DOE/ER-0674

Summaries of FY 1995 Engineering Research

March 1996

U.S. Department of Energy

Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences

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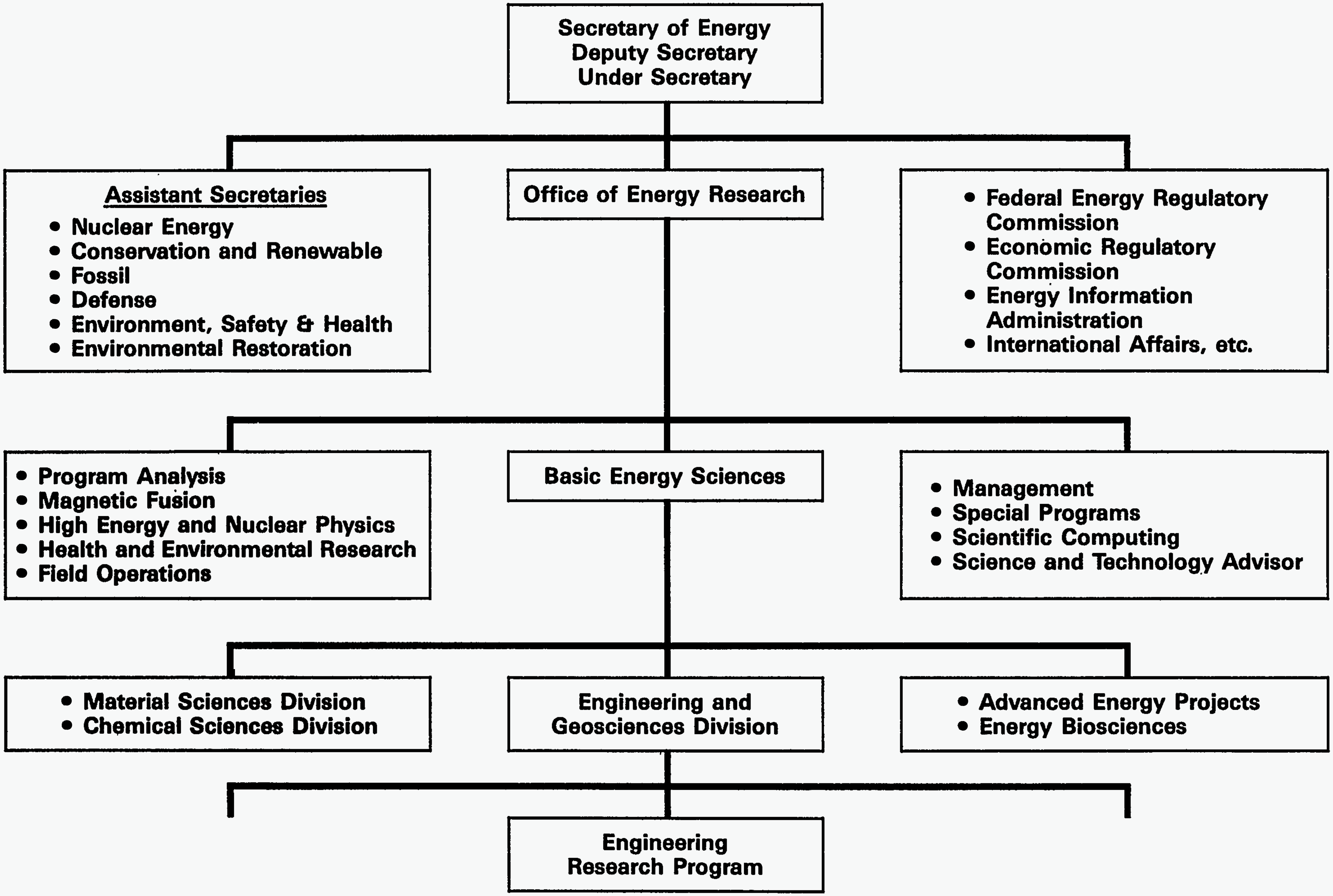
Germantown, MD 20874

Foreword

This report documents the BES Engineering Research Program for fiscal year 1995; 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, by phone at (301) 903-5822 or by fax at (301) 903-0271 (additional information and updates are accessible on World Wide Web, http://er.doe.gov.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1995. The summaries received have been edited if necessary, but the press for timely publication made it impractical to have the investigators review and approve the revised 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 the institutions at which projects were sponsored in fiscal year 1995.

Each project entry begins with an institutional-departmental heading. The names of investigators are listed immediately below the title. The funding level for fiscal year 1995 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. A separate index of Principal Investigators includes phone number, fax number and e-mail address, where available. The fiscal year in which either the project began or was renewed 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., 94-3). The summary description of the project completes the entry.

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 in 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 of 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 nonsteady flows, methodology for reducing vibrations and noise in heat exchangers, and engineering aspects of combustion.

3) Solid Mechanics: continuum mechanics, fracture mechanics, thermomechanical behavior in severe environments, aging & lifetime reliability of 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, 1985 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 in three carefully selected, high priority research areas; namely,

1) Mechanical Sciences including fluid mechanics (multiphase flow and turbulence) heat transfer, and solid mechanics (continuum mechanics and fracture mechanics), but excluding purely computational efforts.

2) System Sciences including process control and instrumentation, and intelligent systems.

3) Engineering Analysis including nonlinear dynamics, data bases for thermophysical properties of fluids, modeling of combustion processes for engineering application, and foundations of bioprocessing of fuels and energy related wastes.

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 previous growth in the program budget an important development took 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 an unstructured environment. Some resources are available for coordinated, more narrowly focussed, related, high quality research at universities and other research centers. All such activities are supported and administered directly by the Engineering Research Program, but some coordination of efforts with the ORNL program may prove useful.

Secondly in FY 1985, a collaborative research effort was started between MIT and Idaho National Engineering Lab. At present, the collaboration is in two distinct areas: Automated Welding, and Fracture Mechanics. Collateral, high quality research efforts at other institutions, including Plasma Process Engineering are supported by the Engineering Research Program.

In the expectation of a future modest growth of this Program, three International Workshops on Two Phase Flow Fundamental 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 proceedings of the two workshops have been published as volumes in the series "Advances in Heat and Mass Transfer" (Hemisphere Publishing Company). A third international workshop held in June 1992 surveyed the status of the field. The proceedings have been published by CRC Publishing Company, also in the series "Advances in Heat and Mass Transfer".

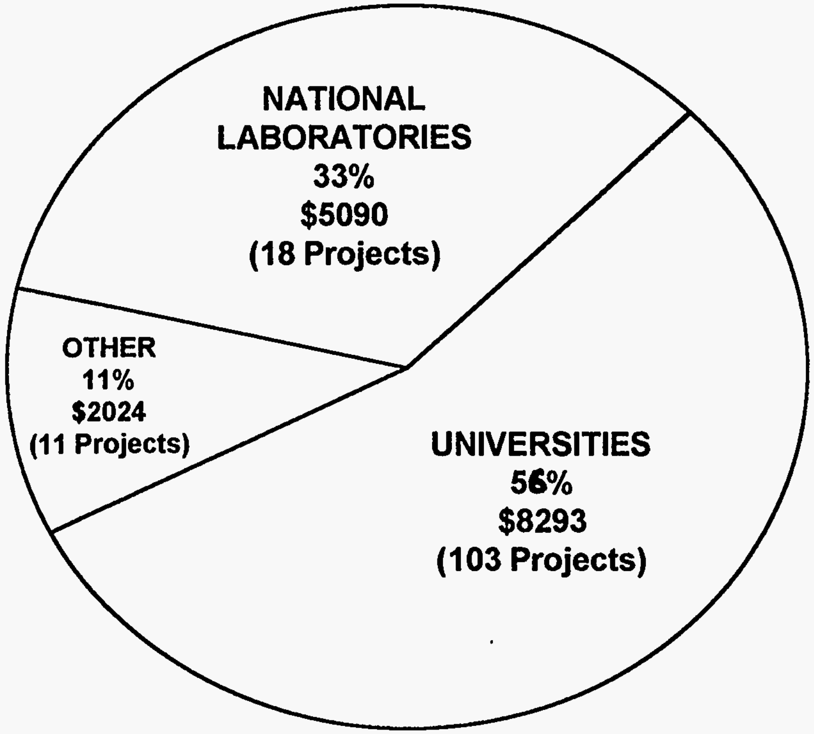
Two additional workshops were held during 1988. The first dealt with possible research opportunities in the field of novel devices using the new high temperature superconductors. The second addressed research needs for bioprocessing of fuels and energy related wastes. Reports of both workshops have been published. Additional funds had been provided in FY 1992 to initiate research in the above mentioned bioprocessing area. Of interest are relevant studies at the intersection of biology, biochemistry, and chemical engineering.

Another workshop aimed at identifying research opportunities to mitigate the effects of aging in energy production and distribution systems took place in October 1992. The proceedings have appeared in Applied Mechanics Reviews.

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. Also there is some interest in addressing the basic foundations of advanced manufacturing processes. In this context 36 three-year (12 per year) doctoral fellowships administered by National Academy of Science-National Academy of Engineering and National Research Council have been sponsored.

Research projects sponsored by the BES Engineering Research Program are currently underway at universities, private sector laboratories, and DOE national laboratories. In fiscal year 1995 the available program operating funds available amounted to about $15.5 million. The distribution of these funds among various institutions and by topical area 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 competitive grant applications. Applications 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 graduate education is an important consideration. Thus projects sponsored at universities are essentially limited to advanced theoretical and experimental studies usually performed by faculty members, staff research scientists, and doctoral candidates.

ENGINEERING RESEARCH PROGRAM
FY '95 BUDGET ($000'S)
BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '95 BUDGET
BY TECHNICAL AREAS

	($000's)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	4722	30.6	55
SYSTEMS SCIENCES	4208	27.3	24
ENGINEERING ANALYSIS	6479	42.1	53

Table of Contents

Table of Contents (continued)

University Of Alabama

Dept of Mathematics **$106,000**
Tuscaloosa, AL 35487 **01-C**
94-3

Hydrodynamic Instabilities and Coherent Structures
A. Frenkel

The objective of this research is to further the fundamental understanding of stability properties of several far-from- equilibrium fluid systems which are relevant to energy engineering sciences. In particular, flows periodic in space and possibly in time are studied as models to gain insights into such turbulence phenomena as large-scale coherent structures, eddy viscosity, and the inverse cascade of energy. Film flows--such as core-annular ones--are important to, e.g., lubricated pipelining of viscous oils. The large-scale evolution equations for the different systems may exhibit common features, such as pattern formation and coherent structures.

Some of the results are as follows: A rigorous iterative method was suggested for the problems of periodic-flow stability. The possibility of negative isotropic large-eddy viscosity was demonstrated, resolving a rather long-outstanding question. A weakly nonlinear Landau-type theory was constructed for an intermediate-scale instability of a periodic flow. The spatial structure of the saturated disturbances of this non-uniform flow is significantly different from previously known, uniform cases.

For film flows, a perturbative method capable of yielding both the evolution descriptions and the parametric conditions of their validity was suggested. A highly nonlinear evolution equation of a wavy flow down a cylinder was obtained. Its numerical simulations yielded an excellent agreement with experiments. They also revealed, for the first time ever in numerical simulations, irreversible coalescences of soliton-shaped coherent structures; these are now thought to play an important role in the wave dynamics of film flows. Also, a theory of a flow down an inclined plane was constructed. Simulations of the evolution equation showed a remarkable agreement with three-dimensional wave patterns observed in recent experiments.

Some fundamental questions concerning commonly used perturbative approaches were clarified. Certain deficiencies of well-known evolution equations were pointed out.

Argonne National Laboratory

Energy Technology Division **$194,411**
Argonne, IL 60439 **01-A**
94-1

Chaos in Fluid-Structure Systems
S. Chen

Energy systems have had a history of dynamic structural instabilities caused by fluid flow resulting in costly component repair and replacement and loss of energy production. Integrated theoretical and experimental studies are being performed to enhance the understanding of nonlinear oscillations and dynamic instability phenomena involving both fluids and solid structures and their coupling. The objectives are to contribute to the explanation of observed phenomena, providing insights into chaotic characteristics of such coupled mechanical systems and ultimately, to the solution of engineering design problems. This is a cooperative research program with Professor F. Moon at Cornell University.

Fluidelastic instability of loosely supported tubes is suspected to be one of the main causes of tube failure in some operating steam generators and heat exchangers. As a vehicle to understand the nonlinear behavior of fluid-structure systems, fluidelastic instability of loosely supported tube arrays in crossflow is being studied in detail. A tube row with a motion-limiting stop configuration has been tested to investigate various response characteristics and a mathematical model based on the unsteady flow theory has been developed to predict the response characteristics of this classical fluid-structure system. Other fluid-structure systems, such as coupled stack/wire dynamics due to wind excitations, have also been investigated. It involves lock-in resonance and parametric resonance of coupled oscillations of guided wires and stack. Analytical results and experimental data agree fairly well.

Tests and analysis of tube arrays are being continued. One of the key elements is the motion-dependent fluid forces which are being measured using the existing water channel with an emphasis on the nonlinear behavior. The motion-dependent fluid forces depend on Reynolds number, reduced flow velocity, and oscillation amplitude. Specific topics being addressed include mathematical models and instability mechanisms, interaction between flow field and oscillating structures, useful applications of fluidelastic instabilities, and control of fluid/structure systems.

University of Arizona

Aerospace & Mechanical Eng **$138,875**
Tucson, AZ 85721 **01-B**
93-3

Film Cooling in a Pulsating Stream
I. Wygnanski, H. Fazel, A. Ortega

Turbulent wall-jets are used for boundary layer control and film cooling. Thus the present investigation endeavors to determine the effects of two-dimensional excitation on skin friction and heat flux in laminar and turbulent wall-jets. The approach includes experiments, numerical simulations, and stability theory. The theoretical analysis at either constant temperature or constant heat flux boundary conditions was completed and validated experimentally in laminar flow. The development of the code for the compressible D.N.S continued. The code is based on the complete compressible Navier Stokes equations in conservation formulation. The wall boundary condition for the temperature was changed to allow for partially cooled or heated walls, where the length of the temperature ramp can be specified. The experimental investigation included simultaneous measurements of mean and fluctuating components of velocity and temperature using hot and cold wire anemometers. The flow was subjected to controlled two-dimensional excitation. Experimental results for the laminar wall-jet show that moderate excition may result in skin friction of 60% and a concomitant increase in heat flux of 30%.

Arizona State University

Mechanical & Aerospace Eng **$50,945**
Tempe, AZ 85287 **01-A**
92-4

Contiuum Damage Mechanics - Critical States
D. Krajcinovic

Objective: Primary objective of the current research program is to examine a variety of critical states in mechanical response of brittle and quasi-brittle solids containing a large number of crack-like micro-defects. More specifically, the focus of the ongoing research is placed on the determination of circumstances (type of loading, confinement level, shape and size of the specimen, thermal and environmental conditions, etc.) leading to the onset of critical states defined as a threshold connectivity at which a solid ceases to support external loads.

Technical Approach: Current applied mechanics/ engineering practice in evaluating the mechanical failures of brittle and quasi-brittle solids emphasizes use of effective continuum theories coupled with the deterministic and highly idealized description of the defect geometry (such as doubly periodic arrays of penny-shaped cracks). In contrast, the approach selected in this research program accentuates the stochastic geometry of the microstructural disorder and its effect on the onset of macro-fracture and the type of the failure mode.

One of the important aspects of this research is to explore applicability of the novel methods of statistical physics (percolation theory, models of self-organized criticality, etc.) to micromechanical models. Some of the already obtained results provide connection between the mechanical parameters such as stiffness and damage variable and the percolation theory concepts such as the order parameter, excluded volume, etc.. This provides a set of rational criteria for the selection of the universal dimensional invariants needed to describe the onset of a certain class of failures. Secondly, use of the statistical methods (such as fractal and multifractal formalism) provide a superior and size-independent (intrinsic) description of the fluctuations in the stress field (stress concentrations) in the vicinity of the critical states. This aspect alone should provide a definitive answer related to the dependence of the order-disorder transition on the microstructural texture and/or boundary conditions. In summary, the selected approach provides the best hope of description of the universal aspects of the stochastic nature of the damage and its evolution in the vicinity of the critical state.

Battelle Memorial Institute

Engineering Mechanics Dept **$23,000**
Columbus, OH 43201-2693 **01-A**
94-3

An Investigation of History-Dependent Damage In Time-Dependent Fracture Mechanics
F. Brust, Jr.

To increase energy efficiency, new power plants must operate at higher and higher temperatures. Moreover, power generation equipment in the US continues to age and is being used far beyond its intended life. Some recent failures have clearly illustrated that current methods for insuring safety and reliability of high temperature equipment is inadequate. Because of these concerns, an understanding of the high-temperature crack growth process is very important.

Critical experiments are performed on materials which are used in these severe high temperature environments. Theoretical models are then developed which attempt to predict the crack growth and failure response of these material components. The models are then exercised, and compared to the experimental results, with modifications/improvements made as necessary. This synergistic interaction between analytical, computational, and experimental disciplines has proven very effective. To date, both sustained and variable high temperature load histories have been investigated in two-dimensional geometries. The model, which is based on the use of advanced constitutive laws and the use of new integral parameters to understand and predict the events leading to failure, has proven quite effective. Current efforts involve investigating different histories, and investigating three-dimensional effects, the latter of which is realistic for service conditions.

Brown University

Dept of Chemical Engineering **$98,919**
Providence, RI 720 **01-A**
95-3

Simulation and Analysis of Dyanmic Failure of Ductile Materials
L.B. Freund

A central goal in the mechanics of materials is the calculation of parameters which characterize macroscopic failure of materials in terms measurable features of the microstructure of those materials. The motivation for doing so is to establish which material and/or geometric characteristics account for macroscopic failure, with a view toward improvement of failure resistance through material selection or microstructural design. Such calculations normally require construction of simple, conceptual models and numerical simulation of more complex, realistic models. In the present project, this is viewed as a modeling issue; existing computational procedures will be applied as tools to extract quantitative interpretations for the models developed. The emphasis will be on the behavior of structural metallic alloys with moderate to high ductility. Thus, the dominant mechanism of plastic deformation is crystallographic slip and material strength degrades through nucleation, growth and coalescence of micro-voids. Plastic strains in such processes can be large so that strain localization issues become important in the analysis of models. Finally, the models will allow for a complete loss of stress carrying capacity of the material associated with the creation of new surface, without the introduction of an additional failure criterion, so that fracture can arise as a natural consequence of the deformation process.

University Of California/B

Dept of Chemical Engineering **$78,440**
Berkeley, CA 94720 **06-A**
94-4

Enzyme Adsorption and Activity at Liquid-Liquid Interfaces
H. Blanch

Protein adsorption at oil/water interfaces is the primary phenomenon governing formation of stabilized emulsions. The homogeneity of the liquid/liquid interface provides an ideal environment to examine the fundamental forces involved in protein adsorption and film formation. The approach taken in this study involves two experimental techniques: pendant drop tensiometry and total internal reflection fluorescence spectroscopy (TIRFS). The combination of these two techniques allows investigation of protein adsorption dynamics as well as providing insight into the structure of adsorbed proteins. Pendant drop tensiometry is used to follow dynamic interfacial tension of several well-characterized proteins under conditions of varying protein bulk concentration, pH, ionic strength, and oil phase characteristics. Surface tension measurements have been employed to monitor protein adsorption, as well as measure the relevant time scales for adsorption. An analysis of unique systems such as disulfide-reduced proteins and short chain poly-amino acids is being undertaken to reveal the magnitude of non-native bond formation and primary structure on adsorption and gelation behavior. We have constructed a liquid/liquid TIRF spectrometer. This apparatus enables quantitation of protein adsorption, and permits changes in the protein secondary structure to be observed based on the intrinsic fluorescence of tryptophan residues. Initial studies using TIRFS have shown shifts in the fluorescence emission spectra of fluorescein conjugated to lysozyme upon adsorption to a heptane/aqueous phosphate buffer solution, indicating the extent of conformational change of the adsorbed protein.

University Of California/B

Dept of Electrical Engineering & Computer Sciences **$90,000**
Berkeley, CA 94720 **06-C**
93-3

Dynamics of Electronegative Plasmas for Materials Processing
A. Lichtenberg, M. Lieberman

The purpose of this project is to study the equilibrium particle and energy balance and the heating mechanisms in electronegative r.f. discharges. Particular attention is given to the formation of non-Maxwellian electron distributions and their effect on the macroscopic parameters. The research includes theoretical, particle-in-cell simulation, and experimental investigations. The sheath heating theory and the simulation results developed for electropositive plasmas are used to guide the investigations. The investigation includes, but is not limited to, the study of oxygen feedstock gas in capacitively coupled, parallel plate, r.f. discharges.

A macroscopic analytic model for a three-component electronegative plasma has been developed. Assuming the negative ions to be in Boltzmann equilibrium, a positive ion ambipolar diffusion equation is found. The electron density is nearly uniform, allowing a parabolic approximation to the plasma profile to be employed. The resulting equilibrium equations are solved analytically and matched to an electropositive edge plasma. The solutions are compared to a simulation of a parallel-plane r.f. driven oxygen plasma and found to give good agreement, provided the two-temperature electron distribution found in the simulation is also used in the model. The results indicate the need for determining a two-temperature electron distribution self-consistently within the model.

University Of California/B

Dept of Mechanical Engineering **$96,460**
Berkeley, CA 94720 **01-B**
95-3

Ultrashort Laser Heating and Phase Change in Liquids
C.-L. Tien

The general objective of this research program is to achieve a better understanding of the fundamental mechanisms of thermal radiation and heat conduction in microscale structures commonly encountered in engineering applications.

When the pulse duration of short-pulse, high power lasers approaches the characteristic molecular time scales of the material with which the laser interacts, traditional models of radiation absorption and energy transport must be re-examined. A complete understanding of heat generation and dissipation during this process is required for precise, efficient laser processing. The research of the past year has resulted in microscopically based models of radiation absorption and thermal transport in liquids, semiconductors, and disordered media. These models have been applied to create novel solutions to important engineering problems.

The model for liquids was developed to include consideration of the short time-scale phenomena of saturable absorption and multiphoton absorption in energy transport calculations. The multiphoton effect was proposed as a novel mechanism for imparting large amounts of energy into normally transparent liquids. Experiments were performed to confirm model predictions. Fractal theory was applied to examine short-time-scale energy transport in random media. On short time scales anomalous diffusion was predicted due to the disorder. Finally, using predictions from models of femtosecond (10-15 s) laser interactions with semiconductors, a new method of releasing failed microstructures through electronically-induced desorption of water was developed and demonstrated.

University Of California/LA

Mech, Aero & Nuclear Eng Dept **$ 0**
School of Eng & Applied Science **01-C**
Los Angeles, CA 90024-1597 **92-3**

Basic Studies of Transport Processes in Porous Media

I. Catton

The objective of this project is to develop an understanding of the governing physical processes at a level appropriate for development of macroscopic models for use in the analysis of engineered energy systems. Current work considers both single-and two-phase flows. Efforts are both theoretical (numerical in some cases) and experimental. Emphasis is placed upon the development of mathematical models for single- and two-phase turbulent transport in highly porous media with regular, non-uniform, isotropic and non-isotropic characteristics. The basis of the the work is a hierarchial heterogeneous medium averaging methodology using fully turbulent models with Reynolds stresses and fluxes in every pore space building from the lowest level. Boundary and interphase conditions are incorporated at various scales leading to descriptions of momentum, heat and mass transport in porous media. Equations for developed flow and diffusive processes in a random, highly porous medium have been developed along with the statistical and numerical methodology needed to treat the fluctuation terms for various assigned random porous morphologies. Models have been developed to describe turbulent flow, diffusion of admixtures, and energy processes in highly porous media. Using second order turbulent models, equation sets have been obtained for laminar and turbulent filtration and two-temperature or two-concentration diffusion in non-isotropic porous media and interphase exchange and micro-roughness. The equations differ from those found in the literature. The models are being used to optimize some heat transfer devices by selecting the surface characteristics that yield high heat transfer and low pressure drop. Flow across or through bundles of roughened tubes is presently being modeled.

University Of California/LA

Mech, Aero & Nuclear Eng Dept **$110,559**
School of Eng & Applied Science **06-C**
Los Angeles, CA 90024 **93-3**

Linear Kinetic Theory and Particle Transport in Stochastic Mixtures

G. Pomraning

The goal in this research is to develop a comprehensive theory of linear transport/kinetic theory in a stochastic mixture of solids and immiscible fluids. Such a theory should predict the ensemble average and higher moments, such as the variance, of the particle or energy density described by the underlying transport/kinetic equation. The statistics to be studied correspond to N-state discrete random variables for the interaction coefficients and sources, with N denoting the number of components in the mixture. The mixing statistics to be considered are Markovian as well as more general statistics.

In the absence of time dependence and scattering, the theory is well developed and described by the master (Liouville) equation for Markovian mixing, and by renewal equations for non-Markovian mixing. The intent of further work is to generalize these treatments to include both time dependence and scattering. A further goal of this research is to develop approximate, but simpler, models from the comprehensive theory. In particular, a specific goal is to formulate a renormalized transport/ kinetic theory of the usual nonstochastic form, but with effective interaction coefficients and sources to account for the stochastic nature of the problem. Numerical comparisons of all models will be made against Monte Carlo simulations which involve a straightforward average of solutions for a large number of physical realizations of the statistical mixing. Contact will also be made with experimental simulations of cloud-radiation interactions currently underway at another institution as part of DOE's global climate modeling initiative.

University Of California/LA

Physics Dept **$77,396**
Los Angeles, CA 90024 **06-C**
93-3

Nonlinear Waves in Continuous Media
S. Putterman

Nonlinear wave interactions in far off-equilibrium fluids are being studied with the goal of understanding the interplay between processes that concentrate energy (e.g. sonoluminescence), randomize energy (e.g. wave turbulence) and form localized states (e.g. solitons). The experimental discovery that strong sound waves generate picosecond flashes of light is now being studied from the theoretical perspective with the goal of understanding how energy can focus by twelve orders of magnitude. Turbulence in nonlinear waves is being studied from both the theoretical and experimental directions. Goals include the development of a Fokker-Planck theory that includes intermittency as well as the observation of collective modes in turbulence that are analogous to second sound. High amplitude waves can also form self-localized states such as the breather and kink solitons, and domain walls which have recently been observed. Current efforts are aimed at extending these findings to systems which are two- and three-dimensional. This work proceeds from the experimental, analytical and simulational avenues of approach.

University of California/SD

Scripps Inst of Oceanography **$ 0**
La Jolla, CA 92093-0402 **06-C**
94-4

Broadband Signals: Signal Processing in Chaos
H. Abarbanel

The analysis of chaotic signals observed in measurements on physical systems is of importance in energy problems ranging from fluidized bed flows in fossil energy applications to determination of the natural climate variability to the uncovering of simple models for complex behavior in fluid flows. This research has developed tools for this analysis which allows one to reconstruct the multivariate state space of a system from observations, time lagged, of a single dynamical variable. The time delay, the dimension, and properties of the strange attractor can all be determined from these data. The concept of unfolding the attractor using the method of global false nearest neighbors and then determining locally the number of dynamical degrees of freedom using the local version of this has brought to the study of complex behavior a robustness which allows it to be used in engineering analysis and design. The algorithms developed for this purpose have also been used in a variety of applications requiring the separation of a chaotic signal from another information bearing signal or 'noise'. The tool kit of these algorithms is being ported to a common interface for use in the energy related sciences.

University Of California/SD

Dept of App Mech & Eng Sci **$127,070**
La Jolla, CA 92093 **06-B**
93-3

Fundamental Studies of Spray Combustion
P. Libby, F. Williams

This research involves a combined experimental and theoretical effort related to the behavior of fuel droplets in well defined but nonuniform flows. A test rig which permits a wide variety of investigations including nonpremixed, premixed and partially premixed systems in both laminar and turbulent streams represents the main experimental setup. A phase doppler particle analyzer which permits measurement of two velocity components, droplet diameter and number density is the principal instrumentation employed in our studies. It is supplemented by a gas chromatograph for measuring species concentrations. We have nearly completed and are writing up for publication our theoretical and experimental research on droplet oscillation in opposed streams, behavior which accounts for the observed bimodality of the probability density distributions of the axial velocity. Experiments on a turbulent spray impinging on a wall and complementary theoretical analysis lead to estimates of the largest droplets which follow the gas including fluctuations and the smallest droplets which ignore velocity fluctuations. When these experiments are repeated for a wall of suitably high temperature, a trimodal distribution of axial velocity is observed; the implication is that droplets of appropriate size impinge on the wall, bounce back and return a second time. At lower wall temperatures entirely different behavior is observed, namely droplet breakup. Our recent work concerns water sprays in a two stage homogeneous flame in order to investigate the removal of the CH-radical by water. Preliminary results on this study were presented at the 31st AIAA Propulsion Conference. Additional experiments on this flow are underway.

University Of California/SD

Dept of Chemistry, 0340 **$ 0**
La Jolla, CA 92093 **06-C**
92-4

Noisy Nonlinear Systems
K. Lindenberg

The broad objective of this project is to investigate the interplay of nonlinear deterministic dynamics with spatial and temporal fluctuations.

Density fluctuations in binary reaction--diffusion processes in low dimensional systems lead to spatial and temporal anomalies. We have extended our mesoscopic approach to obtain the reaction-diffusion equations that are customarily postulated phenomenologically to a broader variety of systems. This approach places a number of theories on a common fundamental basis.

We have begun an investigation into the characteristic manifestations of soft anharmonicity in nonlinear coupled arrays both in and out of thermal equilibrium. In particular, we are interested in various ways in which vibrational energy may become spontaneously localized as a consequence of anharmonicity even in translationally invariant arrays. These include the overpopulation of anharmonic vibrations in thermal equilibrium, the inhibition of dispersion, and the enhancement of spatial coherence.

We have continued our work on a microscopic quantum mechanical model for charge transfer in condensed media. We are able to calculate the reorganization energy and rate prefactor as a function of elementary parameters for some simple model situations.

University Of California/SD

Inst for Nonlinear Science, R-002 **$101,185**
La Jolla, CA 92093 **06-C**
93-3

Structure of Turbulence, Conditional Averaging and Subgrid-Scale Modeling
E. Novikov

Well developed turbulent flows are encountered in many energy engineering enterprises, as well as in environmental, aerospace and naval engineering. The number of degrees of freedom for such flows is enormous and direct numerical simulations (DNS) are impossible now and in the foreseeable future.

One of the major goals of this project is to advance the knowledge of the structure of turbulence, aiming it at a subgrid-scale modeling for the large-eddy simulations (LES).

The developed approach for achievement of this goal includes: conditional averaging of the Navier-Stokes equations (NSE); use of Markov processes with dependent increments (consistent with NSE); breakdown coefficients and associated infinitely divisible probability distributions.

Among the obtained results are: probability distribution for three-dimensional (3D) vectors of velocity increments, which has an unusual form and experimentally observed exponential asymptotics; new scaling for experimentally and numerically observed 3D "vortex strings", 2D coherent vortices and coherent structures of scalar fields; exponential behavior of conditionally averaged vortex stretching as a function of fixed vorticity, which is obtained by DNS on a CM-5 parallel computer, using 6th-order finite differences on $(256)^3$ grid; the whole 3D conditionally averaged vorticity field, obtained by DNS; statistical characteristics of microcirculations; probability distributions and moments of the breakdown coefficients (intermittency), compared with experimental data for the Taylor-scale Reynolds number 3200; a hierarchy of subgbrid-scale models, preliminary tested by DNS and by LES for isotropic, shear-flow and free-surface turbulence.

University Of California/SD

Dept of Physics **$115,000**
La Jolla, CA 92093 **06-C**
93-3

Traveling-Wave Convection in Fluid Mixtures
C. Surko

This research program involves the study of convection in fluid mixtures of ethanol and water, in which the fluid motion takes the form of traveling waves. It is a model system for studying nonequilibrium traveling-wave phenomena that can provide important insights into the behavior of double diffusive systems in which the transport occurs on two different time scales. In this system, the coupling of the concentration field to the velocity and temperature fields results in a wide variety of potentially important phenomena. As a fluid dynamical system, it is closely related to atmospheric and oceanographic flows, and as a model for traveling-wave dynamics, it can provide insights which are useful in the understanding of other traveling-wave systems such as large-aspect-ratio lasers.

Earlier experiments in an annular geometry, which is essentially a one-dimensional system with periodic boundary conditions, led to a basic understanding of the dynamics of uniform and confined states of traveling waves. Current experiments involve a large aspect-ratio two-dimensional convection cell which allows study of the role of defects and grain boundaries in the development of traveling wave patterns. States of intense spatio-temporal disorder can be created which consist of many small domains of plane waves. As the pattern evolves in time, the domains grow until the average domain size is of the same order as that of the convection cell. Thus, the initially homogeneous "turbulence" gives way to a pattern consisting of a few large traveling-wave domains separated by stable domain walls. One basic question to be addressed is whether the model equations commonly used to describe this system can reproduce the transition from the disordered initial state to the ordered multi-domain state. Numerical algorithms have now been developed for characterizing these multi-domain states, and they allow direct comparisons between the experimental patterns and analytical models. These analysis tools are also likely to prove useful in studying traveling-wave patterns in other physical contexts.

University Of California/SD

Institute of Nonlinear Science **$99,990**
La Jolla, CA 92093-0402 **06-C**
95-3

Modeling of Process Control
L. Tsimring

Traditionally, for ease of operation and analysis, technological systems (manufacturing systems, communication systems, etc.) have been *designed* to behave in as linear a manner as possible. Increasingly tight specifications, environmental considerations and economic pressures are pushing the operational windows into regions where assumptions of linearity tend to break down. Despite a flurry of activity in the area of nonlinear dynamical systems (both analysis and control system design) we see very few applications of these new results. One important reason is the lack of suitable nonlinear dynamic models. The objective of this project is the development of tools for building nonlinear models based on input/output data from systems which may exhibit chaotic or nonchaotic dynamics, to implement the algorithms in efficient software packages and to apply them to a wide range of examples, primarily from communications and process control. These examples are not just academic test cases which provide feedback on the direction of the theoretical developments, but constitute by themselves important technological problems. The varied background of the investigators, the interdisciplinary approach, and the emphasis on tools, software *and* applications hold high promise for a broad impact of the proposed research. This is a joint projects with M. Morari at the California Institute of Technology.

University Of California/SB

Dept of Physics **$135,000**
Santa Barbara, CA 93106 **06-C**
93-5

Bifurcations and Patterns in Nonlinear Dissipative Systems
G. Ahlers, D. Cannell

This project consists of experimental investigations of heat transport, pattern formation, and bifurcation phenomena in non-linear non-equilibrium fluid-mechanical systems. These issues are studies in Rayleigh-Benard convection, using both pure and multicomponent fluids. They are of fundamental scientific interest, but also play an important role in engineering, materials science, ecology meteorology, geophysics, and astrophysics. For instance, various forms of convection are important in such diverse phenomena as crystal growth from a melt with or without impurities, energy production in solar ponds, flow in the earth's mantle, geo-thermal stratifications, and various oceanographic and atmospheric phenomena. Our work utilizes computer-enhanced shadowgraph imaging of flow patterns and high-resolution heat transport measurements.

We studied convection in a gas (CO_2) under pressure (about 30 bar) in a very large aspect ratio sample (radius/height = 150). Under non-Boussinesq conditions, the bifurcation from conduction to convection became hysteretic, and the initial pattern consisted of a perfect lattice containing more than 10^4 hexagonal cells. For parameter values where time-independent parallel straight rolls were theoretically predicted for a laterally infinite system, we found a state of spiral-defect chaos.

We investigated convection in a nematic liquid crystal in a horizontal magnetic field H. We found excellent agreement with recent theoretical predictions for the bifurcation line $R_c(H)$, and for the convection-roll orientations as a function of H. We also used this system to study convection when two phases (the nematic and isotropic phase) are present in the cell. Convection in the presence of a first-order phase change is relevant to convection in the earth's mantle; ours are the first quantitative experiments relevant to this important problem.

We have continued our work on binary-mixture convection. For positive separation ratios Ψ we studied square patterns. For negative Ψ, we investigated time formation of localized pulses in two dimensions.

University Of California/SB

Dept of Chemical & Nuc Eng **$107,400**
Santa Barbara, CA 93106 **01-C**
95-3

Wave Turbulence Interactions
S. Banerjee

The work is part of an ongoing research effort aimed at understanding transport processes across a gas-liquid interface. The research includes both experimental and computational components (using direct numerical simulation). In this work, the effects of waves on turbulence in a liquid stream is investigated. The study includes two-and three-dimensional waves, with and without imposed wind shear. Wind flow can be either co- or counter-current to the liquid. The study is experimental, using a 3-D LDA synchronized with acoustic surface position measurements (both non intrusive). These are also synchronized with high-speed video flow visualization using microbubble tracers. Wire gauges are also used for detecting wave length. The waves are generated mechanically.

Results indicate that the turbulence intensity away from the wall channel bottom-wall was substantially increased as a result of the waves. The increase appears to be a consequence of turbulence production in the outer flow region since the turbulence intensity in the wall region was not altered, and it seems that the turbulence wall structures were not affected as well. This, in spite of the fact that the wave-induced orbital motion reached all the way to the wall. Even in predominantly laminar flows, the introduction of 2-D waves causes three-dimensional turbulence in the near-free surface region. Turbulence enhancement in this region is in general found to be proportional to the wave strength. The next phase of the work will focus on the combined effect of wind and waves on the turbulence structure.

California Inst Of Technology

Chemical Engineering 210-41 **$125,000**
Pasadena, CA 91125 **03-A**
91-3

Modeling for Process Control
M. Morari

While many advanced analysis and synthesis techniques have been recently developed for the control of nonlinear systems, few of these results have been utilized in process applications. One key reason may be the lack of suitable models for these systems. The objective of this research program is the development of tools for building nonlinear models based on input/output system data and the implementation of these tools in an efficient software package. The toolkit is specifically intended to assist in problems of nonlinear estimation and control, and monitoring and diagnostics, tasks which can be interpreted as "model validation".

Currently, the modeling methods being examined are similar to those which have shown great success in the identification of self-driven systems. For example, the method of False Nearest Neighbors (FNN) was first developed to determine the dimensionality of autonomous chaotic systems. The FNN method has been extended in order to determine the dimensionality of systems from properties of input/output data. Methods are also being developed for determining the proper sampling time of a nonlinear input/output system. Determining a proper sampling time and model order are necessary first steps for building accurate low order models. This effort is coordinated with L. Tsimring at U.C.-San Diego.

California Institute Of Technology

Graduate Aeronautical Laboratories **$99,664**
Pasadena, CA 91125 **03-A**
95-3

Dynamic Failure Characterization of Ductile Steels
A. Rosakis

To aid in the design and vulnerability analysis of energy systems (e.g., pressure vessels, pipelines, reactors), it is necessary to monitor and quantify the mechanical behavior and failure modes of materials used in such systems under carefully controlled conditions. Because of design constraints and safety issues, energy systems are typically built with corrosion resistant and highly ductile metallic alloys such as stainless steels. However, due to aging of such structures in the energy industry, it is essential to understand the effect of embrittlement, ductile-brittle transition and its influence on the resistance to catastrophic failure, i.e., crack initiation and unstable growth. Relatively little is known regarding dynamic crack initiation and growth in ductile metals. A major challenge which has remained unresolved in this area is the measurement of J-integral under a combination of large scale yielding conditions and dynamic loading. However, recent advances in high-speed diagnostic techniques and computational capabilities has made it possible to investigate and develop a fundamental understanding of dynamic failure in ductile materials such as stainless steels. Failure in such ductile metals is inherently three dimensional (e.g., shear lips, tunneling) and it is necessary to develop adequate modeling tools to understand such phenomena and develop models predicting such behavior.

Carnegie Mellon University

Chemical Eng Dept **$151,854**
Pittsburgh, PA 15213 **03-A**
94-4

Systematic Process Synthesis and Design Methods for Cost Effective Waste Minimization
L. Biegler, I. Grossmann, A. Westerberg

This project is developing a novel integrated approach for process synthesis and design to address recent environmental challenges. The approach provides rigorous trade-offs among raw material and energy costs, capital investment and waste treatment. Issues of waste minimization addressed include:

1. Economic design of reactor networks that minimize conversion of raw materials to waste byproducts.

2. Synthesis of separation sequences to isolate, redirect and recycle byproducts.

3. Integrated synthesis and design of reaction, separation and energy systems with environmental and operability concerns, also dealing with process uncertainty.

Superior reactor designs can have the greatest impact for process improvement, both from an environmental and an economic perspective. A quantitative targeting approach for reactor networks is permitting the reduction of waste byproducts at the source. The second task concentrates on the synthesis of flexible separation processes (displaying azeotropic and liquid/liquid behavior) -- with efforts to overcome the combinatorial explosion of alternatives, each of which requires a very large and difficult optimization be solved. The third task combines structural optimization and problem decomposition at various modeling levels in order to screen alternatives based on economic, environmental and operabilty trade-offs, before complex simulation models are applied. This approach also includes the development of flexible designs that are tolerant to uncertainties related to process conditions and waste treatment requirements.

Carnegie Mellon University

Dept of Elec & Comp Eng **$0**
Pittsburgh, PA 15213 **03-C**
92-3

Research on a Reconfigurable and Reliable Manipulators
P. Khosla, T. Kanade

The goal of our research is to develop basic design theory and methodology that will allow one to determine both the kinematic and dynamic configuration of a manipulator capable of performing a given task. The motivation for this arises from the concept of a modular manipulator system comprising a set of link and joint modules of various sizes which may be assembled together in a desired kinematic configuration to achieve a specific task. The joint and link modules have consistent mechanical and electrical interfaces which will allow either semi-skilled field personnel or another manipulator to rapidly configure a manipulator to meet specific task requirements. Since current manipulator systems are of fixed configuration, they lack the ability to perform widely varying tasks. Further, these manipulators are not fault tolerant - a loss of a degree-of-freedom will result in a significantly reduced capability to perform the task it was deployed for. In pursuing research on a reconfigurable modular manipulator system, our goal is to not only to create the technology but to push basic research for design of non redundant, redundant, and fault tolerant manipulators.

This basic research effort will address the problem of mapping tasks into a manipulator configuration, formulation of control algorithms for the mapped configuration, and experimental verification of the developed ideas. Though it is not the primary objective, we believe that building prototype experimental modules for demonstrating our ideas will also contribute to the technology of modular manipulators. For configuring a manipulator from task requirements, we have developed methodologies that map the task requirements into a specific non-redundant manipulator. The kinematic task requirements are used to determine the link lengths and the orientation of the modules. The dynamic task requirements are translated to obtain the sizes and rating of the actuators or joints.

University Of Chicago

The Enrico Fermi Institute **$165,000**
Chicago, IL 60637 **06-C**
93-3

Fundamentals and Techniques of Nonimaging Optics
R. Winston

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. Our theoretical work on nonimaging designs has led to our group experimentally demonstrating ultra-high flux from sunlight which exceeds previous results by substantial factors. In 1991 we presented the proposal that nonimaging designs be regarded as functionals of the desired irradiance, rather than depending on a static parameter such as the "acceptance angle". The working out of this "tailored edge ray " algorithm has led to many applications in illumination and flux concentration. Current algorithms under study employ methods from non-local optimization as well as application of Lorentz geometry to flow-line designs.

Clarkson University

Dept of Chemical Engineering **$63,125**
Potsdam, NY 13676 **01-C**
94-3

Gas and Solids Holdup in Three Phase Bioreactors
J. McLaughlin

The goal of this research is develop mathematical modeling and tools that can lead to a better understanding of three phase Bioreactors. Fluidized beds that use gel beads containing bacteria are of particular interest. The bead Reynolds numbers are order unity. Thus, models developed for particle Reynolds numbers that are large compared to unity do not correctly predict the hydrodynamics of the Bioreactors.

A goal of the project is to understand the interaction between gas bubbles and gel beads. A fluidized bed has been constructed and used to measure the rise velocity of air bubbles.

Translucent (bacteria free) gel beads make it possible to study bubble trajectories at solids volume fractions up to 50%. An effective viscosity model based on the Thomas correlation appears to be useful for the bubble size range of interest.

A computer simulation program is being used to simulate axisymmetric flow around an isolated bubble. It incorporates the effects of surfactants on the bubble motion. The simulations agree with published studies of bubble motion in both pure and impure water. The simulation program will be used to simulate bubble motion in the fluidized bed using the effective viscosity model to describe the effect of the beads.

Cornell University

Mechanical & Aerospace Eng **$79,012**
Ithaca, NY 14853 **01-A**
94-3

Nonlinear Dynamics of Fluid-Structure Systems
F. Moon

Two principal experiments were carried out under this grant during the second year of this project:

i) Forced vibration of a single flexible tube with internal flow and ii) Cross flow measurements of chaotic vibrations of a flexible tube in a five tube row.

i) In the first set of experiments, begun in the first year, we explored multifractal phenomena, which describe the transition from quasiperiodic to chaotic vibrations. Quasiperiodic vibrations were observed in earlier experiments by Dr. G. Scott Copeland in flow through a long tube with an end mass. These results were reported an a Ph.D. dissertation in Summer 1990. By introducing a periodic-forcing of the tube in an adaptation of this experiment, we were able to more easily study this transition from quasiperiodic to chaotic vibration. This study was motivated by work in the mid 1980's on forced Rayleigh-Bernard flow which showed a linkage between quasiperiodic motion and the circle map.

In the forced tube experiment we were able to show a similar connection to the circle map, and in particular, the multifractal nature of the breakup of the torus in c phase space. A multifractal is a distribution function which is described by a set of points with a continuous set of fractal dimensions. Our observations of multifractal behavior were, we believe, the first to be observed in fluid-structure vibrations.

In January 1992, Mr. George Muntean visited Argonne National Laboratory and reported to Dr. S.S. Chen our findings on muiltifractal measurements. He subsequently presented a paper at the DOE Grantees meeting this past spring. A revised paper has been submitted to the Journal of Fluids and Structures, and is currently under review.

ii) The design of the cross-flow, tube row experiment began last summer and was completed this fall. These experiments parallel the work of Cai and Chen (1992). In the Cornell experiments the center tube of a five-tube set suspended on a flexible rod. The tube motion is limited by motion stops, thus introducing a strong nonlinearity in the tube stiffness. Preliminary experiments were carried out in water. The vibration amplitude versus flow velocity shows the instability onset (Hopf bifurcation) and the vibration saturation when the impact constraints limit the chaotic motion. This response was found to depend on whether the flow velocity was increasing or decreasing.

The vibration frequency was found to depend on the flow velocity. There is some evidence that the periodic motion at the onset of flutter to chaotic motion transition occurs through quasiperiodic vibration.

At the present time we are carrying out the calculations of the fractal nature of the Chaotic motion with the goal of establishing the low dimensional nature of the dynamics. At the same time we will correlate our findings with a similar experiment at Argonne National Laboratory to establish the validity of the fractal dimension technique in determining chaos in such flows. The next stage of this work will involve experiments in cross flow of air past a row of tubes as described in the next section on our proposed research for the third year of this project.

In 1993 a new wind tunnel facility has been constructed and we are investigating nonlinear dynamics of a tube row in cross flow.

Cornell University

Sibley School of Mech & Aero Eng $107,061
Ithaca, NY 14853 01-C
94-3

Experimental Studies of Reynods Number Dependence of Turbulent Mixing and Transport
Z. Warhaft

Our experimental studies of the structure of turbulence and its mixing properties are motivated by a desire to better understand the fluid mechanics of chemical reactions, combustion and environmental pollution.

Turbulence in machinery (such as jet engines and combustion chambers), and in the environment (the atmosphere and oceans), occurs at high Reynolds numbers, R_λ. Basic phenomenological models of turbulence are constructed under the assumption that R_λ is high. Yet one of the greatest difficulties, both experimentally and computationally, has been in generating an isotropic turbulent field of high R_λ. Thus fundamental theory has not been tested under controlled laboratory conditions (although there is broad confirmation from (uncontrolled) environmental measurements). Using a novel active grid approach devised by Makita of Toyohashi University, we have achieved an R_λ of 450, nearly an order of magnitude higher than is typically achieved in conventional isotropic (grid) turbulence experiments. We are in the process of elucidating how the turbulence spectrum evolves and the validity of the traditional statistical models of turbulence. We are also studying the mixing properties of the turbulence, using temperature as a passive scalar. Our preliminary results show a clear evolution in the turbulence spectrum as R_λ is increased with the scaling region first occurring with a slope of approximately -1.3 (at $R_\lambda \sim 100$) and then increasing to -1.6 by $R_\lambda \sim 200$. The slope does not appear to reach the Kolmogorov value of -5/3 even for our highest R_λ (of 450).

Dartmouth College

Thayer School of Engineering $114,726
Hanover, NH 03755 01-C
95-3

Two-Phase Potential Flow
G. Wallis

The objective is to develop a mature science of two-phase potential flow, based on fundamental hydrodynamic theory and tested by experiment.

A theory has been developed for the force on any object, in an inviscid flow with weak vorticity, in terms of the added mass tensor for the object. Measurements of the force on a set of streamlined objects in a shear flow agree with the form of the theory but with coefficients that are 20 to 30% lower than the corresponding added mass coefficients.

A "particle-pressure coefficient" has been derived for rectangular arrays of spheres moving relative to an inviscid irrotational fluid. The coefficient is positive for all aspect ratios in contrast to negative coefficients predicted by Geurst's equations.

Methods have been developed for predicting the dipole moment (polarization) of spheres with any motion in a potential flow. This leads to approximate constitutive equations for the two-phase suspension.

Duke University

Dept of Physics $124,528
Durham, NC 27706 01-C
93-3

Experimental and Analytical Investigations of Flows in Porous Media
R. Behringer, G. Johnson, J. Georgiadis

Research Objectives: The objectives of this project include the characterization, both theoretical and experimental of fluid flows through porous media. The particular focus is on fluid convective flow in porous media. Convection in porous media occurs, for instance, when a layer of fluid-saturated porous media is heated from below.

The characterization of porous convections includes both pure fluids and mixtures of different fluids. Long term benefits will be an improvement in the theortical and practical applications of flow in porous media in the presence of temperature gradients. Relevant practical situations include petroleum and hydrology problems where heating occurs.

Scientific Approach: The primary approach is experimental, and involves the use of Magnetic Resonance Imaging (MRI) as a powerful new tool to see the flow inside of porous media. The project involves the use of a MRI apparatus and a precision thermal apparatus for carrying out the convection experiments. Additional theoretical work now includes an analysis of the convective model equations with the goal of understanding recent experimental results. These results show a strong coupling between the solid structure of porous media and the flow states.

Current Status of Project: Recent work has been described in Shattuck et al. Phys. Rev. 75, 1934 (1995). These experiments show the strong coupling between pore space structure and flow patterns. An additional longer paper is in progress. This work forms the basis of Mark Shattuck's thesis. Continuing work will focus on experimental MRI studies of binary mixture convection in porous media.

Florida State University

Supercomputer Computations Research Institute **$100,000**
Tallahassee, FL **95-5**

Theoretical and Computational Studies of Pattern Formation
J. Vinals

No summary information

Georgia Institute of Technology

Computational Mechanics Center **$61,325**
Atlanta, GA 30332 **01-A**
94-3

An Analytical-Numerical Alternating Method for 3-D Inelastic Fracture and Integrity Analysis of Pressure-Vessels and Piping at Elevated Temperatures
S. Atluri

Current and future power generation plants require efficient operation so that energy savings may be realized. In addition, power generation equipment in the US continues to age, creating operational dangers for the working staff as well as greater potential for power outages. Current methods to ensure safe operation of these plant components which operate in the nonlinear material regime are simplistic, and hence, not very reliable. This program is developing advanced analytical tools which can be used to reliably assure safety of future plants as well as aging plants.

The finite element alternating method is the state-of-the-art methodology for determining stress intensity factors for two and three dimensional crack growth problems. This method has permitted accurate and simple analyses of linear fracture problems to be made so that sophisticated reliability assessments of operating equipment may be made. This program has extended the finite element alternating method so that it may now be used in the nonlinear regime, i.e., the non-linear finite element alternating method. With this new methodology, sophisticated damage and fracture assessments can be made for components which experience failures in the elastic-plastic and high temperature creep regime. This is truly a revolutionary advance to the fracture assessment field.

Currently, sophisticated fracture assessments are being made using advanced fracture theories such as the T*-integral which were previously unattainable. The methods are being verified by comparison of predictions to experimental results. It is anticipated that these advances will permit the designer to make sophisticated fracture assessments in the future with a minimum of effort.

Idaho National Engineering Lab

Applied Physics & Optics Unit **$436,000**
Idaho Falls, ID 83415 **06-A**
93-3

Fundamentals of Thermal Plasma Processing
J. Fincke

The objective of this project is to improve the thermal plasma spray process and the understanding of high-velocity, high-temperature, nonequilibrium plasma processes. High plasma velocities lead to large departures from chemical equilibrium as well as high particle velocities. Higher particle velocities decrease particle residence time, minimize oxidation reactions and produce denser coatings. Ion and dissociated species populations are typically larger than expected at the local kinetic temperature. Since surface recombination increases plasma/particle heat transfer rates producing fully molten particles with less residence time. The desired result is to deliver to the substrate a particle ensemble at higher velocities with less variance in temperature, velocity, molten fraction, and chemical composition. Ultimately this will allow improvements in coating adhesion and strength while other characteristics, such a porosity, can be specified and controlled. This leads to the possibility of engineering new coatings with graded composition, porosity, etc.

Diagnostic techniques include coherent Thomson scattering, Coherent-Anti-Stokes-Raman Spectroscopy (CARS), Laser Induced Fluorescence (LIF), two-photon LIF, degenerate-four-wave-mixing, plasma velocity by direct measurement of Doppler shifted laser scattered light, particle size, velocity, and temperature, and an enthalpy-probe, mass spectrometer combination.

Idaho National Engineering Lab

Materials Science Division **$224,000**
Idaho Falls, ID 83415 **03-A**
93-3

Application of Intelligent Control Systems to Mixed-Culture Bioprocesses
J. Johnson, D. Stoner

The aim of this project is to show that the productivity of mixed-culture bioprocesses can be increased by applying intelligent systems to the process control problem. Controllers are being implemented by combining the tools of intelligent control including fuzzy logic, expert systems, and neural networks. The ability of a mixed microbial culture to adapt to changing conditions will be matched by the ability of the control system to learn about process performance continuously. Sensors will be developed to inform the control system about the activity of the dominant strains of microorganisms in the mixed culture. This will be combined with expert knowledge on the metabolism and biochemistry of these strains incorporated as fuzzy logic rules in the controller.

These control concepts are being demonstrated in the laboratory using the oxidation of ferrous iron by Thiobacillus ferrooxidans as a model system. A controller is being developed first for a pure culture of this organism in a chemostat, the control objective being to maximize the oxidation rate without the appearance of ferric iron precipitates. Currently the controller adjusts the temperature, pH, and dilution rate adaptively, to find the best set points. Later the culture complexity will be progressively increased by adding an acidophilic heterotrophic bacterium that consumes organic matter known to inhibit Thiobacillus, and a protozoa that feeds on the bacteria. Appropriate control rules will be developed and implemented at each step.

Idaho National Engineering Lab

Energy Res & Applications Dept **$210,000**
Idaho Falls, ID 83415 **06-A**
93-3

Modeling of Thermal Plasma Processes
J. Ramshaw, C. Chang

Optimization of thermal plasma processing techniques requires a better understanding of the space- and time-resolved fluid flow and temperature distribution in the plasma, and of interactions between the plasma and injected or condensed particles. The present research is directed toward the development of a comprehensive computational model capable of providing such information. The plasma is represented as a two-temperature multicomponent ideal gas governed by the Navier-Stokes equations. In contrast to much of the earlier work, local thermodynamic equilibrium is not assumed. Multicomponent diffusion is represented by a self-consistent effective binary diffusion approximation, suitably generalized to include ambipolar diffusion of charged species. The further generalization to diffusion in external electromagnetic fields is in progress. Dissociation, ionization, and other chemical reactions are fully coupled to the plasma flow and are treated by a new general implicit chemistry algorithm. Extensions of this algorithm to two-temperature plasmas and heterogeneous reactions (such as particle condensation) are in progress. Discrete particles interacting with the plasma are represented by a stochastic particle model which allows for statistical distributions of particle properties. Applications to date include simulations of plasma spraying in both conventional and modern high-speed torches, as well as studies of chemical, thermal, and excitation nonequilibrium in thermal plasmas. Future applications to plasma synthesis are also planned.

Idaho National Engineering Lab

Materials Technology Group **$687,000**
Idaho Falls, ID 83415-2218 **01-A**
93-3

Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws
W. Reuter, J. Epstein, W. Lloyd

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluations guiding the direction of experimental testing. Tests are being conducted on materials ranging from linear elastic to fully plastic. The latter extends beyond the range of a J-controlled field. Specimens containing surface cracks are used to simulate the fracture process (crack growth initiation, subcritical growth, and catastrophic failure) that may occur in structural components.

Metallography and microtopography techniques have been developed to measure crack tip opening displacement and crack tip opening angle for comparison with analytical models. Moiré interferometry techniques are used to evaluate and quantify the deformation in the crack region. These studies have resulted in the ability to predict crack growth initiation of specimens containing surface cracks using constraint and fracture toughness data obtained from standard fracture toughness specimens. Future research will focus on predicting the stable crack growth process in base metal and the fracture process in weldments.

Diffusion bonded specimens are being used to simulate weldments. These specimens are used to study the ability of existing models to predict the fracture process for weldments. Actual weldments are being fabricated and testing/analysis will be underway soon.

This project is a collaborative program with MIT.

Idaho National Engineering Lab

Materials Technology Group **$477,000**
Idaho Falls, ID 83415 **03-A**
93-3

Intelligent Control of Thermal Processes
H. Smartt, J. Johnson

This project addresses intelligent control of thermal processes as applied to gas metal arc welding. Intelligent control is defined as the combined application of process modeling, sensing, artificial intelligence, and control theory to process control. The intent of intelligent control is to produce a good product without relying on post-process inspection and statistical quality control procedures, by integrating knowledge of process engineering practice and process physics into sensing and control algorithms. The gas metal arc welding process is used as a model system; considerable fundamental information on the process has been developed at INEL and MIT during the past ten years. Research is being conducted on analytical modeling of nonlinear aspects of molten metal droplet formation and transfer, and integration of knowledge-based control methods (including artificial neural networks and fuzzy logic based connectionist systems) with iterative learning control methods. Results are being transferred to industrial partners through a related ER-LTT/EE-OTT CRADA on Intelligent Diagnostics, Sensing, and Control of Thin Section Welding.

This project is part of a collaborative research program with the Massachusetts Institute of Technology.

Idaho National Engineering Lab

Nondestructive Mat'ls Charac Grp **$180,000**
Idaho Falls, ID 83415-2209 **03-B**
93-3

Nondestructive Evaluation of Superconductors
K. Telschow

This project is concerned with the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of materials, particularly high-temperature superconducting materials in tape form. Microstructural and, particularly, superconducting properties, need to be measured non-invasively and spatially in order to aid the fabrication process.

A noncontacting AC induced current measurement technique has been developed that can determine critical currents on a local scale. This technique can be used in conjunction with external applied fields and DC transport currents to determine spatial variations in critical current dissipation. Its operation is based on inducing the critical state and full field penetration into the sample directly under the probe. A new integral equation approach has been found that can be solved iteratively to determine the flux front profile in geometries with azimuthal symmetry accounting that accounts for demagnetization effects. This approach has been applied to configurations involving samples in a uniform field and tapes in the field of an external coil. The capability of high temperature SQUID sensors for measurements in long length tapes is being investigated for induced, leakage and trapped fields.

University Of Illinois

Coordinated Science Laboratory **$128,270**
Urbana, IL 61801 **03-A**
94-3

Model Building, Control and Optimization of Large Scale Systems
T. Basar

This program involves fundamental research on the modeling, control, and optimization of large scale systems. It encompasses both linear and nonlinear models, deterministic and stochastic systems with external and internal uncertainty, systems with weak spatial and weak or strong informational links, and dynamic decision models with multiple criteria. The main theme is goal-oriented model simplification for control and decision making. The overall goal is the development of new and effective methodologies for robust control, stabilization and optimization of large scale systems in the presence of static as well as dynamic uncertainty, and the analysis of such systems using the concepts of multimodeling, decomposition and aggregation.

One area of current research is the optimal and robust control of structurally-changing, large-scale uncertain systems, where the structural changes are stochastic and are modeled by a finite-state Markov jump process, and the additive uncertainties in the system dynamics and measurement channels are deterministic and norm-bounded. Our focus here is on systems where the transition rates from one structure to another exhibit a time-scale separation. Another topic of study at the present is optimally robust control of nonlinear systems with parametric and additive uncertainty, using the robust identification schemes recently developed in the scope of this project.

University Of Illinois

Dept of Chemical Engineering **$145,000**
Urbana, IL 61801 **01-C**
95-3

Gas-Liquid Flow in Pipelines
T. Hanratty

The long range goal of this research is to describe the macroscopic behavior of gas-liquid flows by developing a phenomenological understanding of small scale interphase interactions. The simplified systems of fully-developed flow in vertical and horizontal pipes are being used. Studies are being carried out of drop sizes in vertical flows, of asymmetries in horizontal annular flows, of the behavior of slugs in slug flow and of the role of waves in enhancing transport in stratified gas-liquid flows.

Studies of droplet deposition in vertical annular flows have revealed the surprising result that deposition rates are independent of droplet concentration at large enough concentrations. Dropsize measurements suggest that this is associated with a transition whereby droplet turbulence is hindered by droplet-droplet interactions.

Measurements of the liquid shedding rates of slugs in a gas-liquid horizontal flow have been made. Slug stability may be viewed as a situation in which the rate of liquid accumulation is equal or greater than the rate of shedding. This notion is used to improve predictions of the initiation of slug flow.

University Of Illinois

Dept of Mechanical and Industrial Engineering **$67,419**
Urbana, IL 61801 **01-A**
93-3

Stress Induced Phase Transformations
H. Sehitoglu

The stress-strain behavior associated with austenite → martensite phase transformation of carburized steels and nickel-titanium alloys is studied. Due to a lack of fundamental understanding of the role of stress on transformations in pressure type loadings, advances in these materials and science based-design with these materials have not occurred. Volumetric transformation strains have been measured on 43110 type steels austenitized at 950°C and at 843°C respectively with an initial austenite volume fraction of 35%. The experimental results indicate that the phase transformation strains exhibit considerable sensitivity to the hydrostatic stress with phase transformations occurring under zero hydrostatic stress case and the limit of transformation strains when the fracture of the specimen was delayed under superimposed pressure.

A number of experiments have been conducted on the NiTi alloys that are known to undergo thermo-elastic phase transformations. Unlike steels which exhibit virtually no recoverable transformation strains, the transformation strains in this class of materials are partially recovered upon unloading; depending on the applied strain levels. At low strain rates the transformation occurs through phase boundary motion while at high strain rates, the phase boundary motion was not observed at the macroscale. The stress-strain behavior is shown to exhibit considerable sensitivity to hydrostatic stress under pressure loadings.

Constitutive models proposed in the literature for deformation were evaluated in light of these results. The current models predict that the volume fraction of martensite is solely dependent on the effective stress, and the flow rule is chosen such that the ratio of transformation strain components remain constant during deformation. Our experimental results indicate that there is a dependence of the transformations strain on the hydrostatic stress component and the flow rule assumed in the literature for the transformation is also incorrect. In view of these experimental findings, new transformation models are being developed.

Currently, the research continues to focus on deformation studies under pressure loadings on the carburized steels and on the NiTi alloy. The influence of hydrostatic pressure on the threshold stress for transformation, transformation kinetics, and shifts in the transition (martensite start/finish) temperatures for transformation are being quantified with experiments at several temperatures.

Johns Hopkins University

Mechanical Engineering Dept **$ 0**
Baltimore, MD 21218 **01-C**
92-3

Numerical and Physical Modeling of Two-Phase Flow Phenomena at Large Reynolds Numbers
A. Prosperetti

The ultimate purpose of this study is to develop accurate averaged-equations models of disperse multi-phase flows of engineering significance. Analytical means are used to derive the form of the equations and direct numerical simulations to effect their closure at finite volume fractions.

A new method of phase averaging has been developed and applied to rigid and compressible spheres in potential flow and in Stokes flow. Analytical results have been obtained in the dilute limit and numerical ones for finite volume fractions. The method is quite flexible and general and has also been applied to the derivation of averaged energy equations at small Peclet number and of the particle stress tensor in potential flow. It has also been shown that it reproduces - often with considerably less effort and greater generality - many results in the literature.

Current efforts center on the simulation of suspensions of non-spherical particles in the potential- and Stokes-flow limits. Approximate closure techniques at finite concentrations are also being developed.

Robert H. Kraichnan, Inc.

369 Montezuma 108 **$67,685**
Santa Fe, NM 87501-2626 **01-C**
93-3

Turbulence Theory
R. Kraichnan

Turbulent flow is omnipresent in geophysics and energy-producing devices. Atmospheric turbulent transport plays an essential role in the movement of heat, moisture, and pollutants. Turbulent flows represent an enormous amount of data. Both for practicable computation and for physical understanding, it is necessary to extract the essential information in compact form. This project explores novel approaches to economical and meaningful description and computation of turbulence. During the past two years of this project, explicit statistics have been deduced theoretically for the spottiness of small scales of a contaminant carried by turbulence. This is the first such success for a turbulence problem, and has sparked an international follow-up effort. The work has now been tested numerically, by simulations of unprecedented resolution. A result of this project should be improvement of schemes for economical computation of contaminant dispersal.

Lawrence Berkeley Laboratory

Dept of Physics **$249,000**
University of California **06-C**
Berkeley, CA 94720 **93-3**

Studies in Nonlinear Dynamics
A. Kaufman, R. Littlejohn

Our research concerns the development of methods of modern nonlinear dynamics with applications to problems in physical and engineering sciences. We have been especially involved with Hamiltonian dynamical systems and the application of differential geometric and topological methods. A main area of application is wave systems, in which we have taken a broad, interdisciplinary perspective. Our interests have included the propagation, spectra, mode conversion, and tunnelling of waves. Major divisions of the program are: (1) A study of the properties of coupled wave systems, including elastic waves in solids, electromagnetic waves in optical media or plasmas, nuclear wave functions in molecular physics, and many others; (2) The development of a new method for decoupling coupled wave systems, including systematic adiabatic perturbation schemes for this purpose; (3) The development of asymptotic quantization methods for coupled wave systems, i.e., the determination of normal mode frequencies and eigenfunctions; (4) Investigation of differential geometric and topological concepts such as Berry's phase, gauge structures, and topological singularities (such as monopole strings) which generically occur in coupled wave systems; (5) A systematic study of mode conversion (otherwise called Landau-Zener transitions), in which we apply bifurcation and catastrophe theory to categorize the basic types of mode conversion which can occur; (6) Investigations into coherence and radiometry in optics; (7) The development of theories of mode conversion applicable when nonlinear effects are important; and (8) A study of the non-Abelian gauge fields which occur in the separation of rotational and internal coordinates in the n-body problem (with applications to celestial mechanics, satellite control, and atomic, molecular, and nuclear physics).

Lawrence Livermore National Laboratory

Dept of Physics **$200,000**
University of California **06-A**
Livermore, CA 94720 **94-1**

Steady State and Transient Nucleation Kinetics
G. Wilemski

This research addresses several fundamental issues in homogeneous nucleation theory. The appealing simplicity and wide applicability of classical nucleation theory is offset by its inaccurate predictions of nucleation rates. New molecular theories of nucleation appear capable of providing greatly improved predictions, but practical application of these theories is currently restricted to the simple rare gas systems. One aim of this work is to bridge this gap by developing theoretical expressions for cluster evaporation rates based on computer studies of the energetics and dynamics of small clusters of more complex molecules such as water and methanol. To preserve a modicum of simplicity in the theory, this work will strive to obtain results that depend on only a few readily determined molecular parameters.

Theoretical work will also be performed to test and improve various aspects of binary nucleation theory. Accurate numerical solutions of the birth-death equations will be obtained to simulate binary nucleation kinetics for fluid systems with strong compositional surface enrichment, partial miscibility, and significant vapor phase nonideality. These results will be used to assess the accuracy and applicability of various approximate analytical expressions for the rate of binary nucleation. Attention will be given to the effects of transient behavior on binary nucleation rates and to cases of ridge crossing, i.e., when the major nucleation flux bypasses the saddle point. To improve understanding of the effects of partial miscibility on nucleation, molecular dynamics and Monte Carlo simulations of binary rare gas clusters will be made to investigate how the internal molecular distribution of the two species varies as the different interaction strengths are varied.

The Lovelace Institutes

Institute for Basic and Applied Medical Research **$55,487**
Albuquerque, NM 87108 **03-B**
93-3

Two-Phase Flow Measurements by NMR
E. Fukushima, S. Altobelli, A. Caprihan

The objective of this grant is to apply NMR to study how mixtures of different phases flow. The concentration profile of one or both of the phases undergoing flow as well as velocity profile and other more esoteric quantities such as acceleration and diffusion can be measured without interfering with the flow. The non-invasive measurement of such parameters is especially difficult for concentrated mixtures that are opaque to the standard measurement medium such as light and sound waves but NMR works very well provided we examine proton containing liquids, e.g., water and oil, in nonmetallic containers.

Steady flows of concentrated suspensions in a circular pipe, first with a constant cross-section and then with a step expansion and contraction, have now been studied. Because NMR imaging is a fairly slow method, it is very important to extend the NMR method to faster flows. As a point of reference, velocity images have been made in tens of minutes whereas the achievement of similar results in fractions of seconds will be a specific objective for the next few years.

University Of Maryland

Dept of Mechanical Engineering **$65,524**
College Park, MD 20742 **01-D**
93-3

Characterization of Metal Cutting Dynamics
B. Berger, I. Minis

The development of energy efficient machine tools which produce parts of high quality and require minimum intervention requires the capacity to identify precursors of unstable, chatter states and integrate such identifiers into control system algorithms. Large amplitude oscillations associated with chatter adversely affect surface finish, dimensional accuracy and tool wear often resulting in tool breakage.

This research effort has addressed the fundamental issues involved in the identification and control of chatter through: (i) creation of a data base of over 200 cutting experiments comprising $16 \cdot 10^7$ separate measurements for ranges of values of depth of cut, turning speed and feed rate; (ii) analysis of time series in the data base with a variety of techniques including false nearest neighbors, mutual information, singular value decomposition, time-frequency calculation and polyspectral methods; (iii) identification in the data analysis of three non-dimensional measures of the cutting state which are sufficiently robust for use in the on line control of the cutting machine; (iv) incorporation of the measures of the cutting state into the control system of an existing lathe.

A relationship has been established between the cutting state and the structure of the power spectra of the time series and its envelope. This research has resulted in the development of means for the elimination of chatter in orthogonal cutting.

University Of Maryland

Dept of Electrical Engineering **$95,000**
College Park, MD 20742 **06-C**
92-3

Mathematical Models of Hysteresis
I. Mayergoyz

This research is concerned with the development of mathematical models of hysteresis. These models are phenomenological in nature and, for this reason, they can be applied to the description of hysteresis regardless of its physical origin.

The main research objectives of the ongoing research can be briefly summarized as follows: further development of scalar and vector Preisach type models of hysteresis (superposition models, two-input models for magnetostrictive and piezoelectric hysteresis and their tensor extensions, feedback Preisach-type models), development of Preisach-type models for viscosity (aftereffect), application of Preisach-type models to the description of superconducting hysteresis and evaluation of hysteretic losses in hard superconductors, software implementation of the Preisach hysteresis models, extensive experimental testing and verification of hysteresis models, investigation of penetration of electromagnetic fields into nonlinear hysteretic media. It is hoped that, as a result of this research, the Preisach-type models of hysteresis will emerge as a useful and indispensable tool in engineering research and design problems.

University Of Maryland

Electrical Engineering Department **$ 0**
Baltimore, MD 21228 **03-B**
92-3

Pulse Propagation in Inhomogeneous Optical Waveguides
C. Menyuk

We are presently working on two principal projects. First, we are studying randomly varying birefringence in optical fibers and its impact on both soliton and NRZ communications. We have derived a set of equations (modified Manakov equations) that allow us to simulate the propagation through a fiber with rapidly and randomly varying birefringence on the much longer length scale on which the signals varying due to chromatic dispersion, polarization mode dispersion, and nonlinearity. These equations also yield considerable physical insight into the behavior of these systems. We have benchmarked these codes carefully, and we have demonstrated that they yield the same results as computer codes that use far shorter step sizes and are far less efficient. In addition to Monte Carlo methods, we are now using analytical methods based on the theory of stochastic differential equations to completely characterize the probability distribution functions for the evolution of the signal's state of polarization and the corresponding terms in the modified Manakov equation that describes the complete evolution.

The second project is quasi-phase-matched waveguides. We are using a Green's function approach to determine the rate at which radiation leaks from the quasi-phase-matched guides. In the future we will look at oblique guides and guides with other unusual cross-sections that appear in the experiments to reduce unwanted Bragg reflections.

University Of Maryland

Dept of Mechanical Engineering **$129,319**
College Park, MD 20742 **01-C**
94-3

Contaminant Dispersal in Bounded Turbulent Shear Flows
J. Wallace, P. Bernard, L. Ong

Closely coordinated direct numerical simulations and windtunnel experiments of evolving line-source plumes are being conducted to better understand the physics of the scalar transport and to develop a methodology for the accurate prediction of scalar fields in highly sheared environments. The latter includes a new class of models which more accurately mimic the dynamical processes affecting plume development. Of particular interest is the wall-normal diffusion of the scalar and its connection to vortical structures in the wall region, and the efficacy of the transport models in both canonical boundary layer flows as well as in complex flow geometries with significant flow separation.

A quasi-three-dimensional laser light-sheet tomographic method to visualize the scalar topography of boundary layer plumes has been implemented. A smoke plume seeped into the flow from a wall slot in the windtunnel (idealizing the dispersion of a passive scalar pollutant released from a line source in the atmospheric surface layer) has been filmed at 10 KHz and rendered into a 3-D computer movie of constant concentration surfaces. These images with simultaneous measurements of the velocity and vorticity vectors with a miniature 12-sensor hot-wire probe provide a database for model development and verification.

Massachusetts Institute Of Technology

The Energy Laboratory **$123,688**
Cambridge, MA 02139 **03-B**
94-3

Metal Transfer in Gas Metal Arc Welding
T. Eagar, J. Lang

The objective of this project is to find new control methods to improve metal transfer in gas metal arc welding -- a widely-used manufacturing process. The goal is to develop a faster process that is stable. To gain insight on the complex process, a lumped-parameter mathematical model of drop detachment from a melting gas metal arc welding electrode has been developed and its performance compared to an extensive range of experimental results.

A highly-instrumented gas metal arc welding experiment which modifies the fundamental way metal is transferred in the new welding process has been designed and constructed. The experiment uses mechanical energy as a new control input to the welding process. The metal electrode is vibrated axially while welding at the desired frequency of drop detachment in order to force the detachment of metal drops. The experiment has been used to study vibrated electrode metal transfer, short duty-cycle current pulsing metal transfer, and constant current metal transfer with steel and aluminum electrodes. Very clear high-speed video images of the electrode area provided measurements of the surface tension of the molten steel, the oscillations of drops attached to the electrode, and the dynamics of the drop detachment process.

Experiments show that the electrode model captures the instantaneous geometry and dynamics of drop detachment. Hitherto, dynamic electrode melting models have only sought to capture the average of the process. The model has been used, among other things, to quantitatively explain the effectiveness of current pulsing for improving drop detachment.

Massachusetts Institute Of Technology

The Energy Laboratory **$111,100**
Cambridge, MA 02139 **03-A**
94-3

Synthesis and Optimization of Chemical Processes
L. Evans, P. Barton

The goal of this research program is to develop new systematic methods for the synthesis and optimization of chemical processes. As the chemical industry is one of the largest consumers of energy in the U.S., it is important to find efficient and creative computer-aided design strategies for developing new manufacturing processes, and retrofitting existing plants

The general philosophy of this research is to develop, in an university environment, innovative generic methodologies for solving problems of industrial importance. These methods are then demonstrated by using prototype software to solve problems typical of those encountered in industry.

Research is currently considering three topics. A long term program that focuses on synthesis techniques for achieving increased energy efficiency through better heat and work integration has culminated with an investigation of the simultaneous synthesis and optimization of a chemical process, its heat exchange network, and the utility system. Case studies involving an atmospheric crude tower and the cold end of an ethylene plant demonstrate that the new approach can be used to derive designs very close to those of mature process technologies, thus enabling new process designs to start high on the learning curve. Secondly, a new initiative is addressing the need for process design and optimization technologies for batch/semi-continuous processes. Research is focusing on design tools for rapid and efficient pro- cess development. A prototype process development methodology has been proposed that exploits modeling technology to explore alternatives and ensure feasibility of the design. Finally, a new initiative is investigating improve- ments, such as use of hybrid numerical and symbolic strategies, to the robustness and efficiency of numerical algorithms for process simulation and optimization.

Massachusetts Institute Of Technology

The Energy Laboratory **$152,609**
Cambridge, MA 02139 **03-B**
94-3

Multivariable Control Of The Gas-Metal Arc Welding Process
D. Hardt

The goal of this work is to provide a well-controlled welding process, based on multivariable regulation of several welding attributes. However, previous work encountered several problems that precluded good regulation of the process -- primary among these was the lack of sufficient controllability of the process.

We are taking three approaches to this problem. The first involves development of a more controllable conventional welding process by creating a plasma process that allows independent control of heat and mass transfer to the weld. In addition, a miniature arc-furnace-based droplet producing method has been developed that can control the heat and mass transfer very precisely, but needs an additional heat source for weldment pre-heating. The third supports the other two by investigating applied control theory in the area of distributed parameter control.

The distributed-parameter work has concentrated on formulation of a general heat conduction problem with boundary heating to allow feedback control of the temperature distribution in time and space. Test cases involving both welding and general thermal control in steel processing are being considered. The plasma process and arc-furnace approaches are being pursued analytically, with fluid thermal modeling combined with control systems theory, and experimentally. In the case of the arc-furnace approach, an apparatus is under development to test the concept of "stream welding;" for the plasma approach, a torch with feedback-controlled plasma flow is under design.

Massachusetts Institute Of Technology

National Magnet Laboratory **$88,555**
Cambridge, MA 02139 **01-D**
93-2

Cryotribology (Low Temperature Friction and Wear): Development of Cryotribological Theories and Application to Cryogenic Devices
Y. Iwasa

To advance our understanding of cryogenic-temperature sliding stability, and thereby to improve the reliability of superconducting magnets, we have been examining, experimentally and theoretically, the fundamental mechanisms of frictional stability. The attainment of absolutely stable, positive friction-velocity characteristics at cryogenic temperatures appears improbable because of the lack of thermally-activated steady-state shear creep. We are presently investigating: 1) a force-based approach to magnet design that promotes quench-causing conductor microslips to occur early in the magnet's charging cycle where their consequences are relatively benign; and 2) the cryotribological behaviors at 77K and 4.2 K of several metal/metal and other nonpolymeric sliding pairs, particularly of several hard, creep-resistant, chemically inert materials such as: the Group 8 noble metals, high-strength ceramics and recently-developed sputter-deposited diamond films. Of particular interest is the extent to which hardness, ductility, and chemical compatibility influence cryogenic-temperature sliding behavior.

Massachusetts Institute Of Technology

The Energy Laboratory **$191,628**
Cambridge, MA 02139 **01-A**
94-3

Modeling and Analysis of Surface Cracks
D. Parks, F. McClintock

A methodology for predicting constraint-sensitive plane strain ductile fracture in engineering structures is being developed. At low toughness, the elastic T-stress and K provide a rigorous and straightforwardly calculable two-parameter fracture mechanics. At loads giving moderate to large-scale yielding, a modification to the standard effective crack length formulation accounting for effects of T-stress on plastic zone size gives simple and accurate estimates of J, compliance, and crack tip constraint based solely on elastic K and T calibrations. In fully plastic cracking of low to moderate strength structural metals, asymptotic elastic-plastic crack tip fields fail to dominate the strain over microstructural length scales, suggesting the utility of rigid/plastic models. Such fully plastic cracking is based on limit analysis and a micromechanical model of crack tip opening angle that is sensitive to constraint and an effective slip angle at the crack tip. The corresponding material constraints are being determined from bending and tension tests of both standard and novel design.

All of these models have been incorporated into line-spring finite elements for stationary and growing surface-cracked plates and shells, providing simple and extraordinarily accurate analysis and simulation of these important engineering flaws. Finally, through finite element simulation, the effects of loading, geometry, and material strength differences are being systematically evaluated for mismatched welds containing cracks near and on the fusion surface.

Massachusetts Institute Of Technology

Dept of Mechanical Engineering **$ 0**
Cambridge, MA 02139 **01-C**
92-3

Rheological and Flow Characteristics of Dense Multiphase Slurries Employing a Bimodal Model
R. Probstein

This research aims to develop a rational theoretical and experimental methodology for the rheological and flow property prediction of dense-phase slurries with particles distributed in size from submicron to several hundred microns. The approach models a polydisperse suspension as inherently bimodal, wherein it is considered to be made up of a fine fraction which behaves colloidally and imparts to the suspension many of its important rheological and flow characteristics, and a coarse fraction which behaves as if it were in a pure liquid with the same viscous behavior as the colloidal suspension and raises the apparent viscosity through hydrodynamic interactions. To describe the behavior of the coarse fraction, a viscosity equation based on lubrication concepts was applied to suspensions of non-colloidal particles. The equation derived for monodisperse suspensions was also shown to apply remarkably well to bidisperse and polydisperse suspensions. The polymodal particle size was either uniformly or log-normally distributed, and the broadest size range was 37-212 microns. The maximum packing of these suspensions obtained from viscosity measurements were found to be equal to the dry random packing of the same particles divided by 1.19. This is a new dilatancy factor likely to be associated with lubrication layers between the particles. The viscosity equation was also used to describe the behavior of bidisperse suspensions with a very large particle size ratio. Here, the bidisperse viscosity was simulated using the bimodal model. The viscosity equation again matched well with the simulated data. The calculated values of maximum packing fraction were consistent with the experimental values for smaller size ratios. This lends further support to the validity of the bimodal model. The bimodal approach was next applied to the high-shear-limit viscosity of a polydisperse suspension with a size range from submicron to 40 microns. The separating particle size that divided the distribution into a fine and a coarse fraction was found to be 1.5 microns. It was determined so as to give the best fit between the bimodal model and experiiment. The result for the separating particle size showed that the fine fraction is indeed colloidal.

Massachusetts Institute Of Technology

Dept of Chemical Engineering **$152, 653**
Cambridge, MA 02139 **06-A**
94-3

Development of Principles & Methodologies of Metabolic Engineering
G. Stephanopoulos

Metabolic Engineering is an emerging field of biotechnology aiming at the directed modification of the metabolic pathways of microorganisms, plants and animals using recombinant DNA technology. The overall objective is to achieve overproduction of fuels, chemicals and materials, or biosynthesis of novel products through the amplification of selected biochemical reactions or the introduction of new biosynthetic pathways in metabolic networks. The experimental techniques of metabolic engineering are derived from applied molecular biology and are well advanced. However, interactions of metabolic pathways and the general principles governing metabolic fluxes *in-vivo* are poorly understood. The goal of this research is to contribute to the development of the tools and principles that elucidate the *control of flux* in metabolic networks. As the problem of determining flux control distributions at the individual reaction level is too complex and experimentally intractable, our approach has examined the control of flux exercised by *groups* of reactions. Concepts from metabolic control analysis have been extended to groups of reactions in order to identify the group exercising the strongest degree of control on the production flux. The approach is then repeated within the group until single reactions are identified that are of particular importance to the flux of product formation. This approach has been applied with success to the production of aromatic and aspartate aminoacids in *Corynebacterium* and yeasts.

Massachusetts Institute Of Technology[1]

Dept of Chemical Engineering **$79,862**
Cambridge, MA 02139 **06-C**
95-3

Los Alamos National Lab[2]

MEE-9 **$200,000**
Los Alamos, NM 87545 **06-C**
91-4

Sandia National Laboratories[3]

Engineering Sciences Center **$200,000**
Albuquerque, NM 87008-0834 **06-C**
91-4

Macrostatistical Hydrodynamics
H. Brenner[1], A. Graham[2], L. Mondy[3]

Experimental, analytical, and numerical studies of falling-ball 'tracer' particle dynamics in concentrated suspensions composed of dispersed, neutrally-buoyant spheres and rods comparable in size to the tracer have been continued and extended. Falling ball viscometry was shown to be a useful technique to measure the apparent viscosity of mixtures of particles of various shapes and sizes. When two types of suspended particles (such as spheres and rods) are of disparate sizes, the measured apparent viscosity of the homogeneous mixture could be described successfully by a model which approximated the mixture as one of the fraction of larger particles suspended in a hypothetical suspending continuum with a viscosity identical to the effective viscosity of a suspension of the fraction of smaller particles alone. The pressure 'drop' across a ball falling through a quiescent suspension, which constitutes another useful dynamical suspension parameter, was measured and, in moderately concentrated suspensions, found to agree well with theoretical results for the comparable pressure drop in a homogeneous Newtonian liquid. For a ball falling in a highly concentrated suspension, the pressure drop seems to be a sensitive measure of phase slip at the containing cylinder walls. Also, spinning-ball rheometry in quiescent suspensions has been developed as a useful adjunct to the falling-ball rheometric studies. This technique provides a sensitive measure of phase slip at the spinning ball's surface, as well as another experimental benchmark for ongoing theoretical investigations of slip in disperse systems. Finally, in collaboration with The Lovelace Institutes, nuclear magnetic resonance imaging is being used to study flow-induced particle segregation ('hydrodynamic diffusion') in pipe flow. These data in inhomogeneous flows and complementary video imaging of individual tracer particles in homogeneous flows will provide much needed information on the effects of flow on particle interactions and effective rheological properties at the macroscale.

University Of Minnesota

Dept of Mechanical Engineering **$127,361**
Minneapolis, MN 55455 **01-B**
94-3

Heat/Mass Transfer Enhancement in Separated and Vortex Flows
R. Goldstein

The fluid mechanics and thermal transport in separated and vortex flows are studied to increase our knowledge of heat/mass transfer enhancement mechanisms.

A stepped pin-fin array has been found to be effective for the enhancement of duct flow heat/mass transfer. Detailed flow and mass transfer measurements to understand the related mechanisms have been conducted. A complex vortex system has been observed near the step region. This step-induced vortex system separates from the step toward the endwall and interacts with the main horseshoe vortex system, altering the near-wake flow pattern dramatically. It produces a remarkable acceleration near the endwall and a deceleration near the mid-span, even suppressing the Karman vortex shedding. Enhancement of endwall heat/mass transfer has been found in the region with strong flow acceleration.

Energy separation in vortex flow is being studied with free jets and flow around a cylinder. Energy separation occurring in a free jet, depends on the nature of the vortex structure around the jet periphery and is greatly affected by acoustic excitation. An experiment to measure unsteady temperature fluctuations around a cylinder exposed to high velocity flow is being conducted to examine the difference between instantaneous and time-averaged energy separation. A thin film resistance temperature sensor, which can measure the transient recovery temperature with a frequency of 1000-2000 Hz, is being developed and a special wind tunnel is being assembled.

University Of Minnesota

Dept of Aero Eng & Mechanics **$108,000**
Minneapolis, MN 55455 **01-C**
93-5

Lubricated Transport of Viscous Materials
D. Joseph

The project has as its broad aim the understanding and technological development of lubricated pipelines of heavy oils in core annular flow, and the spontaneous lubrication of oil/water and water/oil emulsions and for slurry transport. The scientific approach relies heavily on experiments and direct numerical simulations. Analytically the problem involves the study of two-phase flows and deals with migration and segregation of lubricating fluid at the wall. The role of inertia in centering density matched core-annular flows and in levitating these flows off the wall when the fluids have different densities has been clarified in recent works sponsored under this grant. Experiments on the effects of different linings and surfactants on the fouling of pipe walls with hydrocarbons were carried out. A patent for a "method of preventing fouling of pipe walls for lubricated transport" was obtained for cement linings (U.S. Patent No. 5,385,175). Another patent for a non-fouling pressure tap is under consideration. It has been found that oil-in-water emulsions used as a coal substitute fluid and stable water-in-oil emulsions used in the processing of synthetic crude oils will lubricate when flow speed is above a critical one and other attainable conditions are satisfied.

University Of Minnesota

Dept of Mechanical Engineering **$ 0**
Minneapolis, MN 55455 **06-C**
92-4

Thermal Plasma Processing of Materials
E. Pfender, J. Heberlein

The objectives of this program are the characterization of plasma reactors used for materials processing, in particular for the deposition of diamond films and the generation of ultrafine particles. The characterization involves diagnostics and modeling of the plasma - reactant flow interactions.

One of the reactor configurations characterized is the liquid injection plasma reactor. Droplet trajectories have been determined with a telemicroscope-laser strobe video combination giving 100ns exposures of a 50 times magnified image. For the highest diamond growth conditions, precursor droplets appear to impinge on the substrate surface before completely evaporating. A model is being developed for identification of the most important physico-chemical effects in this process.

The characterization of rf reactors for ultrafine powder production has concentrated on calculating temperature and velocity profiles for different reactor configurations and operating conditions to provide a basis for optimal reactor design.

The establishment of a diagnostic capability based on laser scattering techniques developed at the Idaho National Engineering Laboratory has produced the first initial results of scattering signals from a plasma jet.

Further modeling has been concerned with determining accurate transport coefficients for gas mixtures, because the importance of these data is increasing for all plasma modeling efforts.

National Academy of Sciences-National Academy of Eng National Research Council

Washington, DC 20418 **$1,249,500**
06-C
Department of Energy Integrated Manufacturing Fellowship Program **95-2**
T. Rozzell

Thirty-six three-year predoctoral fellowships in integrated manufacturing are in place administered by the National Research Council, under the aegis of the National Academy of Engineering, following national competitions. The objectives of the program are to create a pool of PhD's trained in the integrated approach to manufacturing, to promote academic interest in the field, and to attract talented professionals to this challenging area of engineering.

The fellowship program was conceived as one response to the loss of competitiveness of the United States in manufacturing. Two related aspects of the problem are the traditional separation of the product design function from the manufacturing function and the lack of an appreciation for the process of manufacturing as an integrated system.

It is expected that the improved manufacturing methods which this fellowship aims to bring about will contribute to improved energy efficiency, to better utilization of scarce resources, and to less degradation of the environment.

National Aeronautics and Space Adminstration

600 Independence Avenue, S.W. **$107,630**
Washington, DC 20546 **06-C**
94-5
Center for Aerospace Research & Education for Minority Students at Southern University
I. Blankson

Pursuant to an agreement between the Secretary of Energy and the Administrator of NASA, the recommended funds will support the education of minority students at Southern University (an HBCU) in disciplines related to aeronautics and space sciences. Over the five years of this agreement NASA will provide $2,500,000. The education program will be coordinated with a research program addressing Solid mechanics and Finite element Modeling, Composite materials, Aerodynamics and impact, as well as Thermal sciences (Heat transfer and Fluid Dynamics). In more detail examples of specific projects are Improvement of satellite Rendezvous Maneuvers, optimization of gear design, analysis of the wear of diamond tools. Furthermore, these funds will be used to strengthen the undergraduate education in aeronautics at Southern University.

National Institute Of Standards & Technology

Thermophysics Division **$ 0**
Boulder, CO 80303 **06-A**
94-3
Gelation of Dense Silica Suspensions: Effect of Shear
H.J.M. Hanley

The project examines the gel structure of silica by SANS (small angle neutron scattering) and light scattering measurements. The goal is to extend the current understanding of how gels form on a microscopic scale, and to determine what specific changes are induced in the microscopic structure by the influence of an applied shear. Scattered intensity data were taken on the 30 m SANS instruments at the NIST Cold Neutron Research Facility. Samples were aqueous suspensions of Ludox silica particles of nominal diameter 24 nm. Gelation was induced by adjusting the pH and salt content of the suspensions. The series of experiments were repeated with the silica samples loaded into the NIST Couette shearing cell. The results showed that shear most conclusively influences the structure of the gel. On the assumption that an investigation of the decomposition of a system to a solid would lead to an insight into the gelation mechanism, a simulation of a two dimensional Lennard-Jones system was initiated. A striking similarity between the computer results and the SANS data was observed. A scaling relation for the time evolution of the structure factor of a decomposing system has been proposed. The relation will lead to a novel procedure to analyze scattering from dense gels.

National Institute Of Standards & Technology

Thermophysics Division **$416,000**
Gaithersburg, MD 20899 **03-B**
Boulder, CO 80303 **91-5**

Development of Measurement Capabilities for the Thermophysical Properties of Energy-Related Fluids
R. Kayser, J. Levelt Sengers, M. Moldover, W. Haynes

The major objectives of this project are to develop state-of-the-art experimental apparatus for measuring the thermophysical properties of a wide range of fluids and fluid mixtures important to the energy, chemical, and energy-related industries and to carry out carefully selected benchmark measurements on alternative refrigerants and refrigerant mixtures. The specific measurement capabilities completed or under development include new apparatus for transport properties (tantalum-hot-wire thermal-conductivity apparatus, vibrating-wire viscometer), thermodynamic properties (dual-sinker densimeter, high-temperature vibrating-tube densimeter, total-enthalpy flow calorimeter), phase equilibria properties (recirculating phase equilibria apparatus, low and high-pressure ebulliometers, re-entrant radio-frequency resonator), and dielectric properties (concentric-cylinder dielectric-constant apparatus). These new apparatus extend significantly the state of the art for properties measurements and make it possible to study a wide range of complex fluid systems (e.g., highly polar, electrically conducting, and reactive fluids) under conditions which have been previously inaccessible.

National Institute Of Standards & Technology

Electromagnetic Technology Div **$86,000**
Boulder, CO 80303 **06-C**
94-3

High-T_c Superconductor-Semiconductor Integration and Contact Technology
J. Moreland, S. Russek, S. Sanders, J. Ekin

The purpose of this project is to study materials problems faced in integrating high-T_c superconductor (HTS) thin-film technology with conventional semiconducting technologies. The emphasis of the research is to investigate HTS-semiconductor contact systems and novel HTS-semiconductor devices. The ultimate goal is to develop HTS thin-film technology to its fullest potential for multimodule interconnections, future ULSI source and drain connections, and microelectronic microwave filters. These potential applications provide the motivation for a thorough investigation of HTS thin-film materials development of these hybrid systems. Determining the compatibility of HTS thin-film deposition and patteming processing with that of standard Si and GaAs processing is crucial for expanding the applications of these hybrid technologies.

The nanostuctural properties of HTS materials have proven to have a principal influence on the electrical properties of HTS materials and devices. For this reason the use of scanned probe microscopies are being emphasized for evaluating HTS-semiconductor epitaxy as well as electrical conduction in interconnects and contacts to hybrid device structures. The further development of scanned probe microscopies, specifically for electronic device imaging will be invaluable not only for the HTS-semiconductor integration studies but for all developments in microelectronics in the foreseeable future.

The City University Of New York

The City College **$133,639**
The Benjamin Levich Institute **06-C**
for Physico-Chemical Hydrodynamics **95-4**
New York, NY 10031

The Rheology of Concentrated Suspensions
A. Acrivos

This research program aims to investigate the flow of concentrated suspensions of non-colloidal particles from the fundamental point of view. Earlier studies by the Principal Investigator and his associates have shown that the rheology of such systems is strongly affected by the shear-induced migration of particles from regions of high shear to low and from regions of high particle concentrations to low which, by distorting the particle concentration profile, can lead to an erroneous interpretation of the experimental measurements pertaining to the effective viscosity of such systems. This shear-induced particle diffusion is also responsible for the phenomenon of viscous resuspension whereby, in the presence of shear flow, a settled bed of heavy particles can resuspend even under conditions of vanishingly small Reynolds numbers.

A theoretical model of shear-induced particle diffusion, which was developed earlier by the Principal Investigator was tested experimentally in various unidirectional flows by measuring the extent of viscous resuspension and comparing it to the theoretical predictions. Very good agreement was found between theory and experiments even in the case of flow in a tube where strong secondary flows are generated owing to the presence of a non-axisymmetric particle concentration profile. In addition, a technique was developed, using LDA, for measuring the particle velocities in concentrated suspensions. This technique is currently being used to measure instantaneous 3-d particle velocities in concentrated suspensions undergoing a variety of shear flows in order to further test the predictions of the theoretical model.

The City University Of New York

The City College **$ 0**
Dept of Chemical Engineering **03-A**
New York, NY 10031 **94-3**

Partial Control of Complex Processing Systems

R. Shinnar, I. Rinard

There are two research objectives. One is to understand the control of Fluidized Catalytic Crackers (FCC's), an important goal in itself. The second is to use the FCC as an example to learn about the control of complex chemical plants in which the number of variables to be maintained within acceptable limits exceeds the number of manipulatable variables available for control.

The dynamic simulation model of the FCC developed previously has been published and is available on request. The study of multiple steady states and input multiplicities was completed and accepted for publication. In the region of current operation and over a wide range of model parameters, FCC's exhibit only the three steady expected of any exothermic reaction system. Input multiplicities exist and limit control to regions where the process gains are nonzero.

Major attention this year was given to the choice of decentralized control structures for partial control. Based on the FCC, there are several results that should be of wide interest: (1) An FCC can be stabilized and controlled by a 2x2 matrix; (2) A control matrix useful in one domain of operation may not be in a different domain, (3) One must look beyond setpoint tracking performance to judge the suitability of a given matrix; and (4) Linear algorithms are satisfactory for loop tuning but the impact of nonlinearity determines the choice of the primary matrix.

The City University Of New York

The City College **$110,250**
The Benjamin Levich Institute **06-C**
New York, NY 10031 **94-3**

Studies in Physico-Chemical Hydrodynamics of Extended Systems

G. Sivashinsky

The objective of this project is a unified theoretical approach to the description of a variety of physico-chemical hydrodynamics systems characterized by a significant disparity between the spatial scales involved. By appropriately performed averaging over short scales one may considerably simplify the original problem, sometimes even lowering its effective dimensionality and thereby making the latter quite tractable either analytically or numerically.

With all their relative simplicity the emerging reduced models proved rich enough to capture many nontrivial features of the original systems which hitherto resisted description by any other means. Specifically, the scale-separation approach will be applied to (1) the mathematical modelling of stabilization, blowoff and flashback of premixed gas flames; (2) the theory of thermal explosion in the reactive premixture subject to the effects of natural or forced convection; (3) the nonlinear dynamics of the interfacial instabilities in multilayered flows dominated by viscosity effects.

State University Of New York

Department of Physics **$191,012**
Stony Brook, NY **06-C**
95-3

Sub-Electron Transfer of Electric Charge in Semiconductor Nanostructure
K.K. Likharev

The main goal of this project is to carry out a complementary set of experimental and theoretical studies of the continuity of electric charge transfer in semiconductor heterostructures.

The interplay of continuous (sub-single-electron) and discrete transfer of charge in solid state systems is the basis of several new physical phenomena predicted and observed since the mid-1980s, including the Coulomb blockade, Coulomb staircase, single-electron-tunneling (SET) oscillations, Bloch oscillations, etc. These effects are considered as the possible basis of a novel generation of future "single-electron" devices, circuits, and systems. However, to our knowledge, the conditions and limitations of the sub-single-electron transfer of charge, especially in the most important case of poorly-conducting structures of small size, have not been studied. The main objective of this work will be a combined (experimental and theoretical) study of the discreetness of the charge transfer in semiconductor nanostructures, in particular in conditions of space-confined electron hopping.

Northwestern University

Engineering & Applied Science **$91,537**
Evanston, IL 60208 **03-B**
93-3

Thin-Film Characterization and Flaw Detection
J. Achenbach

This work is concerned with the determination of the elastic constants of thin films deposited on substrates, with the measurement of residual stresses in such films and with the detection and characterization of defects in thin film substrate configurations.

There are many present and potential applications of configurations consisting of a thin film deposited on a substrate. Thin films that are deposited to improve the hardness and/or the thermal properties of surfaces are of principal interest in this work. Thin film technology does, however, also include high Tc superconductor films, films for magnetic recording, superlattices and films for band-gap engineering and quantum devices. The studies carried out on this project also have relevance to those applications.

Both the film and the substrate are generally anisotropic. A line-focus acoustic microscope, is being used to measure the speed of wave modes in the thin film/substrate system. This microscope has unique advantages for measurements in anisotropic media. Analytical and numerical techniques are employed to extract the desired information on the thin film from the measured data. Recent results include: (1) use of multiple wave modes to determine thin film constants, (2) measurements of superlattice film constants, and (3) investigation of the effect of surface roughness.

Northwestern University

Dept of Chemical Engineering **$139,916**
Evanston, IL 60208 **01-B**
95-3

Theory of Subcooled Boiling
S. Bankoff, S. Davis

The objective of this work continues to be the study of the dynamics, stability and rupture of thin liquid films, especially with heat and/or mass transfer. These films appear in many engineering processes, such as film coating, gas absorption, condensation, and especially cooling of hot surfaces.

In the long-wave linear stability limit, destabilizing mechanisms are identified. For arbitrary wavenumbers, a shear-mode instability exists that is stable in plane Poiseuille flow. Regions are determined in which the primary instability is to long-wave disturbances. A weakly nonlinear analysis reveals that small-amplitude disturbances are governed by perturbations of the Kuramoto-Sivashinsky equation. Hysteretic transitions are found between smaller- and larger-amplitude traveling wave states. In the strongly nonlinear regime, stable solitary traveling-wave solutions are found when only viscous effects are considered. A criterion for the flooding phenomenon, derived from this analysis, compares qualitatively with phenomenologically-based models, The stability of the solution to three-dimensional disturbances is then investigated. A strongly nonlinear system is derived that determines the evolution of the interface and the pressure field. A linear analysis of this equation provides conditions for three-dimensional instability. A weakly nonlinear analysis concludes that amplitudes of two-dimensional traveling waves are governed by a two-dimensional complex Ginzburg-Landau equation, with the anisotropic nature of the flow displayed in the diffusion coefficients. Stability of the two-dimensional monochromatic wave is examined, and possible three-dimensional patterns are discussed.

The experimental program is designed to confirm the range of validity of the theoretical analysis, and to determine its practical limits. An inclined-plate apparatus has been constructed consisting of a glass sheet 1 m long and 0.5 m wide, with adjustable inclination and radiant heating. Global views of the instantaneous wave structure are obtained by fluorescent illumination and digital imaging. Spatial development of the wave structure and the approach to film dryout are thus obtained.

Northwestern University

Dept of Eng Sci & App Math **$53,762**
Evanston, IL 60208 **01-C**
94-3

Microscopic Interfacial Phenomena During Flow in Porous Media
M. Miksis

The objective of this work is to study the effect of interfacial phenomena on the motion of a fluid in a porous material. In particular, we will be primarily concerned with the micromechanics of the fluid motion and its effect on the macroscopic flow. On the pore scale, we find a moving boundary problem for the fluid/fluid and the solid/fluid interfaces. During this project period, attention will be directed to understanding and modeling the dynamics of these interfaces. In particular, attention will focus on three specific topics: surfactant effects, motion of an interface into an unsaturated porous medium and breaking phenomena.

We have recently investigated how capillarity affects the dynamics of a foam on the microscopic scale using both analytical and numerical methods. Now we will consider how capillary and surfactants affect the stability and mobility of foam flow in a porous media. Also, we will continue a study on how capillary effects on the microscopic scale affect the motion of an immiscible contaminating liquid in an unsaturated porous material. Finally, we will investigate the dynamics of a fluid interface during breaking. Breaking phenomena occur during the dynamics of two-phase flows.

Northwestern University

Dept of Chemical Engineering **$111,000**
Evanston, IL 60208-3120 **06-C**
95-3

Fragmentation and Dispersion of Powdered Solids in Viscous Liquids
J. Ottino

The objective of this work is to produce basic understanding of dispersion and mixing processes. Work under this grant involves two main areas -- Mixing of Viscous Liquids and Mixing of Powders -- these two areas being bridged by work on mixing of concentrated suspensions and pastes. Work in mixing of liquids involving modelling studies in aggregation, fragmentation and dispersion in regular and chaotic flows. Several scenarios have been considered: growth with constant capture radius, compact volume-preserving clusters, and fractal aggregates. Numerical simulations show that the average cluster size of compact clusters grows algebraically, while the average cluster size of fractal clusters grows exponentially; companion mathematical arguments are used to describe the initial growth of average cluster size and polydispersity. It is found that when the system is well mixed and the capture radius independent of mass, the polydispersity is constant for long-times and the cluster size distribution is self-similar. Furthermore, our simulations indicate that the fractal nature of the clusters is dependent upon the mixing. The work in powder mixing involves theory and experiments in non-cohesive systems. Theoretical work involves a combination of geometrically based methods and particle dynamic calculations focusing primarily on slow mixing by tumbling .

Northwestern University

Dept of Eng Sci & App Math **$69,930**
Evanston, IL 60208 **06-C**
95-3

Stability and Dynamics of Spatio-Temporal Structures
H. Riecke

The objective of this project is to improve the understanding of systems exhibiting spatio-temporal chaos by investigating paradigmatic cases. The research encompasses fundamental and applied aspects. Fundamental issues to be addressed are the characterization and classification of states which are disordered in space and time. In applications, spatio-temporal chaos arises in systems ranging from fluid flow to lasers and coupled oscillators. For instance, in wide-area lasers and in laser arrays spatio-temporal chaos can reduce the quality of the laser beam and can even be detrimental to the device itself. Stabilization and control of the beam requires a detailed understanding of the origin and the nature of the chaotic state.

Using analytical and numerical techniques, a number of paradigmatic systems will be studied: parametrically driven waves of different types with special emphasis on the effect of parametric driving on unstable laser beams; the stability and chaotic dynamics of traveling waves as found in convection of liquid crystals; the role of heteroclinic cycles in chaos in rotating convection.

Presently, the dynamics of unstable parametrically driven waves is studied in 1 and 2 dimensions with focus on the unexpected behavior of defects in the wave pattern. Progress towards the characterization of the chaotic state is made. The stability of oblique combinations of traveling waves (traveling rectangles) is studied.

Their stability is found to be quite different than that of single waves. Consequences for experimental observations are investigated.

University Of Notre Dame

Dept of Chemical Engineering **$ 0**
Notre Dame, IN 46556 **01-C**
92-3

Wave Dynamics on Falling Films and Its Effects on Heat/Mass Transfer
H-C. Chang

The funded project is a study of how interfacial waves evolve on a thin falling film and how these waves enhance heat and mass transfer in many industrially important devices like solar energy collectors, desalination evaporators, pollutant scrubbers, distillation columns, etc. Understanding the various wave transitions, from small-amplitude sinusoidal waves with linear dynamics to large-amplitude solitary waves with highly nonlinear and chaotic dynamics, would also be important in the fields of hydrodynamics and dynamical systems.

During the 1995 fiscal year, we have completed the understanding of the wave dynamics. How small-amplitude inlet noise triggers sinusoidal waves, how these waves evolve into solitary waves and how the solitary waves interact to produce wave texture coarsening downstream have been deciphered and quantified. The texture coarsening phenomenon is most important in mass/heat transfer enhancement and the latter subject will be scrutinized next. Our results obtained in FY 1995 are published in the following articles and two additional articles to appear:

(1) Cheng, M. and Chang, H.-C., "Competition between subharmonic and sideband secondary instabilities of a falling film", Phys. Fluid, 7, 34-54 (1995).

(2) Chang, H.-C., Demekhin, E. A. and Kalaidin, E. N., "Interaction dynamics of solitary waves on a falling film", J. Fluid Mech., 294, 123-154 (1995).

Oak Ridge National Laboratory

Engineering Physics and Mathematics Division **$1,233,000**
Oak Ridge, TN 37831 **03-C**
94-3

Center for Engineering Systems Advanced Research (CESAR)
J. Barhen, E. Oblow, L. Parker, N.S.V. Rao

The primary mission of CESAR is to develop, through innovative research, a core of excellence in the areas of intelligent and nonlinear systems technology. By combining long-range future-oriented R&D efforts with near-term, sustained technology transfer to U.S. industry and graduate student education (on-site assignments from universities), CESAR strives to enhance U.S. scientific and technological capabilities in strategic areas vital to energy independence, national security, and international competitiveness.

Beginning in FY 1995, CESAR's efforts emphasize two new basic research areas: computational nonlinear science and cooperating autonomous systems. Research objectives are chosen to address the technology-base requirements for DOE missions that rely on the use of intelligent systems, or require the solution of "grand challenge" problems, where the development of novel algorithms for efficient utilization of high performance computing technology plays a critical role.

We characterize intelligent machines as systems that integrate perception, reasoning, and action to perform tasks under circumstances that either are insufficiently known in advance or dynamically change during task execution. Perception, reasoning, and action, as well as the integration of these modules into working systems, present challenging issues for inter-disciplinary basic research. We continue to investigate a wide variety of such issues in the areas of cooperating agents, mobility, manipulation, intelligent multi-sensory systems, empirical estimation and machine learning.

In the area of computational nonlinear science, CESAR pursues the development of fundamental methods, including neural networks, wavelets, stochastic approximation, global optimization, and parallel processing algorithms for solving complex scientific or engineering problems modeled by partial differential equations and/or involving remote sensing components.

Oak Ridge National Laboratory

Bioprocessing Research and Development Center **$185,000**
Oak Ridge, TN 37831 **06-A**
94-3

A Study of the Mechanisms of Liquid-Emulsion Bioreactor Systems
T. Scott

Biphasic liquid-liquid systems, in which a biocatalyst is in an aqueous phase and the substrate is primarily in an immiscible organic phase, represent an important class of nonaqueous bioprocessing options. The approach at ORNL is to use high-intensity pulsed electric fields to disperse aqueous droplets into immiscible organic phases in order to provide surface area for reaction. Results using horseradish peroxidase suggest that the reaction occurs predominantly at the liquid-liquid interface and that depending on the solvent used enzyme life is enhanced when using a solvent that interacts with the enzyme and provides alternative pathways to suicide deactivation by cofactors. Related studies have shown that the viability of whole cells can be enhanced or remain unaffected or that cells may be killed by manipulating delivery of pulsed electric fields in multiphase liquid systems. Further results in multiphase systems have shown that pulsed electric fields may be used to amplify Rayleigh instabilities in conducting liquid laminar jets. This technique allows for high-capacity production of uniform, millimeter-sized liquid drops from nozzles.

Pacific Northwest Laboratory

Battelle Memorial Institute **$50,000**
Richland, WA 99352 **01-B**
91-4

Radiative Transfer Through Arrays of Discrete Surfaces with Fixed Orientation
M. Drost

Radiative heat transfer in an array of discrete surfaces is an important and poorly understood class of radiative heat transfer problems. The objective of this study is to develop an understanding of the impact of array geometry, surface properties, and incident radiation characteristics on radiation heat transfer in the array. The results of the study will be used to establish criteria for the valid application of participating media models to arrays of fixed discrete surfaces.

The approach consists of using an innovative Monte Carlo model to evaluate radiation heat transfer in arrays of fixed discrete surfaces with a range of array configurations. The Monte Carlo model will be validated by comparison with experimental results being developed at Oregon State University. The Monte Carlo simulations will be used as a benchmark for comparisons with different analytical approaches that model the array as a participating medium.

FY 1994 accomplishments consist of: 1) Based on a comparison of the results of a Monte Carlo model for radiation impinging on an array of discrete surface and a Monte Carlo model of a homogeneous media we have demonstrated that arrays of fixed discrete surfaces cannot, in most cases, be modelled as a homogeneous medium. Most previous investigators have assumed that arrays of fixed discrete surfaces can be modeled as homogeneous media. 2) Completed a model and an evaluation of the impact of polarity on Monte Carlo modeling. The results show that polarity of incident radiation can significantly affect the interaction between the incident radiation and an array of fixed discrete surfaces. 3) The MCLITE cell-to-cell transport Monte Carlo code has been validated against experimental data. 4) One technical paper was published in FY 94 and three journal articles were submitted in to journals for publication in 1994 and two journal articles were accepted for publication.

University Of Pennsylvania

Dept of Mech Eng & App Mech **$15,999**
Philadelphia, PA 19104 **01-C**
95-1

Active Control of Convection
H. Bau

Active, feedback control strategies to alter flow patterns in a fluid layer heated from below and cooled from above (the Rayleigh-Benard problem) are being studied experimentally and theoretically Our objectives are to (i) stabilize the no-motion state of Rayleigh-Benard convection (delay to higher values of the Rayleigh number the transition from the no-motion to the motion state); and (ii) suppress (laminarize) oscillatory and/or chaotic convection. This work is an extension of our earlier research effort in which it was successfully demonstrated experimentally and theoretically that feedback control can be used in a thermal convection loop to tame chaos. The results of our current work may be important to among other things, materials processing and crystal growth applications in which it is desirable to eliminate convective currents or suppress oscillatory convection. Thus far, it has been theoretically demonstrated that, with the aid of a feedback controller, the transition from the no-motion to the motion state and the transition from time-independent to time-periodic convection (Hopf bifurcation) can be significantly delayed. An apparatus for experimental verification of our theoretical predictions is under construction. The apparatus consists of a cylindrical cavity heated from below and cooled from above. The heating surface consists of an array of individually controlled, thermal actuators micromachined on a silicon substrate. What is learned during this research may also be useful for devising control strategies for other non-linear flow phenomena. For instance, a colleague and I have shown theoretically that control strategies similar to the ones developed here can be used to delay or advance the loss of stability of planar Poiseuille flow.

Pennsylvania State University

Mechanical Engineering Dept **$94,981**
University Park, PA 16802 **01-B**
95-3

Research on Combustion-Driven HVOF Thermal Sprays
G. Settles

High-velocity oxy-fuel (HVOF) thermal sprays comprise a promising, relatively-new coating technology combining the fields of materials, manufacturing, combustion, and gas dynamics. HVOF uses combustion to melt and propel solid particles at high speeds onto surfaces to be coated. The goal of this research is to understand and improve the HVOF deposition of corrosion-resistant coatings, which are important in many energy-related industries. Both experiments and modeling are involved. The transfer of technology from rocket propulsion and supersonics is also an important element of this research. An early discovery was the very rapid mixing of the HVOF plume with the surrounding atmosphere.

Experiments on HVOF inert-gas shrouding are now being conducted to gain knowledge leading to a practical shroud for use with commercial HVOF equipment at usual standoff distances for the control and minimization of coating oxides. Further, nozzle design and operating-parameter variations are being exploited to achieve an optimum balance of kinetic and thermal energies of HVOF spray particles, thus to produce desirable coating properties such as high density, low porosity, and high corrosion resistance.

Results of the research are presented yearly at the National Thermal Spray Conference. One Ph.D. (C. Hackett) has been educated thus far under this project.

Princeton University

Dept of Mech & Aero Eng **$90,000**
Princeton, NJ 08544 **06-B**
93-3

Mechanisms and Enhancements of Flame Stabilization
C. Law

The program aims to gain fundamental understanding of the structure and stabilization mechanisms of premixed and nonpremixed flames through theoretical and experimental investigations. The following major projects were completed during the reporting period.

The scalar and dynamic structure of premixed and nonpremixed counterflow methane/air, propane/air and hydrogen/air flames has been experimentally investigated by using non-intrusive laser-based techniques and computationally simulated with detailed chemistry and transport descriptions. Results show that the scalar structure including the thickness of a freely-propagating or freely-standing premixed flame is insensitive to strain rate variations such that the flame cannot be extinguished by strain alone. On the other hand, the thickness of a nonpremixed flame scales inversely with the square root of the strain rate, implying that it can be extinguished by straining. Experimental studies on the dynamic structure demonstrate the need to allow for the effect of thermophoresis on the motion of the seeding particles when using laser Doppler velocimetry in measuring the flow velocity.

The dynamics and geometry of flame surfaces in nonuniform flows have been analytically and computations studied, including the phenomena of stretch, local extinction, cusp formation and broadening, and burning rate augmentation through flame wrinkling.

Princeton University

Dept of Civil Engineering **$101,185**
Princeton, NJ 08544 **06-A**
93-4

Transport Properties of Disordered Porous Media From The Microstructure
S. Torquato

This research program is concerned with the quantitative relationship between transport properties of a disordered heterogeneous medium that arise in various energy-related problems (e.g., thermal or electrical conductivity, trapping rate, and the fluid permeability) and its microstructure. In particular, we shall focus our attention on studying the effect of: porosity, spatial distribution of the phase elements, interfacial surface statistics, anisotropy, 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).

Both theoretical, computer-simulation, and experimental techniques have been employed to quantitatively characterize the microstructure and compute the transport properties of disordered media. Statistical-mechanical theory has been used to obtain n-point distribution functions and to study percolation phenomena in continuum random-media models. For example, the pore-size distribution, lineal path function, and the chord-length distribution function have been investigated and computed. This has led to accurate predictions of transport properties of realistic models of isotropic as well as anisotropic heterogeneous media. Cross property relations have been derived. Rigorous relations which link the fluid permeability to length scales obtainable from Nuclear Magnetic Resonance experiments and the effective electrical conductivity have been derived. Moreover, the effective conductivity has been related to the effective elastic moduli. Recently, 3-D images of a sandstone have been obtained using x-ray tomographic techniques and statistical corrleation funcations have been extracted from them.

Purdue University

School of Mechanical Engineering $103,571
West Lafayette, IN 47907 01-C
93-3

Effect of Forced and Natural Convection on Solidification of Binary Mixtures
F. Incropera

This study deals with the influence of combined convection mechanisms on the solidification of binary systems. A major accomplishment of research performed to date has been the development and numerical solution of a continuum model, which uses a single set of equations to predict transport phenomena in the liquid, "mushy" (two-phase), and solid regions of the mixture. Calculations have been performed for aqueous salt solutions and/or lead/tin alloys involving forced convection, thermo/solutal natural convection, and/or thermo/diffusocapillary convection. The calculations have revealed a wide variety of rich and robust flow conditions, including important physical features of the solidification process which have been observed experimentally but have heretofore eluded prediction. These features include double-diffusive layering in the melt, development of an irregular liquidus front, remelting of solid, development of flow channels in the mushy region, and the establishment of characteristic macrosegregation patterns (regions of significantly different composition) in the final solid. Theoretical and experimental studies have also revealed means by which macrosegregation may be actively suppressed, as, for example, through the application of a magnetic field or intermittent rotation of the mold.

Purdue University

School of Nuclear Engineering $125,000
West Lafayette, IN 47907 01-C
93-3

Interfacial Area and Interfacial Transfer in Two-Phase Flow
M. Ishii

The objective of the research program is to develop instrumentation methods, experimental data base and models for describing the interfacial structure and behaviors of two-phase flows. In terms of the flow structure, the transverse distributions of the local void fraction, interfacial area concentration, fluid particle size and their axial development from the entrance to the exit will be the primary focal point of the experimental research. For the purpose of understanding the dynamic behaviors, the interfacial velocity, fluid particle coalescence and disintegration are studied. The axial changes in the distribution of void fraction and interfacial area give the information on the particle coalescence and disintegration. These are used to quantify the flow regime transitions. The multi-sensor probes are used together with hot-film probes for these measurements. The focus of the modeling effort is to develop an interfacial area transport equation which incorporates the mechanistic models for coalescence and disintegration of fluid particles. This transport equation describes dynamical change of the interfacial structure and replaces the conventional model based on flow regime transition criteria.

Purdue University

School of Mechanical Engineering $119,000
West Lafayette, IN 47907 01-B
93-3

Near-Wall Measurement of Sublayer Dryout and Theoretical Modeling of CHF in Vertical Channels
I. Mudawar

This project targets the development of a theoretical model for critical heat flux (CHF) from long heated walls in vertical flow. Flow boiling pattern is examined with the aid of photomicrographic and high-speed video imaging techniques in order to determine the CHF trigger mechanism. Close-up studies of the wall region have revealed features common to most bulk flow conditions. At fluxes below CHF, the vapor coalesces into a wavy layer which permits wetting only in wetting fronts, portions of the liquid-vapor interface which contract the wall as a result of the interfacial waviness. These waves are generated from the heater's upstream region with wavelengths following predictions based upon the Kelvin-Helmholtz instability criterion. Critical heat flux occurs when the pressure force exerted upon the interface due to interfacial curvature, which preserves interfacial contact with the wall prior to CHF, is overcome by the momentum of vapor at the site of the first wetting front, causing the interface to lift away from the wall. Recent studies have shown this interfacial lift-off criterion facilitates accurate theoretical modeling of CHF in both straight and curved channels. Present studies are focused on extending this model to highly subcooled conditions.

Rensselaer Polytechnic Institute

Dept of Mechanical Engineering, $ 0
Aeronautical Eng & Mechanics 01-A
Troy, NY 12180-3590 91-3

Inelastic Deformation and Damage at High Temperature
E. Krempl

A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of engineering alloys under low-cycle fatigue conditions at elevated temperature. The purpose is to characterize the material behavior in mathematical expressions that are intended for use in inelastic analysis of high temperature components, forming analysis and life prediction.

Modeling of recovery of state and other softening effects observed in modified 9Cr - 1Mo Steel at 538°C within the context of the viscoplasticity theory based on overstress (VBO) has been completed. Analysis of finite deformation experiments revealed that presently existing plasticity and viscoplasticity theories are limited in reproducing the observed, texture based deformation induced anisotropy. Ideas have been developed on how to model the deformation induced anisotropy for elastic and inelastic behavior within the context of VBO.

A set of biaxial, low-cycle fatigue tests with stainless steel tubular specimens at 538°C has been completed. During cycling, changes in the voltage drop were monitored using a reversing direct current potential drop measuring system built at RPI. Data analysis included digital filtering and tensor spline smoothing. Curves of normalized, incremental potential drop vs. circumferential position showed peaks growing in time near cracks formed in the specimen. Theoretical electrostatic potential field models for a through-slit crack in a finite width plate and for a semi-elliptical crack in a semi-infinite medium were analyzed following the method adopted for the experimental data. Comparison of experimental and theoretical results yielded acceptable results in some but not all tests.

Rensselaer Polytechnic Institute

Center for Multiphase Research $126,920
Troy, NY 12180-3590 06-C
94-3

Development of Multidimensional Two-Fluid Modeling Capability
R. Lahey, Jr., D. Drew

The work on the development of a physically-based well-posed multidimensional two-fluid model is continuing. A four-field model has been proposed which is based on conservation equations for the evolution of continuous liquid, continuous vapor, dispersed liquid (droplets) and dispersed vapor (bubbles) fields.

The dispersed model is being extended to include the effects of change of shape on the interfacial forces, including virtual mass and lift. A new feature of the model is the interaction of the continuous vapor and the continuous liquid. Ensemble averaging concepts are being applied to different interface configurations in order to derive closure conditions for interfacial momentum transfer and Reynolds stress. A model for droplet deposition has been developed and work is continuing on entrainment, and coalescence and break-up models.

Conservation equations for the evolution of interfacial area density and curvature are being developed to model the evolution of the interface between the continuous liquid and the continuous vapor fields. The model is being derived for, and qualified against, Taylor bubbles and sinusoidal wavy interfaces.

Rensselaer Polytechnic Institute

Dept of Chemical Engineering **$89,900**
Troy, NY 12180-3590 **01-C**
93-4

Development and Use of Image Scanning Ellipsometer to Study the Dynamics of Heated Thin Liquid Films
P. Wayner, Jr., J. Plawsky

The physicochemical phenomena associated with fluid flow, change-of-phase heat transfer, and drying in ultra-thin (thickness less than 10^{-5} m) liquid films are being studied. In these thin liquid film systems, the interfacial, intermolecular, force field, which controls fluid flow and heat transfer, is a function of the film thickness profile. If the physical properties of the evaporating liquid film are known, the film thickness profile, measured experimentally, can be used to calculate the pressure field and the local evaporative heat transfer rate. To measure the film thickness profile, a novel ellipsometric technique (Image Scanning Ellipsometry, ISE) has been developed. ISE combines classical null ellipsometry with microscopic image processing, to determine simultaneously the thickness of the liquid film at all points on the substrate. Image processing helps identify the precise location on the surface of the liquid film which corresponds to the measured thickness. Thus a 2-D profile of the liquid film can be constructed. Currently, a second generation ISE employing enhanced resolution image acquisition and processing equipment is nearing completion. The augmented processing power of the second generation instrument is expected to help plot more precise thickness profiles. Presently, the study of the formation of thin solid films is being emphasized. Results obtained using the initial design were presented in Applied Optics, 33, pp 1223-1229, 1994, and, Physics Fluids, 6, pp 1963-1971, 1994.

Rice University

Dept of Civil Engineering **$88,000**
Houston, TX 77251 **01-A**
95-3

A Novel Nonlinear System Identification Approach with Applicability to Aging of Energy Production and Distribution Systems
P. Spanos

Nonlinear forces acting on energy systems such as large offshore structures, are studied from a perspective of system identification. The nonlinearities may be induced by ocean waves, and they may become significant in several situations. They are not necessarily assumed to be in the form of Morison's equation. Various wave forces are examined. The force function is decomposed either into a set of base functions, or it is expanded in terms of the wave and structural kinematics. The resulting nonlinear system is decomposed in a number of parallel non-memory, nonlinear systems, each followed by a finite memory subsystem. A Gram-Schmidt orthonormalization procedure is applied to decouple these subsystems; a frequency domain technique involving auto-spectra and cross-spectra is employed to identify the linear transfer function. In conjunction with this problem, an efficient algorithm for representing random processes by auto-regressive-moving-average digital algorithms is pursued for implementation into system identification problems. The analytical results are calibrated by Monte Carlo simulation studies.

University Of Rochester

Dept of Physics and Astronomy **$70,519**
Rochester, NY 14627 **06-C**
95-3

Flux Flow, Pinning, and Resistive Behavior in Superconducting Networks
S. Teitel

The fluctuation of vortices and vortex lines has been shown to be a major source of electrical resistance for superconducting networks when placed in magnetic fields. Systems of particular interest include the new high temperature type II superconductors, and periodic arrays of Josephson junctions. Numerical simulations are being carried out to identify and characterize the nature of the various vortex structures present in such systems, as a function of temperature and applied magnetic field, and to understand the nature of the phase transitions between them.

Particular attention has recently been given to studying the equilibrium fluctuation of vortex lines in models of bulk high temperature superconductors.

Simulations have shown that there can be two distinct phase transitions describing the superconducting ordering parallel versus perpendicular to the applied magnetic field. The loss of order in the perpendicular direction has been associated with a melting of the ground state vortex line lattice. The loss of order in the parallel direction has been associated with the onset of a vortex line tangle percolating throughout the entire system. New simulations, relaxing earlier approximations, are being carried out to clarify this issue. The effect of applied currents and random vortex pinning sites will be added in future work. The dynamic behavior of vortices in two dimensional Josephson arrays has also recently been investigated using a detailed finite size analysis to verify proposed scaling equations.

This research will greatly enhance the fundamental understanding of behavior in strongly fluctuating superconducting materials. The results will have impact in understanding the magnetic properties of the new high temperature superconductors, and in the design of Josephson junction arrays for use as microwave detectors and generators.

University Of Rochester

Dept of Physics and Astronomy **$95,030**
Rochester, NY 14627 **06-C**
93-3

Coherence Effects in Radiative Energy Transfer
E. Wolf

This project is directed towards clarifying the foundations of radiometry and the theory of radiative energy transfer and towards elucidation of the effects of the state of coherence of fluctuating sources of radiation both on the spatial and on the spectral distribution of energy throughout the radiated field. Several significant results have been obtained during the past year. They include derivation of radiometric expressions for the spectral density and the spectral flux vector in fields generated by planar, secondary, quasi-homogeneous sources. The results were applied to elucidate the differences between radiometric quantities associated with Lambertian and with Gaussian correlated sources. A radiometric model was also formulated for the propagation of coherence, which greatly simplifies the determination of the degree of coherence of a partially coherent field at arbitrary distances from the source. New conservation laws for free electromagnetic fields of arbitrary state of coherence were also formulated and some new results on spectral invariance and non-invariance were obtained. Properties of random pulses and of other random fields were also investigated and a relationship between the complex degree of coherence in the space-time domain and in the space-frequency domains were clarified.

The Rockefeller University

Department of Physics **$89,000**
1230 York Avenue **06-C**
New York, NY 10021 **95-4**

Some Basic Research Problems Related to Energy
E. Cohen

The present project is concerned with the following problems.

1. The Newtonian viscosity as well as the visco-elastic (i.e., frequency dependent viscous) behavior of monodisperse hard sphere colloidal suspensions have been computed theoretically for all concentrations in the fluid range. A very simple formula for the Newtonian viscosity is obtained, which agrees very well with experiment. A Pade'-approximant of this formula can facilitate its practical use. Similar expressions are obtained for the visco-elastic behavior, which are consistent with experiment.

2. The investigation of Lorentz lattice gas cellular automata is continued. In this gas a point particle moves on the bonds of a lattice fully or partially

occupied by randomly placed scatterers. For fully occupied lattices a mapping between the particle trajectories and percolation clusters (of a corresponding percolation problem) can be made, in that the former are the hulls of the latter. This implies a scaling behavior of the trajectories. However, also for partially occupied lattices, the same scaling behavior of the particle trajectories is observed, while no mapping to a percolation problem can be made. To what extent this behavior suggest a possible generalization of the notion of percolation clusters, is being investigated.

3. Dynamical weights using expanding Lyapunov exponents, rather than the usual probabilistic (Gibbsian) weights, can be employed to obtain the probability distribution of a many particle system in a nonequilibrium stationary state (e.g. a sheared fluid), which can be far from equilibrium. Successful applications of this new approach to obtain the properties of such a system have been made and are further pursued.

Sandia National Laboratories

Combustion Research Facility — $290,000
Thermofluids Division — 06-B
Livermore, CA 94550 — 93-3

Molecular Mixing and Front Propagation in Turbulence
A. Kerstein

The principal focus of this research program is modeling of turbulent flows in which mixing modifies flow energetics, as in buoyant stratified turbulence and turbulent combustion. Another objective is determination of the structure and mean rate of advance of fronts propagating through turbulence.

For the mixing problem, the modeling approach is an outgrowth of a method developed in work to date for application to turbulent mixing of dynamically passive scalars. That method involves the representation of turbulence by mappings applied to a one-dimensional scalar profile. The mapping sequence is a stochastic process reflecting pertinent features of the turbulent cascade. A generalization applicable to dynamically active scalars is obtained by introducing a velocity profile. Now, the mappings are determined by turbulence energetics based on velocity differences and the dynamically active scalars. The mappings modify the velocity and scalar profiles, yielding a self -contained evolution process.

This formulation will be applied to homogeneous turbulence, free shear flows, boundary layers, and buoyant stratified flows to evaluate its predictive capability, both as a turbulence model and as a model of mixing in turbulent flow. The model will be used to gain mechanistic understanding of turbulent mixing processes involving passive and active scalars.

Sandia National Laboratories

Combustion Research Facility — $25,000
Livermore, CA 94551-0969 — 06-B
90-3

Inverse Diffusion Flames in Supercritical Water-Fuel Mixtures
R. Steeper

This project investigates diffusion flames in high-density fuel-water-oxidizer mixtures. These hydrothermal flames are of practical concern in the development of supercritical water oxidation (SCWO) as a waste destruction process, but the basic scientific understanding of such flames is limited. Sandia has built a laboratory-scale, hydrothermal flame reactor with optical access suitable for imaging, laser velocimetry, and Raman spectroscopy diagnostics. Hydrothermal flames created in this facility at supercritical conditions exhibit characteristics distinct from atmospheric-pressure flames. The program provides an opportunity to extend the basic scientific understanding of diffusion flames by examining the effects of high density and an aqueous environment.

In experiments conducted to date, the range of initial concentrations and temperatures that lead to the spontaneous ignition of methane-water-oxygen and methanol-water-oxygen flames has been mapped. A related series of experiments has determined spectroscopically the concentration histories of methane, oxygen, carbon dioxide, and carbon monoxide in reacting mixtures at concentrations lower than the flame ignition conditions. The latter data have yielded global reaction rates for SCWO of methane as a function of fuel/oxidizer concentrations, temperature, and water density. The global rates are an important component of SCWO process design tools and serve as well to calibrate proposed elementary reaction mechanisms.

University Of Southern California

Dept of Mechanical and Aerospace Engineering **$127,359**
Los Angeles, CA 90089 **01-C**
93-3

A Combined Experimental and Numerical Investigation of Multiphase Porous Media Flow Dynamics

T. Maxworthy, E. Meiburg

Experimental and computational results have been derived for the displacement of a more viscous fluid by a less viscous one in a capillary tube and in a plane channel. For large values of the Peclet number Pe, a quasisteady state forms, in which a finger of the less viscous fluid proceeds down the center of the tube, leaving behind a film of the more viscous phase on the wall of the tube. The finger tip is well defined and displays a steep concentration front. For Atwood numbers near unity, the film thickness is approximately equal to the value found by Taylor and Cox for immiscible fluids and large capillary numbers. In this parameter regime, experiments and computations show excellent agreement. The film thickness decreases with At and depends only weakly on Pe. The quasisteady state persists for some time after the concentration boundary layers diffuse to the center of the tube at t~Pe. Eventually, the finger tip decays, and the state of Poiseuille flow and Taylor dispersion is approached asymptotically.

For intermediate and lower values of Pe, there are some discrepancies between the numerical simulations, which assume a constant diffusion coefficient, and the experiments, which show diffusion coefficients that can vary with concentration by almost two orders of magnitude. Further numerical simulations with variable diffusion coefficients have been carried out, and they lead to significantly improved agreement with the experiments. In particular, the variable diffusion coefficient simulations exhibit quasi-steady fingers at much lower values of Pe, in agreement with the experiments. These issues show that true dynamical similarity of different flows can only be obtained if the dimensionless diffusion coefficient-concentration relationships are identical.

For very small Pe and constant diffusion coefficients, the simulations show that a quasisteady state never forms. The finger tip soon becomes less well defined, and Taylor dispersion in Poiseuille flow is approached asymptotically. The unsteady evolution of this flow can be described based of some of Taylor's original arguments. In particular, our results show that the asymptotic state is approached after a time of O(Pe), when the dimensionless concentration front thickness has reached a length of O(Pe).

Stanford University

Dept of Mechanical Engineering **$75,805**
Stanford, CA 94305-3030 **01-A**
93-3

Structure and Modelling of the Three-Dimensional Boundary Layers on a Rotating Disk

J. Eaton

The objectives of this work are to develop improved understanding of the effect of mean flow three dimensionality on convective heat transfer through detailed experiments on turbulent transport mechanisms. Experiments have been conducted in two geometries, a large disk rotating in still air and a highly skewed wind-tunnel boundary layer. New miniaturized probes have been developed to measure the turbulent heat flux in the disk boundary layer. The probe uses a cross-wire anemometer with 2.5 micron diameter wires and a separate resistance thermometer. A technique has been developed for frequency compensation of resistance thermometers that allows their use to higher frequencies than previously possible. Temperature profiles have been recorded and heat flux measurements are underway. An extremely high resolution laser-Doppler anemometer system was developed which provides a 35 micron diameter by 60 micron long measurement volume in a laboratory scale wind tunnel. Reynolds stress measurements deep into the sublayer of a skewed boundary layer were acquired using this system. The results showed close alignment of the shear stress and strain rate vectors near the wall. This contradicts previous assumptions that were made in the absence of any reliable data. The remainder of the grant period will be used to complete the heat flux measurements and interpret them in terms of available models.

Stanford University

Dept of Mechanical Engineering **$135,000**
Stanford, CA 94305-3030 **01-A**
95-3

Stress and Stability Analysis of Surface Morphology of Elastic and Piezoelectric Materials
H. Gao, D. Barnett

During the past year the part of our project on stress-induced surface instability has entered a new phase with the completion of the Ph.D. degree by C-h Chiu who, in his thesis, presented a comprehensive review of the state-of-the art understanding of the formation of cusp-cracks by stress-controlled diffusion in solids. Simultaneously an experimental study of surface evolution in heteroepitaxial thin films has been initiated. These experiments include Atomic Force and Electron Microscope studies of annealed Si-xGe-1-x/Si (100) films with varying composition and thickness. Subcritical film thicknesses have been considered to separate dislocation nucleation processes from cusp formation processes. The goal of these experiments is to check existing theoretical predictions and further investigate the effect of surface instability on dislocation nucleation. The condition for stability/instability of surfaces in piezoelectric materials of arbitrary elastic anisotropy has been determined and this work has been accepted for publication in Proceedings of the Royal Society (London). It has been shown that piezoelectric coupling may either stabilize or destabilize a flat surface, so that, in theory, piezoelectric coupling could be utilized to control diffusive initiation of surface defects. Experiments will be needed to verify the current theoretical model. Future work will be directed toward corroborating theory with experiments and thereby identifying the need to develop better theoretical models for defect generation during stress-driven surface diffusion.

An investigation of Stoneley wave modes confined to the interface between two piezo-crystals (crystals exhibiting elastic-electric-magnetic coupling) either bonded together or separated by an air gap or a superconducting layer has been completed. The new degrees of freedom introduced by electric and magnetic coupling lead to localized waves which can be significant in device design decisions. A second study of dislocations in purely elastic joined anisotropic crystals has revealed the existence of configurations in which dislocations on either side of the bi-crystalline interface will be attracted to the interface. Such a situation (which we call mutual attraction) is not possible when anisotropy is neglected and may play a significant role in the trapping of dislocations at internal interfaces. A new study has focussed attention on determining the equilibrium arrangements of large numbers of dislocations in solids subjected to inhomogeneous plastic deformation. The most interesting arrangements to initially examine are those at equilibrium under zero applied stress, which corresponds to dislocation configurations existing after unloading. We have developed an expression for the interaction energy between two dislocations in an anisotropic solid as a necessary ingredient for comparing a conjugate gradient method with more direct "zero-force" methods in numerical determinations of the equilibrium set. The effect of different constraints (pinned dislocations, glide constraints, stacking faults) on the determination of the equilibrium arrays will also be investigated during the coming year.

Stanford University

Edward L. Ginzton Laboratory **$145,000**
Stanford, CA 94305-3030 **03-B**
93-3

Optical Techniques for Superconductor and Thin Film Characteriztion
G. Kino

Photothermal measurements are used to study diffusion and fluctuation phenomena in high temperature superconductors. Phase delay measurements yield the thermal diffusion, and measurement of the reflectivity of the probe beam yields a quantity closely related to the specific heat. Measurements have been made in individual crystallites 20-50 micrometers across. Below T_c, the peak value of the diffusion constant within a grain is much higher than in other measurements, and it is in good agreement with theory. Above T_c, a very large temperature drop is observed across grain boundaries in YBCO, indicating phonon reflection at the grain boundary. We also observe a diffusion constant within an individual crystallite of twice the normally measured bulk value. Diffusion measurements below T_c in YBCO show good agreement with experiments on measurements of normal electron density as a function of temperature. The amplitude of the probing signal yields a quantity closely related to the specific heat. In YBCO and $Bi_2Sr_2CaCu_2O_8$, measurements show a large peak at T_c and a rapid fall-off from the peak value, in excellent agreement with the second-order phase transition theory for fluctuations near the critical point. Similar measurements of charge density waves in $NbSe_2$ give good agreement with two-dimensional phase transition theory.

Stanford University

Mechanical Engineering Dept — $206,887
Stanford, CA 94305 — 03-B
92-4

Advanced Diagnostics for Plasma Chemistry
C. Kruger, T. Owano

This research is concerned with optical diagnostics for plasma chemistry and plasma processing, with an emphasis on methods that allow for departures from local thermodynamic equilibrium (such as finite chemical reaction rates, nonequilibrium electron densities and temperatures, and radiation loss effects). Studies in an induction plasma facility show significant nonequilibrium within a downstream reactor, and suggest the possibility of erroneous results when using conventional diagnostics that assume local thermodynamic equilibrium.

Advanced laser-based methods are being developed for measurement of plasma parameters including species concentration and temperature. The primary technique under study is the application of Degenerate Four-Wave Mixing (DFWM) to atmospheric pressure plasma environments in order to assess the importance of nonequilibrium effects under conditions of interest to plasma chemistry. Cavity Ring-Down Spectroscopy (CRDS) is also under investigation as another non-intrusive diagnostic.

To investigate the application of advanced laser diagnostics to a realistic and promising form of plasma processing, experiments have been undertaken on the reacting plasma boundary layer of a substrate placed in a diamond producing plasma flow. Linear growth rates up to 50 µm/hour have been demonstrated in these environments, and are over an order of magnitude greater than those characteristic of low-pressure systems.

Recent experiments using DFWM to probe CH and C_2 within the reacting plasma have demonstrated the ability to provide sensitive (ppm level) detection with submillimeter spatial resolution in the measurement of vibrational temperatures, rotational temperatures, and species concentrations.

Stanford University

Dept of Chemistry — $140,892
Stanford, CA 94305 — 06-C
95-4

Topics in a Thermodynamic and Stochastic Theory of Nonlinear Processes Far from Equilibrium
J. Ross

Research focuses on the thermodynamic and stochastic theory of hydrodynamic processes, such as combinations of chemical reactions, diffusion, thermal conduction, and viscous flow. Such theories have been formulated for each of the individual processes, both linear and nonlinear. Progress has been made on combinations of these processes for a simplified form of the Navier-Stokes equations, the so-called Lorenz equations. The theory leads to a formulation of an excess work expressed in terms of thermodynamic functions, which provides a Liapunov function, necessary and sufficient conditions of stability, criteria of relative stability, and relations to fluctuations. An extensive model of chemo-taxis has been formulated with detailed accounts of extensive experiments. The model accounts quantitatively for exact adaptation, initial response, and chemical thermodynamic motion.

Stanford University

Dept of Chemistry — $ 0
Stanford, CA 94305 — 03-A
92-4

Degenerate Four-Wave Mixing as a Diagnostic of Plasma Chemistry
R. Zare

This research pioneers a new absorption technique, called cavity ring-down spectroscopy (CRDS), as a means to provide highly sensitive measurements of absolute concentrations of species in plasmas and other luminous media. A CRDS apparatus has ben designed to measure the trace radical species generated in a hot-filament reactor for diamond film deposition and the *in situ* measurement of methyl radicals in the reactor has been successfully carried out under various growth conditions. A radial profile of the CH_3 absolute concentration near the hot filament has been determined by CRDS using the Abel inversion of the spatial profile of CH_3 absorbance.

The research includes the determination of the conditions under which CRDS can be used for quantitative measurement of absolute concentrations of molecular species. The conditions useful for CRDS diagnostics have been estimated by analyzing how the absorption loss measured by CRDS varies with the sample absorbance for various ratios of the laser pulse linewidth to the absorption linewidth. A wide range of conditions was found in which the sample absorbance (and, consequently, absolute number densities) can be recovered from the CRDS spectrum.

University Of Texas At Austin

Ctr for Studies in Statistical Mech and Complex Systems **$ 0**
Austin, TX 78712 **06-C**
94-3

The Behavior of Matter Under Non-Equilibrium Conditions: Fundamental Aspects and Applications
I. Prigogine, T. Petrosky

Both classical and quantum mechanics can be described either on the individual level (in terms of trajectories or wavefunctions) or on the statistical level using the Liouville operator. It has traditionally been assumed that these two descriptions are equivalent; however, this is no longer true for unstable dynamical systems such as associated to deterministic chaos or to Poincare nonintegrable systems with continuous spectrum (so-called Large Poincare systems, LPS). Practically all systems studied in statistical mechanics belong to this class. To describe these systems, one has to introduce delocalized ensembles that lie outside the Hilbert space. Once the Liouvillian is extended outside the Hilbert space, complex, irreducible spectral representations are obtained. Complex means that the time symmetry is broken as the result of complex eigenvalues of the extended Liouvillian. Irreducible means that these representations cannot be implemented by trajectories or wavefunctions; therefore, laws of nature take a new form, as they have to be formulated on the statistical level. They express "possibilities" and no longer "certitudes." For integrable systems, our theory recovers the usual formulations of classical or quantum mechanics. Hence, this extension of dynamics permits us to unify the two concepts of nature, based one on dynamical time-reversible laws and the other on the evolutionary view associated to entropy. It also leads to a unified formulation of quantum theory, avoiding conventional dual structure based on Schrodinger's equation on the one hand, and on the "collapse" of the wave function on the other. There is striking parallelism between classical and quantum theory. In general, for LPS, both a "collapse" of trajectories and of wave function exist; this theory predicts a number of new phenomena for LPS, as well as chaotic maps, which have no correspondence in the traditional description by trajectories or wavefunctions. It also goes beyond phenomenological kinetic theory. Numerical simulations verify our predictions.

University Of Texas At Austin

Dept of Physics **$358,475**
Austin, TX 78712 **06-C**
93-5

Complex Spatiotemporal Patterns in Nonequilibrium Systems
H. Swinney

The formation of time-dependent spatial pattems is being studied in chemical and physical systems maintained far from equilibrium. The goal is to understand what features of behavior are common in diverse pattem-forming systems. What kinds of patterns arise spontaneously as the stress is increased on an initially homogeneous system? What kinds of transitions are permitted between different patterns? What is the role of symmetries in the boundary conditions and the equations of motion? These issues are being addressed in laboratory experiments and numerical simulations on reaction-diffusion systems, vertically vibrated granular media, a convecting fluid, and chemical electrodeposition. The experiments on chemical patterns have yielded new examples of spatial and spatiotemporal symmetry breaking transitions. An experiment on a vertically vibrated shallow layer has revealed transitions to striped, square, hexagonal, and disordered patterns; a model with a single dissipative layer yields insight into this transition sequence. Comparison of the laboratory observations with simple models provides general insights into the formation of spatiotemporal patterns.

Tufts University

Dept of Mechanical Engineering **$ 0**
Medford, MA 02155 **01-A**
92-3

Effective Elastic Properties and Constitutive Equations for Brittle Solids Under Compression
M. Kachanov

Work done under the contract concentrated on the following problems.

1. Investigations of the mechanics of defects in an anisotropic environment. This investigation, rather broad in scope, includes the following topics:

(a) The impact of matrix anisotropy on the mechanics of crack interactions. It was found, in particular, that the matrix anisotropy enhances the interactions if loading is applied along the stiffer direction of the matrix, and that it weakens the interactions if loading is applied along the softer direction of the matrix. This effect is strongly asymmetric; the enhancement effect is much more pronounced than the weakening effect.

(b) The mechanics of crack-microcrack interactions in an anisotropic environment. A variety of representative geometries was examined and the impact of different elastic constants of the matrix was analyzed.

(c) The effective elastic properties of anisotropic matrices with arbitrarily oriented and interacting cracks.

2. Work on the effective elastic properties of materials with holes of arbitrary shapes was started. Preliminary results have been obtained for holes of elliptical shapes.

University of Washington

Dept of Mechanical Engineering **$69,975**
Seattle, WA 98195 **01-A**
94-3

3-D Experimental Fracture Analysis at High Temperatures
A. Kobayashi

The objective of this three year research project is to assess experimentally, the validity of T* integral and its applicability to quasi-static and dynamic ductile fracture analyses. During this first year, the surface displacement fields, which was determined by moire interferometry, of A606 HSLA steel single-edge notched (SEN) specimens with small stable crack growth of $\Delta a = 2$ mm, were used to compute directly the T* integral for various domain integrals surrounding the crack tip. J was also obtained for several outer contours. The smallest inner contour, G_e, of the domain integral was limited to 6 mm due to the dense moire fringes in the immediate vicinity of the crack tip. Elastic-plastic finite element analysis (FEA), which was conducted at Georgia Institute of Technology under a parallel DOE grant, of the same SEN specimen for a larger crack extension of $\Delta a = 8.5$ mm showed that J was highly path dependent but T* remained path independent with stable crack growth. Also the experimentally determined T* were in good agreement with the corresponding values obtained by FEA. The computed and measured CTOA were in excellent agreement and remained a constant 15° after dropping from an initial high of 30°. possibly due to crack tip blunting.

A series of experiments using a moire grating of 10 lines/mm on central notched (CN) specimens will be undertaken shortly. It is hoped that this coarser grating on a specimen configuration with larger constraint will provide moire interferometry fringes closer to the crack tip, i.e. about 1 mm, and also for a longer crack extension of about Da = 6 mm.

Washington University

Department of Systems Science and Mathematics **$77,434**
Saint Louis, MO 63130 **03-A**
93-3

Visually Guided Control Systems: A New Generation of System Analysis and Design
B. Ghosh

The main objective of the proposed project is to study dynamical systems that are controlled with the aid of CCD cameras. Such a class of systems, called "Visually Guided Control Systems," have the capability to use visual information to provide sutomatic feedback control to a dynamically moving system. An example of such a system is a robotic manipulator with a set of cameras attached operating in an unstructured environment.

We propose a new dynamical systems approach to vision and to vision-based control system design problems that is new both to the area of Computer Vision and to the area of Control System Design. The propsed project, based on a new theory of "Prospective Systems," promises to enrich the field of Computer Vision especially in the area of Motion and Shape estimation of dynamically moving objects in an environment. It also introduces new challenges in System Theory, wherein feedback control is generated by visual sensors based on the theory of nonlinear regulation and nonlinear optimal control. The proposed project undoubtedly broadens the technology and conceptual base while introducing some new promising approaches to visually-guided control systems.

Washington State University

Dept of Mech & Matls Engineering **$74,420**
Pullman, WA 99164-2920 **01-B**
94-3

Coupled Particle Dispersion by Three-Dimensional Vortex Structures
T. Troutt

The primary objective of this research program is to obtain understand concerning the role of three-dimensional vortex structures in the dispersion of particles and droplets in free shear flows. This research study builds on previous studies which focused on the nature of particle dispersion in large scale quasi two-dimensional vortex structures which are a dominant component of free shear flows. Although three dimensional vortex structures can be quite complex in nature time scaling quantities such as Stokes number can still be expected to be important for understanding the experimental and numerical results concerning the particle dispersion process.

This research program is employing time dependent experimental and numerical techniques to provide information concerning the particulate dispersion process produced by three- dimensional vortex structures. The free shear flows investigated include modified plane mixing layers, and modified plane wakes. The modifications to these flows involve slight perturbations to the initiation boundary conditions such that three-dimensional vortex structures are rapidly generated by the experimental and numerical flow fields. The particulate dispersion process associated with these three-dimensional flow structures will be intensively studied to obtain understanding which may lead to improving the design and performance of many energy conversion systems.

University Of Wisconsin

Mechanical Engineering Dept **$122,000**
Milwaukee, WI 53201 **01-C**
93-3

Interfacial Area and Interfacial Transfer in Two-Phase Flow Systems
G. Kojasoy

The objectives of the proposed research program are to develop instrumentation methods, an experimental data base, and an analysis leading to predictive models for describing the interfacial structure and behaviors of horizontal two-phase flows. In terms of the flow structure, the transverse distributions of the local void fraction, interfacial area concentration, fluid particle size and their axial development from the entrance to the exit will be the primary focal point of the research. For the purpose of understanding the dynamic behaviors, the interfacial velocity, wave characteristics, fluid particle coalescence and disintegration will be studied. The axial changes in the distribution of void fraction and interfacial area give the information on the particle coalescence and disintegration. These will be characterized by the collision frequency and interfacial energy and turbulence in the liquid.

A special emphasis will be placed on the further improvement of the multi-sensor resistivity probe method which has been successfully developed and cross-calibrated against other global techniques. The multi-sensor probes will be used together with hot-film probes for the liquid turbulence measurements. These new measurements will give sufficient information to evaluate the local relative velocity and momentum interaction between phases. Final focus of the modeling effort is to develop interfacial area transport equation which incorporates the mechanistic models for coalescence and disintegration of fluid particles. This transport equation describes dynamical change of the interfacial structure and replaces the conventional model based on flow regime transition criteria.

The proposed research program will provide: a) a new scientific instrumentation method for studying detailed interfacial characteristics of two-phase flow, b) benchmark data for the local interfacial area concentration, void fraction distribution, interfacial wave structure, relative velocity and wave propagation velocity for horizontal two-phase flow systems, c) mechanistic models for fluid particle coalescence and disintegration, and d) interfacial area transport equation.

University Of Wisconsin

Dept of Chemical Engineering **$119,340**
Madison, WI 53706 **03-A**
92-3

New Process Modeling, Design, and Control Strategies for Energy Efficiency, High Product Quality, and Improved Productivity in the Process Industries
W. 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, (1) the resilient design and control of chemical reactors, and (2) the operation of complex processing systems, will be investigated. Major emphasis in part (1) will be on two important classes of chemical reactors: polymerization processes and packed bed reactors. In part (2), 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.

Budget Number Index

Mechanical Sciences:

01-A Solid Mechanics: macroscopic aspects of elastic and plastic deformations, and crack propagation
01-B Heat Transfer
01-C Fluid Mechanics
01-D Tribology

Control Systems and Instrumentation:

03-A Control systems, large scale systems
03-B Instrumentation for hostile environment, and NDE
03-C Intelligent systems

Engineering Data and Analysis:

06-A Thermophysical properties and processes
06-B Combustion
06-C Non-linear dynamics and engineering analysis

Budget Number | **Page Number**

01-A

01-B

01-C

01-C (cont'd)

01-D

03-A

03-B

03-C

06-A

06-B

06-C

06-C (cont'd)

Principal Investigators

Principal Investigators (cont'd - pg. 2)

Principal Investigators (cont'd - pg. 3)

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