and multi-component fluids. They play an important role in such energy-related issues as crystal growth from a melt with and without impurities, the catastrophic inversion of salt lakes such as the Dead Sea, energy production in solar ponds, and various oceanographic phenomena.

The work utilizes computer-enhanced shadowgraph imaging to visualize the convective flow patterns. The technique can detect the flow field even when the convective threshold is exceeded by only 0.1%. In parallel, high-resolution heat-flux measurements are made with a resolution of 0.05%. Thus, the relationship between the pattern and the heat transport can be studied in great detail.

In pure fluids, we are investigating the stability of various relatively simple convection patterns in containers with simple side-wall geometries. We expect that this experimental information will help in the development of the theoretical models for pattern stability.

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

22. INVESTIGATION OF FLUID DYNAMIC PHENOMENA \$ 94,000
NEAR GAS-LIQUID INTERFACES 01-C
S. Banerjee, H. Fenech 85-3

The objective of this project is to study the structure of turbulence in liquid streams bounded by a solid surface and a gas-liquid interface. The program proceeds in stages with initial investigations focused on phenomena in the absence of shear at the interface followed by work on systems with shear imposed by either cocurrent or countercurrent gas streams. The velocity field is measured using either 10-25 micron oxygen bubbles as tracers together with high speed video and still photography, or using a photochemically activated dye which forms streaks that can also be followed by photography. A three-dimensional laser anemometer with a 30 micron spot size has been specially designed, constructed and installed to complement the photographic techniques. In parallel, numerical computations involving direct solution of the Navier-Stokes equation by pseudospectral techniques are underway to aid in the interpretation of experiments and understanding of the mechanisms for turbulent transport across the interface. Experimental results to date indicate that the dominant phenomenon results from bursts generated at the wall, involving the ejection of low-speed fluid towards the interface.

The next phase of the program will concentrate on structures that develop when shear is imposed on the interface. Questions to be answered are whether bursts will be formed in this region of high vorticity and if so will they propagate and mix with the bulk fluid and interact with bursts formed at the solid wall?

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

23. STRATEGIES FOR OPTIMAL REDESIGN IN A CHANGING ENVIRONMENT \$150,000
L. T. Biegler, I. E. Grossmann 03-A
G. L. Thompson, A. W. Westerberg 85-4

As the chemical industry matures it is important to consider the redesign of existing processes. Redesign problems are harder to solve than "grassroots" problems because constraints dealing with the existing process need to be considered and 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) Flowsheet optimization for process redesign - The first two years of the project were devoted to development of optimization and heat integration strategies for complex simulation models. More recently, operating or rating models were developed and a redesign strategy was demonstrated for flowsheets with fixed topologies.

(2) Primal/dual linear (LP) and quadratic programming (QP) algorithms. These new algorithms for solving LP and QP problems were developed during the first two years of this project. Computational tests showed that codes based on these algorithms were at least 10 times as fast as currently available codes, and they are especially effective for problems having more constraints than variables.

(3) Redesign of energy management systems - recently developed strategies for grassroots heat exchanger network synthesis are being extended to cover the redesign problem. New formulations of mixed integer linear and nonlinear programs have been developed that make use of the existing network and equipment as much as possible while ensuring maximum energy recovery.

(4) Redesign for flexibility and controllability - based on recently developed strategies for evaluation of process operability, optimization strategies are being developed for improving operability through structural modifications.

(5) Redesign of multicomponent separation sequences - an existing flowsheet and a separation task different from the original flowsheet are given. The objective is to modify the flowsheet so as to accomplish the new separation task at minimum cost.

CARNEGIE MELLON UNIVERSITY
Mechanical Engineering Department
Pittsburgh, PA 15213

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| 24. | EXPERIMENTAL AND THEORETICAL STUDIES | \$100,000 |
| | OF VERTICAL ANNULAR LIQUID JETS | 01-C |
| | N. Chigier, J. I. Ramos | 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

25. TOPICS IN FINITE-TIME THERMODYNAMICS \$ 78,000
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 reemission 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

26. FUNDAMENTALS AND TECHNIQUES OF NONIMAGING OPTICS FOR SOLAR ENERGY CONCENTRATION \$150,000
R. Winston, J. J. O'Gallagher 06-C
81-6

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

27. NUMERICAL STUDIES OF COHERENT EDDIES IN WALL-BOUNDED FLOWS \$ 58,000
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.

COLORADO SCHOOL OF MINES
Department of Chemical Engineering
and Petroleum Refining
Golden, CO 80401

28. AN AUTOMATED FLOW CALORIMETER FOR HEAT CAPACITY AND ENTHALPY MEASUREMENTS AT ELEVATED TEMPERATURES AND PRESSURES \$ 35,000
Victor F. Yesavage 03-B
87-2

The need for thermal property data at process conditions in the design of petrochemical and synfuel plants has been well documented. As such, the primary objective of this work is to construct an automated flow calorimeter to measure isobaric heat capacities and enthalpies of vaporization over the range 0-30 MPa and 300-700 K with an anticipated accuracy of 0.1%. The method of measurement is by the traditional electrical power input technique with a unique calorimeter design utilizing a concentric coil/radiation shield structure which minimizes heat loss errors and simplifies the replacement of plugged components. Flow generation is accomplished with a precision Ruska pump eliminating the need for on-line flow rate measurement. In addition, the proposed instrument will be fully automated minimizing the need for highly skilled operators which had previously been a severe limitation with this type of instrument.

Assembly of the automation hardware is complete and construction of the calorimeter itself should be finished shortly. During the next year the automation and data acquisition software will be written and the completed unit will be tested with water and n-Butane.

DARTMOUTH COLLEGE
Thayer School of Engineering
Hanover, NH 03755

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| 29. | SUBCOOLED SPRAYS IN A VAPOR ENVIRONMENT-TESTS OF THE
TWO-FLUID MODEL FOR TWO-PHASE FLOW
G. B. Wallis, H. J. Richter | \$160,000
01-C
86-3 |
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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-dimensional 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.

G. A. TECHNOLOGIES, INC.
P. O. Box 85608
San Diego, CA 92138-5608

30. HIGHER DIMENSIONAL NONLINEAR DYNAMICS \$ 75,000
John M. Greene, 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 this 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, this study emphasizes the information available in the rates and directions of separation of nearby orbits, or realizations. The methods are being developed and tested using the Lorenz model. The knowledge gained this way is being applied to the Kuramoto-Sivashinsky equation, a simple partial differential equation with chaotic solutions. The object is to develop representations in which these solutions can be most simply expressed.

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

31. PREDICTIVE MODELING OF URANIUM ROLL TYPE DEPOSITS \$ 50,000
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 goethite 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
Applied Optics
Idaho Falls, ID 83415

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| 32. | IN-FLIGHT MEASUREMENT OF THE TEMPERATURE | \$133,000 |
| | OF SMALL, HIGH VELOCITY PARTICLES | 06-A |
| | J. R. Fincke | 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 two wavelength pyrometry technique. In addition, simultaneous particle size is obtained by a light scattering technique. The requirement of coincidence between sizing and pyrometry signals insures that only particles for which temperature data are available will be sized. The technique has been demonstrated on laboratory scale plasma torches. The influence of particle size, injection rate, torch power, etc., are currently being examined in detail. In addition methods of simultaneously obtaining particle size, velocity and temperature are under development.

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

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

33. EXPERT SYSTEM AIDS FOR ANALYSIS CODES \$262,000
V. H. Ransom, R. K. Fink, R. A. Callow 06-C
T. K. Larson, J. D. Ramshaw 85-3

The objectives of this research are to establish the impact that expert systems will have on the architecture of engineering analysis codes and to assess the potential benefits for such an application. At the outset of this research the tasks of physical system modeling, input preparation, output analysis, and code execution were identified as potential applications for expert systems. However, initial findings identified programming language compatibilities and inter-computer communications as key issues in implementation of such systems. In particular, the preferred situation for the modeling and input functions is that the expert systems be accessible through an engineering work station and, especially for the execution control application, the expert system should reside on the same computer system as the analysis code. Only the conditions for the modeling and input functions are generally achievable at this time.

The potential benefits of expert systems for the modeling and input functions were explored by development of an expert system aide for ATHENA, a general purpose thermal hydraulic transient simulation code. The results of this research demonstrated that significant productivity improvement can be achieved, both by relieving the analyst of burdensome tasks, and by providing expertise relative to application of the code in a user convenient form. In experiments, the Athena AIDE resulted in reduction of the time required to produce a model and input deck by fifty to eighty percent. Development of such expert systems is recommended for existing as well as new engineering analysis codes which have a sufficient user base. The results of this research have been documented in several conference and journal articles.

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

34. ELASTIC-PLASTIC FRACTURE ANALYSIS \$ 439,000
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
Materials Technology Group
Idaho Falls, ID 83415

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| 35. | EXPERIMENTAL MEASUREMENT OF THE
PLASMA/PARTICLE INTERACTION
C. B. Shaw, S. C. Snyder, L. D. Reynolds | \$319,000
06-A
85-3 |
|-----|--|---------------------------|

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

36. INTEGRATED SENSOR/MODEL DEVELOPMENT \$450,000
FOR AUTOMATED WELDING 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
Sensors and Diagnostics Group
Idaho Falls, ID 83415

37. NONDESTRUCTIVE CHARACTERIZATION OF FRACTURE DYNAMICS AND CRACK GROWTH \$183,000
John A. Johnson, Basil A. Barna, Randall T. Allemeir 03-B
83-5

The purpose of this research is to develop instrumentation and models to measure and predict the emission and interaction of ultrasound from growing cracks in engineering materials and to investigate methods of sensing the properties of growing cracks. A high speed digital acoustic emission (AE) data acquisition system is being developed and applied to fracture mechanics experiments that are part of the Elastic-Plastic Fracture Analysis program at INEL and the Modeling and Analysis of Surface Cracks program at the Massachusetts Institute of Technology. In addition, numerical methods are being used to model the interaction of acoustic emission stress waves with real crack geometries.

The AE detection system is being developed and is capable of detecting and digitizing AE signals with a larger bandwidth and with less dead time 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. Automatic analysis methods are being developed for source location and source identification for each of the large number of acoustic emission events received in a typical fracture mechanics experiment. Other work includes transducer design, transducer calibration, generalized ray theory analysis (Green's functions), source location algorithms, and inverse source identification algorithms.

Models of the ultrasonic field/crack interaction are based on a numerical (finite element) solutions to the partial differential equations (PDE) describing the system. In the finite element model, a source of acoustic emission 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. These boundary conditions include the geometry of the macrocrack near the source of acoustic emission and thus calculate receiver signals which include effects that cannot be calculated using generalized ray theory.

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

38. VIBRATIONAL CONTROL OF CHEMICAL REACTORS: SELECTIVITY \$ 80,000
ENHANCEMENT, STABILIZATION AND IMPROVEMENT OF TRANSIENT 03-A
BEHAVIOR 84-3
Ali Cinar

The objective of this project is to develop novel applications of the vibrational control theory to various types of chemical reactors. 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. Research is focused on three areas of application:

- (i) Selectivity and yield enhancement in parallel reactions with desirable and undesirable products. The oxidation of ethylene over supported silver catalysts to ethylene oxide and carbon dioxide is used as a test reaction.
- (ii) Stabilization of nonadiabatic and autothermal tubular packed-bed reactor operation at an otherwise unstable steady state. The CO oxidation reaction is used as a test reaction.
- (iii) Improvement of transient behavior of nonadiabatic and autothermal tubular packed-bed reactors by relocation of system zeros using vibrational-feedback control.

The theoretical developments will be tested experimentally on pilot scale equipment in the laboratory. Vibrational control will be implemented by introducing forced periodic oscillations in the input concentrations and flow rates. The effects of multiple vibrating inputs will be analyzed and the contributions of the phase relationships between the forcing functions of various inputs will be investigated. This study will provide techniques for improving selectivity and yield in complex chemical reactions and for reducing the overall control effort in reactor configurations used in the industry.

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

39. INTERFEROMETRIC MEASUREMENTS IN DOUBLE-DIFFUSIVE SYSTEMS \$ 0
William M. Worek*, Zalman Lavan 03-B
84-3

The objective of this 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 is 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.

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UNIVERSITY OF ILLINOIS
Energy Resources Center
Chicago, IL 60680

40. HEAT TRANSFER TO AQUEOUS POLYMER SOLUTIONS \$ 78,000
J. P. Hartnett 01-B
85-2

The goal of the research is to study the fluid mechanical and heat transfer behavior of viscoelastic aqueous polymer solutions. The ultimate objective is to provide a basis for predicting the performance of such fluids. At the present time, two basic investigations are underway:

- a.) Pool boiling behavior of aqueous solutions of two high molecular weight polymers, hydroxyethyl cellulose and polyacrylamide and a comparison with the pool boiling performance of deionized water.
- b.) Combined free and forced convection to two viscoelastic fluids (aqueous solutions of hydroxyethyl cellulose and polyacrylamide) in laminar flow through a 5:1 rectangular channel, and a comparison with Newtonian fluid performance.

To date the following results have been found:

- a.) High concentrations of the aqueous hydroxyethyl cellulose solutions yield higher values of the boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature difference. In contrast, aqueous polyacrylamide solutions yield lower values of boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature. These results are being analyzed to establish a rational basis for the observed differences in behavior.
- b.) Laminar heat transfer results for two Newtonian fluids, oil and water, and for the two viscoelastic fluids, have been obtained. There is clear evidence of secondary flows for both classes of fluids and efforts are underway to determine the nature of the secondary motion.

UNIVERSITY OF ILLINOIS
Department of Chemical Engineering
Urbana, IL 61801

41. GAS-LIQUID FLOW IN PIPELINES \$106,000
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 when slug flow will exist in horizontal gas-liquid flows, (2) to obtain a better understanding of the interfacial wave patterns in stratified gas-liquid flows, (3) to obtain improved predictive methods for horizontal and vertical annular flows. Vertical flow experiments are being conducted in pipelines with diameters of 3/4 in., 1 1/2 in., and 2 1/4 in. The horizontal flow facility, which has pipelines of 1 in., 2 in., and 4 in., was completely renovated during the past year so that it can operate with a wide range of liquid viscosities and at inclinations of +2 degrees.

A linear theory has been developed that predicts the initiation of slugs at low gas velocities by examining the stability of a stratified flow. During the past year some success has been experienced with an alternate approach that establishes necessary conditions for the existence of slugs.

The results of a comprehensive study that relates interfacial stress to wave structure in horizontal flow was published during the past year. On the basis of these results new design methods for stratified flows have been developed. These results will be tested in inclined pipelines.

Techniques have been developed to measure the rates of atomization and deposition in vertical annular flow. A theoretical understanding of these rate processes is being obtained through measurements of wave patterns and droplet motions. These measurements are being used to develop better predictive methods for entrainment.

Previous measurements of entrainment for air-water flow in a horizontal one inch pipe will be extended during the next year to include 2 inch and 4 inch pipelines and high viscosity liquids.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

42. APPLICATIONS OF MOLECULES AS HIGH-RESOLUTION, HIGH-SENSITIVITY THRESHOLD ELECTRON DETECTORS \$ 78,000
A. Chutjian, S. H. Alajajian, O. J. Orient 03-B
86-3

Measurements and theoretical calculations are carried out of electron attachment cross sections $\sigma_A(\epsilon)$ and rate constants in molecules at electron energies below 200 millielectron volts (meV). Measurements are carried out at extremely high energy resolution (5-8 meV, FWHM) using the krypton photoionization technique developed at JPL. This electron energy region is accessible by no other experimental technique, and previously-published JPL results have clearly shown the s-wave threshold behavior in which $\sigma_A(\epsilon)$ diverges as $\epsilon^{-1/2}$. The molecules $c-C_5F_8$ and $c-C_6F_{10}$ have shown extremely narrow, delta-function like widths for attachment of zero-energy electrons. This feature makes them suitable as high-sensitivity threshold electron detectors useful in, for example, obtaining threshold photoelectron spectra of atoms and molecules. Experimental results in F_2 (published), and theoretical calculations in $CFCO_3$ and CCO_4 (to be published) have shown significant discrepancies with calculation and other experiments as to energy dependence of the $\sigma_A(\epsilon)$, and temperature dependence of the rate constants. These properties have bearing on the plasma-assisted etching process, and on soot (and/or electron density) reduction in combustion plasmas. To this end, experimental work on attachment to CO_2 will be initiated, calculations in $CFCO_3$ and CCO_4 completed, and attachment properties of about six other molecules, currently being tested elsewhere as electron "sinks" or soot reducers in combustion plasmas, will be studied.

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

43. STUDIES IN NONLINEAR DYNAMICS \$155,000
Allan N. Kaufman and Robert G. Littlejohn 06-C
86-3

This project involves studies of fundamental properties of nonlinear dynamical systems which arise in physical situations of importance to energy research. Three subjects are being explored. First, theoretical work is in progress to explore several different aspects of wave phenomena. Special focus is given to wave packets, the use of the Maslov index in multidimensional quantization problems, and linear mode conversion. Recent progress includes the establishment of the general relationship between wave packet evolution and quantization, the use of wave packets for the computation of multidimensional problems, an exploration of the relation between the Maslov index and the phase space structures of nonlinear Hamiltonian dynamical systems, and the first treatment of mode conversion phenomena for multidimensional systems, involving novel "reduction" techniques. Emphasis is given to the use of a phase space approach to wave phenomena in all these applications. Second, a new formulation of conservative dissipative processes is being explored, in which the entropy and energy functionals jointly generated 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 systematically.

LOS ALAMOS NATIONAL LABORATORY
Theoretical Division
Los Alamos, NM 87545
Trust. for Admin. - Lattice Simulations

44. LATTICE GAS HYDRODYNAMICS: THEORY AND SIMULATIONS \$ 90,000
Brosi Hasslacher, Uriel Frisch, Yves Pomeau 01-C
87-3

Lattice gases, operating as cellular automata and amenable to massive parallelism, which simulate the Navier-Stokes equation in two and three dimensions, were introduced in 1985 by the principal investigators (Phys. Rev. Lett.). Such lattice gases are formed of "Boolean molecules" with discrete time, space, and velocity. Their collision laws are designed to conserve particle number and momentum. Macroscopic momentum averages satisfy the incompressible Navier-Stokes equation, in a suitable physical limit. Groups in the United States and in France are already engaged in theory, simulations, and hardware projects for lattice gas hydrodynamics. Preliminary results indicate that the method is easy to implement (with or without boundaries), robust, and reproduces known hydrodynamic phenomena. It may eventually yield a new simulation strategy for complex turbulent flows, with many practical applications.

It was proposed that the lattice gas method be evaluated, and that modified models with higher Reynolds numbers be studied. Two-dimensional computer models were created to run on the CRAY-XMP, the CRAY II, and on the Connection Machine II (a computer with 65,000 central processors). These models ran at the rate of 80,000,000, 10,000,000, and 2,000,000,000 cell updates per second, respectively. Comparisons with other calculational methods have been done. A three-dimensional program has been developed which produced the highest Reynolds numbers attainable with 24 bits required per cell. Flow past a square plate has been successfully modeled by this code. Summaries of this and other recent work have been published in several articles in the August issue of Complex Systems. Lattice gas methods for solving partial differential equations appear useful and promising. Expectations of their capabilities on future machines are now being estimated.

LOS ALAMOS NATIONAL LABORATORY
Mechanical and Electronic Engineering Division
Los Alamos, NM 87545

45. DEVELOPMENT OF THERMIONIC INTEGRATED CIRCUITS (TIC's) \$100,000
D. Wilde, R. Lemons, D. Lynn, D. Brown, R. Dooley, 03-B
C. Mombourquette, J. Pafford 82-6

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 is 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. Large numbers of these devices fabricated on a substrate are interconnected to achieve useful circuit functions. High-temperature tests have been conducted at 500°C with no degradation in device characteristics. Current research is focused on improving cathode lifetime, emission, linewidth, and chemical stability to ensure the reliability, functionality, and manufacturability of TIC technology for application in high-temperature and high-radiation environments.

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

46. THE USE OF OPTICAL FLOW FIELDS IN ESTABLISHING STEREO CORRESPONDENCE \$ 78,000
J. H. Duncan 01-C
87-2

The major difficulty in the analysis of stereo images is establishing correspondence, i.e., finding features in one image that correspond to given features in the other image. For static stereo pairs, a number of methods have been developed to establish correspondence. These methods are time consuming and difficult to implement at the edges of objects where the range is discontinuous. In many applications, there is relative motion between the camera pair and the objects in the field of view. In these cases, it is possible to obtain an optical flow field in the left and right images. Since the relative motion between the cameras is known, equations can be derived relating the left and right image flow fields. One relation is obtained by subtracting the flow fields; the resulting equation for the rate of change of disparity is called the binocular flow equation. Preliminary calculations and experiments for rigidly attached, parallel camera-pair configurations have shown that this relation is promising as a guide for establishing correspondence: potential matches can be tested by substituting the measured positions and velocities of the features into the equation. In the present study, the binocular flow equation is being explored in detail to find the limits of its usefulness in establishing correspondence in terms of camera-pair motions and surface shapes.

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

47. STUDY OF MAGNETOSTATIC PROBLEMS IN NONLINEAR MEDIA WITH HYSTERESIS
I. C. Mayergoyz
- \$ 68,000
06-C
83-4

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

48. TURBULENT PREMIXED FLAME STUDY \$135,000
Wai Cheng, James Keck 06-B
Steve Pope (Cornell University) 86-3

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
The Energy Laboratory
Cambridge, MA 02139

49. METAL TRANSFER IN GAS METAL ARC WELDING \$120,000
Thomas W. Eagar 03-B
85-3

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.

Current research emphasizes understanding of the forces controlling droplet detachment in gas metal arc welding. Experimentally, a laser back lit viewing system has been developed which permits viewing of anode and cathode jet phenomena. Welds have been made with a variety of different metals (steel, aluminum and titanium) in different shielding gases (argon, helium, carbon dioxide). It is seen that the anode spot behavior changes dramatically with changes in both metal and gas composition.

This experimental information is being coupled with a model of the forces controlling metal transfer. These include gravitation, surface tension, aerodynamic drag, electromagnetic (Lorentz) force and plasma jet momentum. Initial studies show that globular transfer can be described quantitatively by previous theories which were presented originally in only a qualitative manner. Quantification of previous explanations of spray transfer depart markedly from the experimental observations. A new model of the globular to spray transition has been hypothesized and is currently being studied with a finite element model.

It is believed that this work will ultimately be useful in understanding metal transfer in pulsed current gas metal arc welding. This study also interfaces with the experimental and theoretical gas metal arc welding control models being developed at MIT by Professor D. Hardt and at INEL.

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

50. PLASMA REDUCTION OF METALLIC OXIDE PARTICLES \$119,000
J. F. Elliott, J. Szekely, R. E. Spjut 06-A
85-3

The objective of this research is to characterize reactions in composite carbon-metal oxide particles and the possible reduction of metal oxide particles injected into the tail flame of a thermal 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 rapidly moving projectile. 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.

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
Department of Materials Science and Engineering
Cambridge, MA 02139

51. HIGH TEMPERATURE GAS-PARTICLE REACTIONS \$140,000
J. F. Elliott, R. E. Spjut, P. O. Bolsaitis 06-A
85-3

The objective of the research program is to examine the physico-chemical behavior of individual inorganic particles for conditions simulating those to which particles are exposed in thermal 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 measurements of the strength of the field permits determination of the weight of the particle before and after its exposure to the laser beam. 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.

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.

Experiments are in progress to (a) develop means of extracting the reacted particle for examination by various means, (b) study phase transformations, particularly solidification of alloys and ceramic materials at high rates of cooling, (c) study behavior of carbon-oxide particles in simulated plasma conditions, and (d) study ignition and combustion of metal particles.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Energy Laboratory
Cambridge, MA 02139

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| 52. | DEVELOPMENT OF AN EXPERT SYSTEM | \$ 93,000 |
| | TO SYNTHESIZE HEAT AND WORK | 03-A |
| | INTEGRATION SYSTEMS FOR PROCESS PLANTS | 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
Energy Laboratory
Cambridge, MA 02139

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|-----|--|---------------------------|
| 53. | A PARITY SIMULATOR FOR NUCLEAR
POWER PLANT DYNAMICS
K. F. Hansen | \$214,000
06-C
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
Laboratory for Manufacturing and Productivity
Cambridge, MA 02139

54. MULTIVARIABLE CONTROL OF THE GAS-METAL ARC WELDING PROCESS \$166,000
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 here is to treat the comprehensive problem in a dynamically coupled, multivariable sense. Our work to date has been divided between modelling and control for weld bead geometry and for thermal characteristics.

In the geometry control problem, a four state, non-linear dynamic model has been derived on the basis of previous process analysis work and empirical data. This model relates the conventional welding controls: supply voltage, wire feedrate and welding speed to bead width, depth and reinforcement height. It has been found that not only is the model non-linear, it is extremely sensitive to the operating point used for any local linearization. This leads to the need for a true non-linear control approach, and the current candidate for this is Sliding Mode Control, which can directly incorporate the non-linear model. We are also developing an experimental facility to perform model verification and, eventually, control system studies.

A parallel effort has concentrated on the multivariable control of thermal characteristics including the heat affected zone width, gross cross-section of the pool and centerline cooling rate. A fully non-linear, finite difference model has been developed that captures the thermal dynamics for these outputs and the model has been verified experimentally. An equivalent linear transfer function matrix has been derived from simulation on this model, and again the linear equivalents are non-stationary, but in a less catastrophic manner than with geometry. However, they are variable enough that our control work has mandated the use of a discrete Model Reference Adaptive Control Method. Control experiments are now underway using direct IR sensing of top surface temperatures for real-time feedback.

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

55. THE DEVELOPMENT OF A FRICTION MODEL \$ 0
PREDICTING THE SLIDING BEHAVIOR OF 01-D
MATERIAL PAIRS, ESPECIALLY AT LOW TEMPERATURES 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 knowledge will contribute to a more reliable operation of superconducting magnets.

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

56. IN-PROCESS CONTROL OF RESIDUAL STRESSES AND DISTORTION IN AUTOMATIC WELDING \$110,000
Koichi Masubuchi 03-A
85-3

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

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

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

Phase 2-1: Analytical and experimental studies of thermal stresses during welding and forces acting on tack welds.

Phase 2-2: GMAW process control to minimize interference from tack welds.

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

Phase 2-2 has been added since July 1986. The research efforts thus far covered all phases but Phase 3, which will be done at the end of the program.

The major effort under Phase 1 has been to study means for reducing distortions and residual stresses in girth-welded pipes. It has been found that an application of internal pressures during welding is an effective means of reducing radial distortion.

The major effort under Phase 2-1 has been to study transient thermal stresses and metal movement during butt welding of steel and aluminum plates. It has been found through experiments that forces acting on tack welds can be significantly reduced by additional heating by oxyacetylene torches placed alongside the welding arc. Through an analytical study it has been found that the most effective way is to heat wide areas to relatively low temperatures so that (a) the counter metal movement produced by the additional heating is significant, but (b) the supplementary heating does not produce additional residual stresses.

Under Phase 2-2, basic research has been conducted on possible ways for minimizing interference of tack welds by increasing penetration of the main root-pass welding.

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

57. MODELING AND ANALYSIS OF SURFACE CRACKS \$185,000
David M. Parks, Frank A. McClintock 01-A
85-3

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 of nonlinear fracture mechanics in these crack configurations as they are influenced (principally) by material strain hardening, load magnitude, 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.

To date, detailed non-linear three-dimensional finite element studies of surface cracks under predominant tension show that the asymptotic HRR stress fields of power law hardening materials typically dominate for normal stress levels up to $\sim 75\%$ of yield strength, with a rapid loss of dominance at higher load levels. Calculated crack front deformations are in good agreement with experimental measurements made at the Idaho National Engineering Laboratory. The line-spring has been generalized to include elastic/power law behavior, and resulting solutions are within a few percent of corresponding continuum solutions requiring more than an order of magnitude more computation.

Finally, detailed three-dimensional studies of through-cracks in "thin" sheets has accurately quantified the stress intensity variation through the thickness, as well as the boundary layer structure near the intersection of the crack front with the free surface.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, MA 02139

58. ENERGETICS OF COMMINUTION \$124,000
Carl Peterson 01-A
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 Materials Science and Engineering
Cambridge, MA 02139

59.	MATHEMATICAL MODELLING OF TRANSPORT PHENOMENA	\$115,000
	IN PLASMA SYSTEMS	06-A
	J. Szekely	85-3

The purpose of this investigation is to develop a comprehensive mathematical representation of the electromagnetic force field, the velocity field, and the temperature field in plasma systems.

The problem has been formulated through the statement of the appropriate transport equations and an extensive set of numerical results has been generated. These results describe the velocity field, the temperature field and the mixing characteristics of non-transferred arc plasma jets, both in the absence and presence of swirl. The theoretical predictions were found to be in excellent agreement with measurements conducted both at the Idaho National Engineering Laboratory and at the University of Limoges in Limoges, France.

These computed results are generating a hitherto-unavailable basic understanding of the behavior of plasma systems, and should be helpful in providing the basis for the rational design of plasma reactors.

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

60. A DESIGN AND SYNTHESIS PROCEDURE \$ 42,000
FOR HOMOGENEOUS AND HETEROGENEOUS 06-A
AZEOTROPIC DISTILLATIONS 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 synthesizing optimal separation sequences for multicomponent azeotropic mixtures.

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

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|---|---------------------------|
| 61. SCREENING ALTERNATIVE CONTROL STRUCTURES FOR
PLANT CONTROL SYSTEM
J. M. Douglas, M. F. Malone | \$120,000
03-A
83-6 |
|---|---------------------------|

An interactive computer code that helps the user to develop a conceptual design of a petrochemical process has been completed, and a similar code that helps the user to retrofit a process is about 75% complete. A code that estimates the incremental costs associated with the steady state control of the process is currently being developed. That is, the code helps to identify the dominant disturbances, it checks to see if an adequate number of manipulative variables are available for control (and it calculates the costs associated with modifying the flowsheet to ensure that the process is controllable), it assesses if equipment constraints are encountered when disturbances enter the process and manipulative variables are changed to compensate for these disturbances (and it estimates the costs required to remove these constraints), and it suggests control system alternatives that give close to the optimum operating costs.

We are also building dynamic models of complete processes in order to determine the effect of control system alternatives on the total operating costs of the complete process. We intend to use the results of these studies to develop short-cut procedures for screening control system alternatives. Some short-cut models have been developed, but these need to be tested against rigorous simulations.

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

62. MIXING: STRETCHING, BREAKUP, AND CHAOTIC MOTION \$ 55,000
OF IMMISCIBLE LIQUIDS 01-C
J. M. Ottino 85-3

In spite of its universality and practical implications, the understanding of fluid mixing remains largely empirical and little theoretical foundation exists at the present time. The goal of our research focuses on two aspects of mixing problems with the long range objective of establishing a sound background for the analysis of such processes: (i) theoretical and experimental investigations of the conditions that determine the onset of chaos in deterministic two dimensional flows, and (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 focusing on deformation and breakup in Lagrangian (linear) time dependents flows. The breakup depends in a complicated way on the balance between elongation and vorticity at small scales; on the other hand, the dispersion is effective if the large scale flow is chaotic.

During the past year we concentrated primarily on (i). The strategy was to study rather thoroughly a simple prototype flow - a periodically operated cavity flow - in order to extract as much information as possible about the behavior of two-dimensional chaotic fluid flows in general. We focused on the asymptotic behavior of coherent structures, such as holes and large scale structures (folds) produced by the mixing, as well as the structure of periodic points and sequences global bifurcations. Besides the obvious relevance to mixing of viscous liquids these results can be useful in the understanding of problems as diverse as mixing in the earth's mantle, and mixing of shear sensitive biomaterials. On a more speculative level, the problem might serve as a prototype for coherent structures in turbulent flows.

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

63. MULTIVARIABLE AND DISTRIBUTED CONTROL \$ 59,000
OF NON-LINEAR SYSTEMS 03-A
E. Ydstie 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

64.	NONLINEAR VISCOELASTIC CHARACTERISTICS OF POLYMERIC MATERIALS	\$ 76,000
	S. K. Clark	01-D 86-2

This research has as its objective the development of greatly improved methods for the analytical description of the nonlinear viscoelastic response of textile cords commonly used in reinforced elastomeric products. Such cords are characterized by their sensitivity to frequency, temperature, strain history and moisture. Typical materials of this class are nylon, polyester, and aramid. While linear theories are capable of providing first-order approximations for small strain ranges, more complete material description can only be obtained by considering nonlinear effects of the reinforcing materials.

While generalized three dimensional viscoelastic equations are available for the response of the stress tensor to strain under isothermal conditions; these are so cumbersome when expanded in multidimensional form as to be extremely difficult to confirm experimentally. For this reason, the one-dimensional case exemplified by twisted textile cord provides an excellent opportunity to assess the adequacy of these published theories. This is being done by comparison of the one-dimensional form of these theories with experimental data, which can be obtained readily on such cords. This will give valuable insight into the adequacy of two and three-dimensional models for more complex situations. A significant experimental program is being carried out using both twisted and untwisted textile reinforcing elements under a variety of temperature, strain and frequency conditions. Creep effects, nonlinear elastic effects and hysteretic properties are being assessed through the entire range of these variables. Once the constants of the analytical model are obtained, the adequacy of the model will be evaluated by comparing predictions made with experimental data taken on load histories differ from those used in obtaining the model constants.

At the present time experiment equipmental has been fabricated for carrying out these tests and data is currently being collected and analyzed.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, MN 55455

65. THE IMPACT OF SEPARATED FLOW ON HEAT AND MASS TRANSFER \$116,000
R. J. Goldstein 01-B
87-4

In many real flow systems separation occurs either intentionally or unintentionally. Such separations, often unsteady by nature, tend to result in three-dimensional and secondary flows. Heat and mass transfer in some situations can be unsteady; there can be energy separation in the flow and often large gradients in heat and/or mass transfer occur which are difficult to measure. The proposed study will include a variety of flow situations involving separation and also the development of special measurement techniques to study the heat and mass transfer in the presence of large gradients. Situations to be studied include the flow over two and three-dimensional steps, separation of the flow around circular and square cylinders projecting from surfaces including the influence of a horseshoe vortex and localized fins, flow through a porous medium represented by a simple flow, and the vortex rings formed around a jet as it flows out of an orifice or nozzle. These include the development of precision microsensors for highly localized measurements of the heat flux, and further development of techniques for local mass transfer measurement.

UNIVERSITY OF MINNESOTA
Department of Aerospace Engineering and Mechanics
Minneapolis, MN 55455

66. LUBRICATED PIPELINING \$ 70,000
Daniel D. Joseph 01-C
87-3

This project has as its aim the understanding and control of water lubricated pipelining of viscous crude oils, coal-oil dispersions and other viscous materials. The basis for this work is that there are domains of parameters in which water lubricated transportation of viscous materials is stable. The lubricated configurations can introduce enormous savings of energy in the form of reduced pressure gradients for enhanced transport. The studies underway are theoretical and experimental. The experimental studies are on the transportation of coal oil dispersions, on the properties of emulsified solutions at large shear, and on stable wavy interfaces arising from nonlinear interactions. The problem of coal-oil dispersions is to know if the coal can be made to stay in the oil under conditions of lubricated transport. Stability calculations underway are designed to identify the windows of parameters in which core annular flow is stable and to calculate maximum growth rates for unstable flow. Future studies will concentrate on extensions to include effects of oil wetted walls, gravity and nonlinear mechanisms.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, MN 55455

67. THERMAL PLASMA PROCESSING OF MATERIALS \$125,000
E. Pfender 06-A
85-3

The objective of this research project is a combined analytical/experimental study of the interaction of particulate matter with thermal plasmas, including chemical reactions in the vapor phase.

The analytical work is primarily concerned with heat, mass, and momentum transfer of particulates in thermal plasma flows and with the chemistry involved in the production of fine ceramic powders. A recent literature survey and a critical analysis of available heat transfer data shows that the disagreement between various proposed correlations and experiments may exceed an order of magnitude. This is a clear indication that more work is needed for establishing realistic heat transfer correlations.

Over the past year, some general rules have been established for the thermochemistry of chemical reactions in thermal plasmas and these rules have been applied to the synthesis of silicon nitride. The formation of free silicon in the liquid phase around 2,500 K and high supersaturation ratios of silicon are detrimental for achieving high silicon nitride yields.

The major objective of the experimental work is the development and diagnosis of a new plasma reactor with three cathodes which should solve the problems of particle injection, particle confinement, and particle dwell time in the plasma. Spectrometric measurements are in progress showing temperatures up to 16,500 K in pure argon (1 atm) and pronounced off-axis peaks close to the cathode.

Because of severe limitations of the present reactor, a new reactor is being designed, offering enhanced flexibility in terms of spacing and orientation of the cathodes, and increased power levels.

NATIONAL BUREAU OF STANDARDS
Chemical Engineering Science Division
Center for Chemical Engineering
Boulder, CO 80303

68. RESIDENCE TIME DISTRIBUTION APPROACH TO THE STUDY OF FREE CONVECTION IN POROUS MEDIA \$110,000
Michael C. Jones, R. A. Perkins 01-C
87-2

In this project, the object is to apply the principles of Residence Time Distribution (RTD) analysis to the study of free convection in porous media. The advantages of this technique are that it is nonintrusive, the data are quickly generated, and a large amount of information, distributed in the time domain, is obtained. The disadvantage is that a model must be used to infer the flow pattern from the RTD. It is proposed to apply the same modeling approaches that have been used successfully in mixing tank studies and to interpret the flow patterns in terms of similar mixing model parameters. Correlations would then be sought with the global parameters of the porous medium like Rayleigh, Peclet and Nusselt numbers.

An experimental program will be undertaken in which tracer responses will be obtained for a variety of buoyancy-induced flow conditions to obtain the mixing model parameters. Single point tracer responses as well as multiple point responses on the medium boundaries will be obtained. It is hoped that the latter will lead directly to a description of the cellular flow patterns.

NATIONAL BUREAU OF STANDARDS
Thermophysics Division
Boulder, CO 80303

69. NEUTRON SCATTERING FROM A SHEARED LIQUID: A PROPOSAL TO CONSTRUCT THE SHEARING APPARATUS
H. J. M. Hanley
- \$ 87,000
06-A
87-2

The project aims at the development of equipment to measure the microstructure of liquids out of equilibrium. The objective of the research is to investigate, via neutron scattering, liquids subjected to a shear. The work will focus on the examination of the variation of the structure with respect to a universal parameter, the relaxation time. The relaxation time is the key to characterizing the complexity of the fluid (i.e., complex versus simple) and how it will behave out of equilibrium.

Two shearing cells will be constructed to handle fluids representing a wide range of viscosity, from about 10^{-2} Pa s to about 10^{10} Pa s. The viscosity is proportional to the relaxation time. Experimental problems due to viscous heating and to limits on the force that can be applied to the liquid will be addressed. A feature of the cells will be that they will operate in a transient mode. The structure of the liquid will be inferred from intensity patterns scattered from incident neutrons when the fluid is at rest and when it is sheared. Of particular interest is the possible structure or molecular correlation which may extend over several molecular diameters. Candidate fluids for initial measurements are supercooled molecular fluids and colloidal suspensions.

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

70. THERMOPHYSICAL PROPERTY MEASUREMENTS IN FLUID MIXTURES \$390,000
N. A. Olien, J. M. H. Levelt Sengers 03-B
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-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.

The most recently completed apparatus include a variable volume vapor-liquid equilibrium apparatus for moderate temperature ranges; a Langmuir film balance for use with aqueous, hydrocarbon, and biopolymer systems; a magnetic suspension densimeter for high temperatures and pressures; a torsional crystal viscometer for high temperatures and pressures; and a transient hot-wire apparatus for thermal conductivity measurements at high temperatures. The latter two apparatus are capable of reaching pressures near 70 MPa.

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

71. TOPICS IN PHYSICO-CHEMICAL HYDRODYNAMICS \$250,000
Evgeny Levich 01-C
80-8

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 27695-7911

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| 72. | ANALYSIS OF TRANSPORT MECHANISMS IN DENSE FUEL | \$ 67,000 |
| | DROPLET SPRAYS | 01-C |
| | C. Kleinstreuer | 87-3 |

Of interest are the effects of droplet interaction on the droplet dynamics, droplet vaporization and trace gas entrainment in spray systems. The dense spray portion is conceptualized as two or three streamers of several closely spaced droplets in a non-isothermal environment. Using a boundary-layer type approach for the high to moderate Reynolds number range of interest, the governing equations for the droplet dynamics, fluid mechanics and heat/mass transfer are derived and solved numerically. The fundamental analysis of multiple droplet systems is important for the physical understanding of dense spray processes and for the improved design of fuel droplet combustion as well as spray cooling, coating and separation.

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

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| 73. | TRANSPORT PROPERTIES OF DISORDERED POROUS MEDIA | \$ 94,000 |
| | FROM THE MICROSTRUCTURE | 06-A |
| | S. Torquato | 86-3 |

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 or electrical conductivity and the fluid permeability) and its microstructure. In particular, we shall focus our attention of 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 effective properties of models of both unconsolidated media (e.g., soils and packed beds of discrete particles) and consolidated media (e.g., sandstones and sintered materials).

A theoretical formalism has been developed to represent a general n-point distribution function from which one may compute any of the various types of correlation functions that have arisen in the literature. An efficient computer-simulation technique has also been developed to obtain these statistical quantities. Employing such lower-order n-point distribution functions, sharp bounds on the conductivity, elastic moduli, and permeability of models of porous media have been computed. The rigorous bound on the permeability for random beds of spheres is relatively close to the well-known Kozeny-Carman empirical formula. Finally, the study of percolation of phenomena in continuum random-media models has recently begun.

NORTHWESTERN UNIVERSITY
Department of Civil Engineering
Evanston, IL 60208

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| 74. | EFFECTS OF CRACK GEOMETRY AND NEAR-CRACK MATERIAL
BEHAVIOR ON SCATTERING OF ULTRASONIC WAVES FOR QNDE
APPLICATIONS
J. D. Achenbach | \$ 67,000
03-B
86-3 |
|-----|---|---------------------------|

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 are also valuable in interpreting scattering data for the inverse problem.

From the mathematical point of view an open crack is a surface which does not transmit tractions. The implementation of this statement in a mathematical formulation generally involves a number of idealizations. In work on this project, the usual mathematical modeling of ultrasonic wave scattering cracks is being extended to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks.

Results have been reported that display the effect of deviations from a mathematically perfect simple crack geometry. Most of the results have been obtained by formulating a set of singular integral equations for the fields on the boundaries of the scattering obstacles. These equations have been solved numerically by the boundary element method, and the scattered fields have subsequently been obtained by using representation integrals. 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

75. THINNING AND RUPTURE OF A THIN LIQUID FILM ON A HORIZONTAL HEATED SOLID SURFACE
S. G. Bankoff
- \$ 0
01-C
86-3

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

76. CENTER FOR ENGINEERING SYSTEMS ADVANCED RESEARCH (CESAR) \$1,075,000
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 1987 research initiatives resulting in publications have included: (1) Robot navigation learning in unexplored terrain, (2) Virtual-time operating system functions for robot control, (3) Inverse dynamics position control of a compliant manipulator, (4) Stability, capacity, and design of non-linear continuous networks, (5) 3-D world modeling based on combinatorial geometry, (6) Methodologies for dynamic task allocation in man-machine systems, (7) O-Theory: a probabilistic alternative to fuzzy set theory, (8) Real-time expert systems for control of autonomous robot navigation in the presence of moving obstacles, (9) Combinatorial optimization of the computational load balance for a hypercube computer, and (10) Inclusion of 1-9 within a systems integration framework encompassing concept demonstration and feasibility.

PRINCETON UNIVERSITY
Department of Mechanical and Aerospace Engineering
Princeton, NJ 08544

78. FUEL DROPLETS SUBJECT TO STRAINING FLOW \$ 27,000
Forman A. Williams 01-C
87-3

This research, which has only been underway for several months, involves a theoretical and experimental investigation of fuel droplets in a well-defined straining flow, that associated with a nonpremixed flame, established in counterflowing streams of gaseous fuel and oxidizer. The initial purpose of this effort is to determine the validity of current theories of droplet burning under dynamically changing velocity and ambient conditions. Existing theories are based on highly idealized models of such burning and have been evaluated only under conditions closely approximating those assumed in the theory. The question arises as to their applicability to conditions which prevail in applications, typically in turbulent flows involving fluctuations in velocity and composition. Follow-on studies will be concerned with improved theories of droplet burning, if called for, and with droplet loadings sufficiently large so that a significant interaction between the droplets and the flame occurs. The experimental effort is complemented by appropriate theoretical investigations. Thus, the trajectories and histories of the droplets in the initial experiments will be compared with calculations based on a series of descriptions of increasing completeness in order to establish which, if any, of the theories predicted the observed behavior. Subsequent theoretical work will involve application to the counterflowing configuration of the spray equation which contains more of the aerothermochemical details of droplet behavior than the equations of coexisting continua.

The initial effort will study the behavior of individual droplets of hexane injected on the fuel side of a methane-air flame. An appropriate counterflow burner and droplet injection system have been designed and constructed. The photographic system which involves a camera and stroboscopic light of high repetition rate and intensity is being assembled. The complementary theoretical effort concerned with the calculation of droplet trajectories and histories in a methane-air flame is underway.

This entire research program is being pursued jointly with Paul A. Libby and K. Seshadri at the University of California, San Diego.

PURDUE UNIVERSITY
School of Mechanical Engineering
West Lafayette, IN 47907

79. EFFECT OF FORCED AND NATURAL CONVECTION ON SOLIDIFICATION OF BINARY MIXTURES \$ 89,000
F. P. Incropera 01-C
87-3

This study deals with the influence of combined convection mechanisms on the solidification of binary mixtures in both rectangular and cylindrical geometries. The mechanisms include natural convection driven by temperature and solute concentration gradients, as well as forced convection due to an externally imposed flow or a rotating surface. In the rectangular geometry, solidification is induced at one or both of opposing planar walls, with the ends capped, allowing for natural convection, or open, allowing for passage of an imposed flow and therefore combined convection. For the cylindrical geometry, solidification is induced in the annular cavity between cooled inner and/or outer tube walls, and the ends are capped. Combined convection is studied by solidifying at one tube wall while rotating the other wall. In addition, the effects of convection are studied under conditions for which the inner cylinder is removed and solidification is induced at a stationary or rotating end wall.

A primary objective of the work is to develop and validate a novel model for predicting the effects of convection on solidification in binary mixtures. Treating solid, mushy and liquid regions as a single continuous domain, the model applied continuum theory to solidification in mixtures with convection. Working with two-dimensional numerical solutions, calculations will be performed to determine phase front development and related velocity, temperature and concentration fields over a wide range of operating conditions. Predictions will be validated through comparison with experimental results obtained for transparent binary mixtures. The experiments will involve visual determinations of phase front development and flow within the melt, as well as temperature and concentration measurements. The results are expected to provide important insights concerning the effects of convection on solidification phenomena such as macrosegregation, while validation of the model should provide a useful computational tool for industrial processes involving the casting of binary materials.

PURDUE UNIVERSITY
School of Mechanical Engineering
West Lafayette, IN 47907

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| 80. | HEATING AND EVAPORATION OF TURBULENT LIQUID FILMS | \$115,000 |
| | Issam Mudawwar | 01-B |
| | | 85-4 |

This project aims at studying transport phenomena associated with turbulent liquid film flow. Experiments have been performed with films undergoing sensible heating or interfacial evaporation and correlations have been developed for a wide range of operating conditions. To better understand the effects of interfacial waves on film motion a new high resolution film thickness probe has been developed. Instantaneous measurements of film thickness have been obtained for adiabatic film flow, and a modified probe design is expected to provide film thickness measurements on an electrically heated test section. The remaining tasks of this project will involve obtaining simultaneous measurements of film thickness and liquid temperature to better understand the transient variation of the heat transfer coefficient associated with film waviness. Parallel to this study, simultaneous measurements of the instantaneous longitudinal and transverse velocity components and of film thickness will be used to correlate a time-averaged eddy diffusivity profile which accounts for interfacial wave activity.

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

82. AN ANALYSIS OF THE CLOSURE CONDITIONS \$120,000
FOR TWO FLUID MODELS OF TWO-PHASE FLOW 01-C
R. T. Lahey, Jr., D. A. Drew 86-3

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.

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

83. SOME BASIC RESEARCH PROBLEMS RELATED TO ENERGY \$ 96,000
E. G. D. Cohen 06-A
81-6.

The project is concerned with the following objectives: 1. The prediction of the transport coefficients, such as viscosity, thermal conductivity and diffusion coefficients for mixtures of real fluids, using a new form of the modified Enskog theory. 2. To develop a kinetic theory that allows a computation of the transport properties of polydisperse fluid mixtures, based on an extension of the Enskog theory for hard sphere mixtures. 3. To study the forced modes and the eigenmodes in binary hard sphere fluid mixtures in thermal equilibrium for all mass ratios and densities. While the forced modes determine the response of the fluid to an outside disturbance of given frequency, the eigenmodes determine the response of the fluid to an internal disturbance of given wavenumber, such as a density fluctuation. The study will be based on the generalized Enskog theory. The results will be compared with laboratory and computer experiments. 4. A comparison of binary disparate mass mixtures in the gaseous state--such as the noble gas mixtures He-Xe--and in the liquid state--such as in $\text{Li}_{0.8}\text{-Pb}_{0.2}$ mixtures--will be made to study the occurrence of a new type of sound, fast sound, in these mixtures. 5. A critical study of cellular automata fluids will be undertaken, to ascertain their applicability to describe the flow properties of real fluids.

SANDIA NATIONAL LABORATORIES
Device Research Division
Albuquerque, NM. 87185

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|-----|------------------------------|-----------|
| 84. | HIGH-TEMPERATURE ELECTRONICS | \$120,000 |
| | 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°C) electronics for energy technologies. Included are sensors, passive components, and active semiconductor devices which provide electronic gain or control. Earlier 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

85.	DYNAMICAL PERCOLATION PROCESSES	\$135,000
	AND APPLICATIONS	06-C
	A. R. Kerstein	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 analytical 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

86.	DYNAMICS OF MULTICOMPONENT LIQUID FUEL DROPLETS	\$135,000
	B. R. Sanders, H. A. Dwyer	06-B 81-7

The overall objective of this program is the development of a comprehensive model of multicomponent liquid fuel droplet vaporization and combustion. Experimental evidence suggests that multicomponent liquid fuels can undergo disruptive behavior and microexplosive combustion; however, there is no detailed model available to explain such dynamic events. Disruptive behavior and microexplosive phenomena are of intense practical interest as secondary atomization methods to provide rapid fuel droplet disintegration, vaporization and combustion. Multicomponent fuel droplets also exhibit dramatically different ignition and extinction criteria than single component liquid hydrocarbon fuels droplets, and these differences can be used to advantage in promoting the combustion of low volatility fuels.

The technical approach consists of a complete description of a single liquid droplet undergoing vaporization and combustion in a strong convective gas environment. The model under development is based on the finite-difference solution of the full set of transport equations for transient mass, momentum and energy exchange in the liquid and gas phases. Global chemical reactions are specified by an Arrhenius rate expression, and adaptive gridding is used to resolve regions of large gradients, such as occur in the temperature field near the flame front.

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

87. ASPECTS OF TURBULENCE IN NONLINEAR SYSTEMS
E. Frieman, William Hagan

\$ 0
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.

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

88. SHEAR-INDUCED INSTABILITIES \$ 95,000
IN A DOUBLE-DIFFUSIVE 01-C
PARTIALLY STRATIFIED FLUID 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

89. TRANSPORT CHARACTERISTICS OF CONCENTRATED SLURRIES
Andreas Acrivos

\$ 73,000
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

90. HEAT TRANSFER IN THREE-DIMENSIONAL TURBULENT BOUNDARY LAYERS John Eaton	\$ 63,000 01-B 86-3
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Most boundary layers in practical systems are three-dimensional while most basic research on convective heat transfer has focused on two-dimensional flows. Previous measurements have shown that the turbulent stress field is strongly perturbed by the imposition of mean flow three dimensionality. The objectives of this work are to determine what, if any effects three-dimensionality has on the heat transfer behavior and how these effects may be modeled. A series of flows with successively stronger three-dimensionality are being examined. Work to date has examined two-dimensional boundary layers with large-scale embedded longitudinal vortices. The primary mechanisms governing the heat transfer rate were unaffected by relatively weak single vortices. Pairs of vortices provide stronger boundary layer perturbations and allow study of the effects of lateral divergence and convergence on the boundary layer. Detailed data including all components of the mean velocity and Reynolds stress, spatially resolved heat transfer, temperature profiles and skin friction have been obtained. Analysis of the vortex data is proceeding as the wind tunnel facility is modified for study of a strong three-dimensional boundary layer. Fluid mechanics measurements in the fully three-dimensional flow indicate that the important near-wall layers are strongly perturbed.

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

91. ENERGY CHANGES IN TRANSFORMING SOLIDS \$165,000
George Herrmann, David M. Barnett 01-A
86-4

The objective of this research is to investigate problems of stressed deformable solids in which computations of energy changes and associated thermodynamic (or configurational) forces have important implications.

An anisotropic elastic boundary integral method has been developed and used to predict the existence of stable void lattices in irradiated FCC and BCC metals; numerical results are in close agreement with experimental observations quoted in the literature. An apparent paradox in the dislocation literature has been resolved. Although it should be well-known that the energy of a (Volterra) dislocated solid is independent of the cut used to create it, virtually all such calculations in the literature are not cut-independent and are incorrect. Our resolution of this paradox has important implications for the appearance of misfit dislocations in epitaxial systems. A new investigation of energy changes and forces associated with dislocations in anisotropic layered media is being undertaken, and the theory of interfacial waves in anisotropic elastic media is being extended to include piezoelectricity.

An integral equation method has been developed to study problems of interaction between holes and defects in elastostatics, including the calculation of energy release rates. An elementary theory of defective beams in bending and of bars in tension, compression, and torsion has been developed. Based on an extended circle theorem originally established in potential flow theory, the temperature distribution in an infinite region containing a circular cavity (defect) was determined in terms of the distribution existing in the same region without the cavity. The stress distribution induced by the presence of the defect was shown to be universal, i.e., it depends essentially only on the magnitude of the heat flux vector existing at the center of the defect before it was created.

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

92. TOMOGRAPHIC OPTICAL DATA ACQUISITION SYSTEMS FOR	\$ 85,000
COMBUSTION RESEARCH	03-B
L. Hesselink	85-3

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 analysis allows 3-D reconstruction of the density or species concentration field. All 36 holographic interferometry projections are recorded simultaneously in 300 usec and after development the film is digitized for digital processing.

A Fourier transform technique is used for evaluation of the interferogram. Convolution back projection is used to reconstruct a volume of 7x7x7 cm of a coflowing he-air jet, approximately 6 diameters downstream of a 2.5 cm jet. The velocity ratio is 2.5:1 between the inner helium (8 m/sec) and outer air flow. Excellent 3-D maps of the he concentration have been obtained in the transition region of the jet ($Re \approx 2500$).

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

93. NONDESTRUCTIVE TESTING \$120,000
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

94. FLEXIBLE AUTOMATED OPTICAL SENSING SYSTEMS FOR \$200,000
THE STUDY AND CONTROL OF ENERGY CONVERSION PROCESSES 03-B
C. H. Kruger 85-3

Optical sensors integrated with computers are needed for the study and control of energy conversion processes. This program aims to develop systematic methods for combining the capabilities of optical sensors and computers to generate advanced optical sensing systems. This research is interdisciplinary and involves investigation of sensors, optical signal analysis, computer integration, as well as the development of facilities for proof of the sensor systems.

Several approaches and sensor types have been brought to a fruitful position where proof-of-concept experiments have been performed and the results reported externally at symposia and in the literature. These include a fiberoptic evanescent field absorption sensor, a reflection-based fiberoptic displacement sensor, a miniature fiberoptic probe for optical particle sizing, and a low cost real-time programmable hybrid correlator for industrial applications.

In the continuing research, consolidation of the experimental activities being pursued with emphasis on plasmas is providing a rich environment for the investigation of sensor techniques. Of particular interest are the measurement of electric fields in low-pressure plasma discharges and diagnostics for the study and control of plasma chemistry. The latter area includes research on two-dimensional imaging techniques for plasmas, which would provide the as yet unrealized capability of visualization of plasma reactivity and assessment of the importance of nonequilibrium effects.

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

96. MOMENTUM AND HEAT TRANSFER IN A COMPLEX BUT WELL-DEFINED \$ 94,000
TURBULENT FLOW 01-B
Robert L. Street, Jeffrey R. Koseff 87-1

A basic study of a three-dimensional, recirculating flow with variable density effects is being conducted in a lid-driven cavity. The overall objectives of the research are (1) an improved understanding of the influence of the Taylor-Gortler-like (TGL) vortices on heat transfer in the cavity and of the interaction between forced and natural convection processes, and (2) three-dimensional numerical simulation of recirculating, natural, and mixed-convection flows. Present emphasis is on understanding the interaction between buoyancy and shear phenomena in mixed convection flows, with particular attention on the effects of cavity geometry on these phenomena and the resulting heat transfer parameterization. The physical experiments are being performed in a unique, lid-driven cavity facility using water as the working fluid. Measurements include those obtained by laser-Doppler anemometry, microthermocouples, heat-flux meters, and liquid crystal and rheoscopic flow visualization techniques. In addition, numerical experiments are being performed in support of the specific experiments and on the interesting side-wall heated natural convection flow. The numerical experiments are being conducted using the SEAFLOS1 code which is significantly faster and more efficient than the REMIXCS code used for earlier cavity simulations. Both implicit and explicit versions of SEAFLOS1, which features a revised QUICK formulation for non-uniform grids and the use of the Incomplete Cholesky Conjugate Gradient Method for solving the pressure equation, are in use.

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

97. GLOBAL OPTIMIZATION OF NON-POSYNOMIAL DESIGN MODELS \$ 86,000
Douglass J. Wilde 03-A
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 primaldual 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 unimodel subproblems.

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

98. INVESTIGATION OF TRANSITIONS FROM ORDER TO CHAOS IN DYNAMICAL SYSTEMS
George Schmidt
- \$ 64,000
06-C
87-4

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. This work is nearly completed and we are tooling up to study more complex systems with many degrees of freedom.

We have determined the dynamics of transition from Hamiltonian to dissipative systems in the chaotic regime. As the Hamiltonian limit is approached, strange attractors disappear in an orderly fashion as dissipation is reduced. There exist a set of universal Jacobians J_n , where the 2^n piece strange attractors disappear. This phenomenon is universal as we have proven using renormalization calculations, in the vicinity of the universal Hamiltonian function T . In fact we have shown that all phenomena possess a universal scaling in the K - J parameter space, where K is the strength parameter and J is the Jacobian.

We studied universal strange attractors, homoclinic and heteroclinic crises, Liapunov exponents and windows. Everything scales along fan lines in parameter space in a well defined manner.

Physical systems that produce two dimensional maps are of course different from the universal ones. We have found recently that such systems exhibit extremely rapid convergence to the universal sequence of J_n values. Among the systems studied were the driven damped pendulum, the bouncing ball, the particle in the standing wave field. All systems studied exhibited the rapid convergence to the universal system as predicted. 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

99. THE BEHAVIOR OF MATTER UNDER NONEQUILIBRIUM CONDITIONS: FUNDAMENTAL ASPECTS AND APPLICATION IN ENERGY-ORIENTED PROBLEMS I. Prigogine \$ 60,000
06-C
81-6

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 occurring 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
Department of Physics
Austin, TX 78712

100. PERTURBATION AND CHARACTERIZATION OF NONLINEAR PROCESSES \$135,000
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 nonlinear 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.

UNIVERSITY OF TEXAS
Department of Mechanical Engineering
and Center for Energy Studies
Austin, TX 78712

101. SELF-SHIELDING OF SURFACES IRRADIATED \$134,000
BY INTENSE ENERGY FLUXES 01-B
Philip L. Varghese, John R. Howell 87-3

The objective of this work is to study the interactions between high-temperature, high velocity plasmas and solid surfaces. There are two main thrusts in the program: numerical modeling and experimental testing of model predictions. This calibrated modeling procedure will provide information for reliable predictions of plasma-surface interactions with extremely high energy fluxes. The work will be conducted in unique facilities at the University of Texas at Austin. Plasmas at high temperatures (greater than 10,000 K) and densities (10^{15} cm^{-3}) will be accelerated in capacitor or homopolar generator driven rail guns. These plasmas will be studied using high speed emission spectroscopy and laser induced fluorescence in order to determine the composition and temperature of the plasma, and to detect the development and influence of the vapor shield produced by the surface when it is heated rapidly. The experimental results will be used to modify and refine the numerical model so as to provide an accurate and reliable predictive tool. The model will characterize the basic physical processes that govern the interaction between a surface and a transient energy flux. Because it is fundamentally based, rather than empirical, the model will be more readily adaptable to a wide range of situations in which surfaces are irradiated by intense energy fluxes. The model developed during the course of this work will allow better design of devices such as high current density brushes and switch gear, arc welding apparatus, rail guns, and fusion reactors.

TUFTS UNIVERSITY
Department of Mechanical Engineering
Medford, MA 02155

102. EFFECTIVE ELASTIC PROPERTIES OF CRACKED SOLIDS \$ 55,000
M. Kachanov 01-A
86-2

The knowledge of effective elastic properties of solids with cracks appears to be of increasing engineering importance. Extensive microcracking in structural elements working under conditions of high temperatures or irradiation, microcracking in composite materials under fatigue conditions may noticeably reduce the stiffness of the material and make it anisotropic. Understanding and prediction of these changes are essential for proper design and strength and lifetime assessments.

A new approach to many cracks problems based on interrelating the average tractions on individual cracks is introduced. Its advantages are that it yields simple analytical results which are quite accurate up to very high crack densities and that it can be applied to crack arrays or arbitrary geometry. Relation between deterioration of elastic properties and "damage" is discussed.

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

103. LASER DIAGNOSTICS OF PACVD PROCESSES \$185,000
W. C. Roman, J. H. Stufflebeam, F. A. Otter 06-A
A. C. Eckbreth 86-3

The objectives of this research are to perform a comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process applicable to hard face coatings. Based on its superior erosion resistance, TiB was selected as the initial coating for deposition onto a titanium alloy substrate (Ti-6Al-4V). In task I, novel non-intrusive laser diagnostic techniques (e.g. optical emission and absorption spectroscopy, Laser Induced Fluorescence Spectroscopy (LIFS), and Coherent Anti-Stokes Raman Spectroscopy (CARS) are being used to determine, in situ, the reactive plasma composition, temperature, and species concentration and distribution in the gas phase. The second task includes use of Auger Electron Spectroscopy (AES), Ion Scattering Spectroscopy (ISS), Secondary Ion Mass Spectroscopy (SIMS) and other complementary techniques for detailed coating characterization. These are being combined with physical measurements of coating surface smoothness, density, hardness (state-of-the-art nanoindenter apparatus) and adherence (UTRC custom built pin-on-disc apparatus). 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. Results to date include: 1) fabrication of a 5 kW rf PACVD reactor system integrated with a completely oil-free, high vacuum system (ultimate 10^{-8} torr); 2) exploratory spectral emission surveys for major molecular band and atomic line identification; 3) development of a colinear, scanned, narrowband CARS system and 4) implementation of a ultramicrohardness tester and adhesion test apparatus.

UNIVERSITY OF WISCONSIN
Mechanical Engineering Department
Milwaukee, WI 53201

106. INTERFACIAL AREA AND INTERFACIAL TRANSFER \$100,000
IN TWO-PHASE FLOW SYSTEMS 01-C
G. Kocamustafaogullari, M. Ishii (ANL) 87-3

The research program is a joint effort by the members of the University of Wisconsin-Milwaukee and Argonne National Laboratory. The objective of the research program is to develop instrumentation techniques, a data base and predictive methods for describing the interfacial structure of horizontal and vertical two-phase flow, such as flow pattern transitions, interfacial area concentration and interfacial wave structure. The special emphasis will be placed on developing local interfacial area concentration measurement techniques, and two-phase flow-pattern transition criteria. The latter include 1) scaling criteria in terms of systems size and fluid properties 2) entrance geometry and developing flow effects, and 3) rational procedure and design criteria for predicting these effects.

To achieve the objectives, the technical approach is divided into three parts. The first part deals with theoretical modeling of the interfacial area and flow-pattern transitions based on physical mechanisms. The second part is concerned with designing and performing horizontal and vertical two-phase flow experiments to generate benchmark data using flow visualization and objective measurements. Finally, the third part deals with incorporating the results of theoretical and experimental studies to examine and verify the validity of proposed flow-pattern transition mechanisms and interfacial area concentration modeling.

The results of this research program will provide information in horizontal and vertical two-phase flow fundamentals and information critical to the design of advanced two-phase flow systems.

UNIVERSITY OF WISCONSIN
Department of Chemical Engineering
Madison, WI 53706

107. 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
86-3.
- 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 studied 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.

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