DOE/ER-0635

Summaries of FY 1994 Engineering Research

December 1994

U.S. Department of Energy

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

DOE/ER-0635

Summaries of FY 1994 Engineering Research

December 1994

U.S. Department of Energy

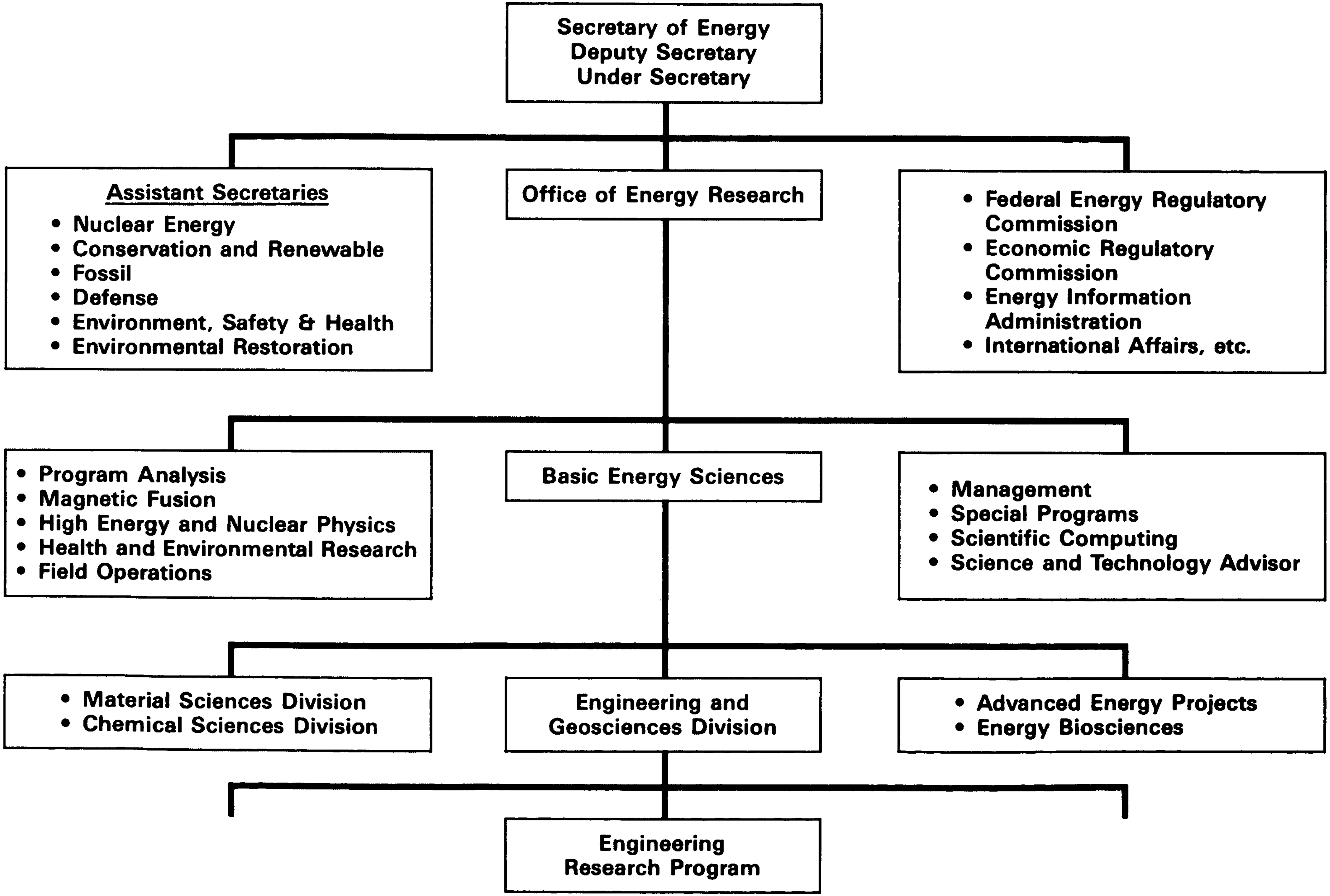
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences
Washington, DC 20585

Foreword

This report documents the BES Engineering Research Program for fiscal year 1994; 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.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1994. 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 1994.

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 1994 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., 91-3). 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.

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 three distinct areas: Plasma Process Engineering, Automated Welding, and Fracture Mechanics. Collateral, high quality research efforts at other institutions 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 will be published by CRC Publishing Company.

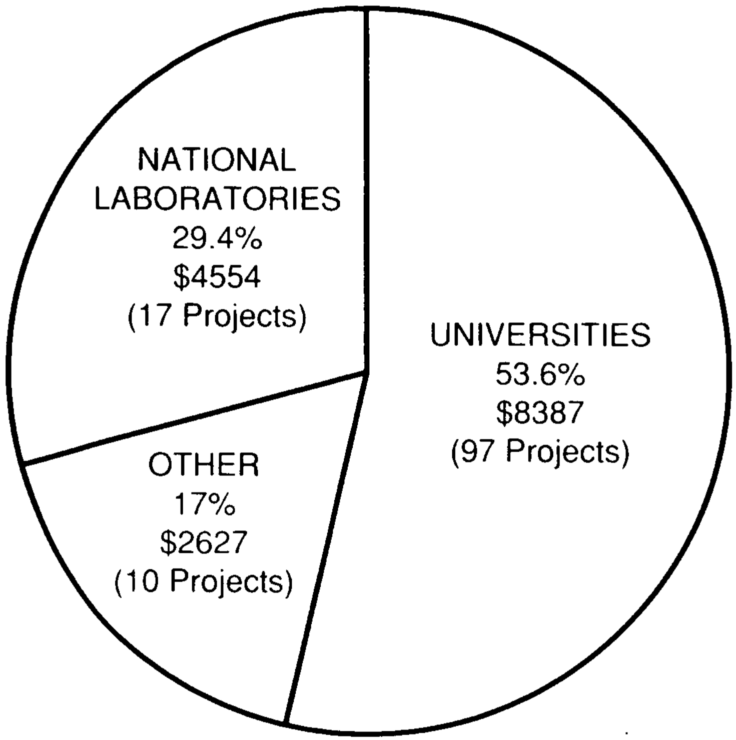
Two additional workshops were held during 1988. The first dealt with possible research opportunities in the field of novel devices using the new high temperature superconductors. The second addressed research needs for bioprocessing of fuels and energy related wastes. Reports of both workshops have been published. Additional funds have 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 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 1994 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 '94 BUDGET ($000's) BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '94 BUDGET BY TECHNICAL AREAS

	($000's)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	4531	29.3	53
SYSTEMS SCIENCES	4918	31.7	23
ENGINEERING ANALYSIS	6038	39.0	48

Table of Contents

Table of Contents (continued)

University Of Alabama

Dept of Mathematics **$105,576**
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. Secondary instabilities of nonlinear waves in liquid films can be studied with methods developed for periodic flows.

Some of the results are as follows: A rigorous iterative method was found for the problems of periodic-flow stability. The possibility of negative isotropic eddy viscosity was demonstrated, resolving a rather long-outstanding question.

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 for large-amplitude regimes of a wavy flow was obtained. Its numerical simulations yielded an excellent agreement with experiments. In addition, it revealed interacting coherent structures with rich and unique dynamics.

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 **$134,000**
Argonne, IL 60439 **01-A**
94-3

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 Comell University.

Fluidelastic instability of loosely supported tubes, vibrating in a tube support plate-inactive mode, 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 series of tube arrays with a motion-limiting stop configuration are being 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, are also being investigated. 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 will be measured using the existing water channel with an emphasis on the nonlinear behavior. Specific topics to be addressed include interaction between flow field and oscillating structures, mathematical models and instability mechanisms, and intelligent control of fluid/structure systems. Experimental efforts are focused on characterizing and controlling chaos and validating analytical models.

Argonne National Laboratory

Reactor Engineering Division **$137,000**
Argonne, IL 60439 **01-A**
94-3

Bounds on Dynamic Plastic Deformation
C. Youngdahl

Analytical studies are being performed to develop methods for approximating or bounding the dynamic plastic deformation of structures. In many applications where the load is transmitted to the structure through a fluid, details of the load history and spatial distribution significantly affect the final plastic deformation. The objective of the program is to devise mode approximation methods and load correlation parameters which can be used to predict the final deformed shape and characterize the effects of the load without resorting to detailed numerical analyses. These approximation methods have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events.

Mode approximation methods and load correlation parameters are hypothesized and their usefulness in predicting final plastic deformation is determined. Optimum modes have been determined for the dynamic plastic deformation of simply-supported, clamped, and cantilevered beams made of a rigid, strain hardening material. The modes are expressed in terms of amplitude and plastic zone size functions which are determined for arbitrary loadings by the numerical solution of sets of coupled, non-linear differential equations. Computational times are of the order of seconds rather than the hours usually spent on dynamic plasticity problems. Qualitative features of the response are analogous to perfectly plastic solutions. The concentrated hinges in perfectly plastic problems become variable curvature regions, and hinge bands become uniform curvature regions, with time dependent curvature and region size.

University of Arizona

Aerospace & Mechanical Eng **$137,500**
Tucson, AZ 85721 **01-B**
93-3

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

We are concerned with the coupling between the fluid mechanics and the convective heat transfer occurring in a pulsed, and therefore actively controlled, wall jet flowing over an isothermal surface having a different temperature than the fluid. Calculations have shown that the heat transfer from a surface depends on the mean velocity distribution and on the resultant stability characteristics of the flow. However, both quantities are strongly affected by the temperature distribution near the surface. We used the linear stability theory in order to predict the passage frequency and the scale of the most unstable eddies responsible for most of the convected heat. The calculations reveal that heating enhances the rate at which the velocity profile spreads while cooling hinders it, heating also de stabilizes the flow while cooling stabilizes it. In general there are two, highly coupled instability modes in a wall-jet. One is dominant near the surface. It contains higher prevailing frequencies and is affected by viscosity while the other prevails in the outer flow close to the outer inflection point of the mean velocity profile, and is essentially in an inviscid mode. Heat transfer influences the viscous mode much more strongly than the inviscid mode. The main influence of temperature gradient on the stability stems from its modification of the unstable region without affecting the critical Reynolds number in any significant manner. Resonant interactions between the modes are feasible and are being considered.

Arizona State University

Mechanical & Aerospace Eng **$50,441**
Tempe, AZ 85287 **01-A**
92-4

Contiuum Damage Mechanics - Critical States
D. Krajcinovic

The objective of this research project is to determine the critical states of brittle solids weakened by a large number of microcracks. This objective is pursued using the methods of applied mechanics, thermodynamics and statistical physics. The thermodynamic studies of the loose bundle parallel bar model were used to define possible expressions for damage variables and conjugate forces. The failure criterion was derived in the form of a generalized Griffith's criterion. A distinction was made between the force controlled processes, in which the failure is a second order phase transition, and the displacement controlled processes. Universal character of scaling laws and percolation thresholds are guaranteed only in the first case.

Another task was to determine the scaling law for the effective stiffness of a two-dimensional continuum weakened by a random distribution of rectilinear slits. The solution was derived (within the node-link-blob model) for the elastic and elasto-plastic materials using the exact stress fields at the crack tip. A rather careful search of the literature indicates this to be the first solution for the elasto-plastic solid.

Battelle Memorial Institute

Engineering Mechanics Dept **$93,125**
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 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 exercized, 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.

University Of California/B

Dept of Chemical Engineering **$77,663**
Berkeley, CA 94720 **06-A**
94-4

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

The approach taken in this research, joint with ORNL effort, is to study the liquid-liquid interphase transport and reaction phenomena important to biphasic bioreactors by using a model enzyme system. The system is comprised of an aqueous-phase horseradish peroxidase (HRP) that is activated by hydrogen peroxide to carry out the oxidation of *p*-cresol that is contained in an immiscible organic phase, toluene. Tasks in the research program involve study of aqueous-phase reaction kinetics, interaction of HRP with the liquid-liquid interface, and modelling of a continuous liquid-liquid contactor that uses high-intensity electric fields to create micron-sized aqueous drops for the enzymatic reaction. Work on this project began in June 1994. Detailed kinetics studies indicate that the presence of toluene in the aqueous phase appears to stabilize the HRP due to an interaction with the active sight of the enzyme. Tests with the electrostatic bioreactor indicate that the electric field does not deactivate the enzyme and that significant portions of *p*-cresol can be removed from the organic phase by a continuous biphasic system. Future work will involve the use of a precision two-phase flow device that will allow investigation of interfacial effects on the enzymatic reaction.

University Of California/B

Dept of Electrical Engineering $184,369
& Computer Sciences 06-C
Berkeley, CA 94720 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 $62,565
Berkeley, CA 94720 01-B
92-3

Thermal Radiation and Conduction in Microscale Structures
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. Recent research has resulted in a microscopically based model of the radiation absorption and thermal transport for metals in both bulk and thin-film form. This model was used to design novel thin-film laser mirrors with improved damage thresholds. Experiments were performed to confirm the model predictions. Currently short pulse, high power laser-material interactions are being investigated for other important engineering materials, including amorphous metals, liquids, and semiconductors.

Fractal theory has been applied to examine short-time-scale energy transport in amorphous materials. On short time scales there exists anomalous diffusion, since carriers travel a distance comparable to the disorder length in the material, and are thus inhibited by this disorder. The impact of anomalous diffusion in short-time-scale applications such as high-frequency, short-pulse laser-material interactions has been shown. Experiments are being planned to demonstrate the importance of this phenomenon in these applications.

University Of California/LA

Mech, Aero & Nuclear Eng Dept $90,816
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 research seeks to develop the methods necessary to model turbulent transport processes for both single- and two-phase flows in highly porous media. Emphasis is placed upon the development and theoretical study of integro-differential transport equations, with special attention given to morphological factors. Research has focused upon (1) single-phase, two-temperature turbulent transport in porous media, and (2) turbulent transport of momentum and energy in a channel with regular rough walls.

Dependence of the Darcy and quadratic terms upon the convective and diffusion terms' assumed version has been shown, as has the connection between the diffusion and drag resistance terms in the flow equations. The closure models allowed associations between bulk process experimental correlations and the current simulation representations to be exploited in the numerical procedures. Subsequent numerical investigations displayed the equations' sensitivity to the assumed morphology and the transport coefficients' descriptive ability for high solid/fluid phase thermal diffusivity ratios and high void fractions.

Two-dimensional capillary patterns and spherical structures were analyzed using an irregular four-coordinate lattice with varying bond orientations and random lattice patterns. Prescription of the medium's statistical structure allowed transformation of the integro-differential transport equations into differential equations with probability density functions governing the spatially varying stochastic coefficients and source terms. Combination of space averaging and random morphology process theories resulted in realistic explanation of processes in porous media.

University Of California/LA

Mech, Aero & Nuclear Eng Dept **$109,464**
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 **$76,630**
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 **$193,457**
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 relaed to the behavior of fuel droplets in well defined but nonuniform flows. Our current research concems fuel sprays in opposed and impinging streams which result in flat flames. A test rig which permits a wide variety of investigations including nonpremixed, premixed and partially premixed systems in such streams has been put into operation. By installing an appropriate grid in one or both ducts, sprays in turbulent streams can be studied. 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. Our theoretical research on the phenomena of droplet oscillation in opposed streams is continuning with the aim of describing the observed bimodality of the probability density distributions of the axial velocity. Experiments on a turbulent spray impinging on a wall without combustion in order to determine the relative velocity between gas and droplets of various sizes has been completed and submitted for publication. Additional experiments in this flow with a flame present have been completed; data analysis and interpretation are underway. An interesting phenomena involving the behaviour of droplets impinging on a hot wall has been observed; at suitably high wall temperatures the droplets rebound rather than wet the wall. This presentation of the results of these experiments and complementary theory was made at an AIAA symposium.

University Of California/SD

Dept of Chemistry, 0340 **$198,897**
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 formulated a mesoscopic approach from which we obtain the reaction-diffusion equations that are customarily postulated phenomenologically. This approach places a number of theories on a common fundamental basis.

We continue to develop approaches to the response of nonlinear systems to colored noise. Our newest methods rely on the analysis of the trajectories that lead a system to improbable events such as passage over a high barrier. Some or our most novel results deal with systems driven by quasimonochromatic noise.

We have investigated the mean exit time of a free inertial random process from a region in space.

The acceleration alternatively takes the values +-a for random periods of time governed by a common distribution psi (t). The most striking feature of this system is the discontinuity of the mean exit time as a function of the initial conditions.

We have begun to formulate a microscopic quantum mechanical model for charge transfer in condensed media. We are able to calculate the reorganization energy as a function of elementary parameters for some simple model situations.

University Of California/SD

Inst for Nonlinear Science, R-002 **$95,982**
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; 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 **$219,120**
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. This is a model system for studying nonequilibrium, traveling-wave phenomena that can provide important insights into the behavior of doubly 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. Examples of practical interest include solar ponds and atmospheric and oceanographic flows.

Earlier experiments in an annular geometry, which is essentially a one-dimensional system with periodic boundary conditions, have led to a basic understanding of the dynamics of uniform and confined states of traveling waves. Our current experiments involve a large-aspect-ratio two-dimensional convection cell. Among the issues to be addressed in this system are two-dimensional wavelength instabilities and the dynamics of defects and grain boundaries which occur in this two dimensional system. In smaller systems, patterns are typically locked in by the cell geometry. In our experiment, which has an aspect ratio of 50:1, the characteristic domain size of patterns is smaller than the cell, so that we can observe the dynamics of defects which do not interact strongly with the cell boundaries. This leads to a greater variety of phenomena and should facilitate comparison with theoretical predictions. We have also observed interesting transients such as single and multi-armed spirals and these patterns will be compared with the predictions of model equations.

University Of California/SB

Dept of Physics **$264,290**
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 **$106,300**
Santa Barbara, CA 93106 **01-C**
91-3

Turbulence Structure and Transport Processes in Wavy Liquid Streams
S. Banerjee

The objective of this work is to investigate the interaction between waves and turbulence structures, and attendant effects on transport of heat and mass, between gas and liquid streams. The work is motivated by the remarkable variety of industrial and environmental problems in which transport processes across fluid-fluid interfaces between turbulent streams play a major role, e.g., condensers, gas-liquid contactors, evaporators, aeration of rivers, and air-sea interactions.

The research consists of experiments in a horizontal open water channel with either co- or counter-current air flow. Waves are generated on the water stream by a wave-maker such that the wave amplitude and length can be varied. The wind shear stress can also be varied by changing the air flow rate.

The facility is equipped with a variety of velocity measurement and flow visualization instruments. Most notably, a 3-dimensional laser Doppler anemometry (LDA) system with specially-built optics, allowing a spot size of about 50 microns, which gives reliable measurements at distances of less than 100 microns from the interface or the wall. Ultrasonic and wire gauges follow the interface position in conjunction with the LDA. The flow visualization techniques are based on electrolytically generated microbubble tracers with two high speed imagers (Ektapro 1000), capable of 1000 full frame images per second and up to 6000 split frames per second.

To date, experiments with 2-dimensional wavy flows, with and without air flow, have been performed and the facility is currently being set up for work with 3-dimensional waves. Results indicate that waves strongly affect the turbulence structures, and that wind shear strongly enhances these effects, possibly to a point where structures which have not been previously observed are formed.

California Institute Of Technology

Chemical Engineering 210-41 **$ 0**
Pasadena, CA 91125 **03-A**
91-3

Modeling for Process Control
M. Morari

One key difficulty which stands in the way of application of many advanced control techniques in the chemical process industries is the need for a model to describe the dynamic behavior of the process to be controlled. The objective of this research program is the development of a range of new modeling techniques, in particular development of techniques for building physics-based, low-order, nonlinear models with physically meaningful parameters, specifically for the purpose of (robust) linear and nonlinear controller design; and development of methods for the identification of linear black box models and the associated uncertainty description suitable for robust control system design.

This research program emphasizes methods that are both mathematically lucid and industrially effective. The developed techniques build on results from nonlinear time series analysis, classical statistics and chemometrics. The False Nearest Neighbor methods was shown to be useful for determining the order of a nonlinear ARMAX model, and the local linear structure of the input/output map was explored via PLS (Partial Least Squares or Projection to Local Structures). By putting PLS in the general context of "significance regression" it was possible to deal effectively with collinear data sets involving errors on inputs ("Measurement Error Model") and outliers ("Robust Regression").

Carnegie Mellon University

Chemical Eng Dept **$150,350**
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 seeks to develop a novel integrated approach for process synthesis and design that addresses recent environmental challenges. Specifically, these synthesis approaches will provide rigorous trade-offs among raw material and energy costs, capital investment and waste treatment. To address the problem of waste minimization at the design stage, major issues 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 with environmental concerns, also dealing with process uncertainty.

The first topic will be handled through a quantitative targeting approach for reactor networks, which deals with the generation of waste byproducts at the source. Here, by developing superior reactor designs we see the greatest impact for process improvement, both from an environmental and an economic perspective. The second topic considers the recovery and reuse of small amounts of byproducts, which can have a significant impact on waste treatment costs. Performing this task will require more exacting designs for systems with nonideal mixtures, such as the generation of flexible solvent recovery systems. Finally the third task combines structural optimization and problem decomposition at various modeling levels in order to screen alternatives before complex simulation models are applied. This approach will also include the development of flexible designs that need to be tolerant to uncertainties related to process conditions and waste treatment requirements.

Carnegie Mellon University

Dept of Elec & Comp Eng **$101,747**
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 **$324,000**
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. This is accomplished by applying the concepts of Hamiltonian optics, phase space conservation, thermodynamic arguments, and radiative transfer methods. In the early nonimaging designs the mighty edifice of aberration theory was dismantled and replaced by a single key idea. According to this, maximum concentration is achieved by ensuring that rays collected at the extreme angle for which the concentrator is designed are redirected, after at most one reflection, to form a caustic on the absorber. This principle proved sufficiently elastic to accommodate most boundary conditions in two dimensions (i.e., linear geometry). Ideal solutions in three dimensions have also been formulated. Our work on vector flux has led to a reexamination of the foundations of radiometry with emphasis on observable effects. Our theoretical work on nonimaging designs has led to demonstration of ultra-high flux from sunlight which exceeds previous results by substantial factors. Design algorithms have been developed for reflectors that are functionals of the desired irradiance. This permits new solutions which solve classical problems in illumination from extended sources. The theoretical understanding of radiance has been extended to remove unphysical negative values and more closely aproximate classical radiometry.

Clarkson University

Dept of Chemical Engineering **$62,500**
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 that are being developed in the Bioprocessing Research and Development Center at Oak Ridge National Laboratory. The Bioreactors are liquid fluidized beds with gel beads that contain immobilized bacteria. In contrast with most fluidized bed reactors, the bead Reynolds numbers are order unity. Mathematical models developed for particle Reynolds numbers that are large compared to unity do not correctly predict the hydrodynamics of the Bioreactors.

Some reactions, such as the production of ethanol, liberate gas bubbles. Such bubbles can lead to undesirable vertical mixing within the reactor. A goal of the project is to understand the interaction between the gas bubbles and the beads. In the production of lactic acid, negatively buoyant adsorber beads can remove the product and increase efficiency. A second goal of the project is to develop a better understanding the hydrodynamic interaction between adsorber beads and gel beads.

The experimental portion of the project involves measurements of bubble rise velocities, observations of gel beads in bubble wakes, and measurements of adsorber bead settling velocities. The mathematical portion of the project involves a combination of asymptotic and numerical work. The usefulness of effective medium concepts for the fluidized beds will be assessed by comparison with experimental measurements.

University Of Connecticut

Dept of Mechanical Engineering **$50,440**
Storrs, CT 06268 **01-A**
92-3

Engineering Science Software

315 Log Road **$51,332**
Smithfield, RI 02917 **01-A**
92-3

A Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding
E. Jordan, K. Walker

In the first goal of this program polycrystalline viscoplastic behavior was successfully predicted from single crystal properties and experimentally verified.

The current goal is to predict the degree of heterogeneity and verify the predictions experimentally. A self-consistent (SC) and a Green's function (GF) model have been developed where the effects of neighboring grains are respectively represented in an average sense and explicitly. Histograms of grain stresses have been constructed for both models. The SC model yields non-symmetric narrow histograms compared to the symmetric wider histograms from the GF model and the experiments. Both models underestimate the heterogeneity at yielding. Inaccurate constitutive modeling now being corrected may be responsible for the underestimation.

Unique neutron diffraction experiments were done at Argonne Labs. Limited results were produced because large detector height (being corrected) compromised resolution. Moire' strain experiments were done at INEL in which the strain of the entire surface was recorded. Histograms of grain strains have been constructed. The orientations of all the grains in the samples were obtained using a SEM technique available at TSL, Inc.

Conclusions: The SC model is not very successful while the GF model was successful in predicting heterogeneity. The remaining challenge is to obtain better predictions for the inelastic case.

Cornell University

Mechanical & Aerospace Eng **$78,230**
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 **$106,001**
Ithaca, NY 14853 **01-C**
94-3

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

Our experimental studies of passive scalar mixing and transport in turbulent flows are motivated by a desire to understand better the fluid mechanics of chemical reactions, combustion and environmental pollution, all of which occur in turbulent background flows. Towards this end we are studying passive thermal dispersion in a jet, and mixing of temperature fluctuations in homogeneous grid generated turbulence.

A question of particular importance is in what way does the scalar mixing depend on the Reynolds number of the flow, i. e. on the relative intensity of the inertial forces to the dampening viscous forces. For example as the Reynolds number increases, do the nature of the small scale scalar statistics change? Do they become more isotropic, reflecting less the overall nature of the flow or do they have inherent anisotropy? We note that chemical reactions occur at the smallest length scales.

Our preliminary investigations have shown that even in isotropic grid turbulence, the scalar is anisotropic both in the second and third moments, and this is independent of the Reynolds number, over the limited range that can be achieved in grid turbulence (up to Re = 130). We are presently developing new techniques using active grids to study turbulence up to a Reynolds number of Re = 400-500. This will enable us to probe many basic aspects of turbulence and mixing at Reynolds numbers much greater than can be achieved in the largest computers, both now and in the foreseeable future.

Dartmouth College

Thayer School of Engineering — **$122,726**
Hanover, NH 03755 — **01-C**
92-3

Two-Phase Potential Flow
G. Wallis

The objective is to develop theorems for two-phase potential flow analogous to those existing for single phase flow.

Using one function, the "exertia," which describes the external fluid inertia due to relative motion of suspended particles, it has been possible to derive the average stress tensor, kinetic energy, overall momentum flux tensor and equations of motion for uniform systems of particles and the effective Bemoulli equation for the fluid flowing through a stationary array of particles.

Recent developments include more general descriptions of the mean particle stresses and the averaged Bemoulli equation for the fluid when both phases have a general motion. Links have also been established between this approach and Guerst's variational methods including the derivation of equations of motion for each phase, it being possible for the dispersed phase to be compressible. The equations of motion for each phase have also been expressed in terms of a mutual "interfacial pressure tensor" that is related to both the average stress in the dispersed phase and the net force on the continuous phase. This interfacial pressure tensor is also closely coupled to the Reynolds stresses in the continuous phase.

The exertia and added-mass coefficients have been computed for various geometrical arrangements of spheres, both in an infinite array and in tubes. Comparable measurements were made by measuring the natural frequency of oscillation of such arrays in water. Future experiments are planned in which more properties, such as pressure fluctuations, are measured.

Theoretical and experimental efforts are underway to obtain realistic interphase forces including the effects of viscosity and drag. Computations show that the effects of pressure gradient, added mass, phase change and drag do not add linearly except at low Reynolds numbers. This has implications for the transient response and stability of fluidized beds.

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

The research objectives of this project are to characterize flows through porous media, including convection-driven and pressure driven flows. Flows in porous media have significant technical applications ranging from the recovery of oil and gas, to geothermal energy, and to the effectiveness of insulation. The current specific objective is to characterize experimentally the onset of convection and chaos in fluid-saturated porous layers heated from below. The experiments exploit the novel technology, Magnetic Resonance Imaging (MRI) and also include high-resolution thermal measurements of temperature and heat transport. Convection experiments have been carried out on a variety of convection layer geometries and with different kinds of media. The results have been the first velocity images of the pattems in porous convection. Steady roll patterns are seen where predicted, but a number of features, including the roll wave length, and the time-dependent states are at variance with theory. Current experiments are directed toward understanding convection of binary mixtures in porous media.

Georgia Institute of Technology

Computational Mechanics Center $60,718
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 Temperature
S. Atluri

The objective of this research project is to assess experimentally, the validity of T^* integral and its applicability to quasi-static and dynamic ductile fracture analyses. The surface displacement fields, which will be determined by moire interferometry, of two- and three-dimension fracture specimens will be used to compare directly the T^* integral for various contours surrounding the crack tip. Single-edge notched and surface flawed, A533B steel specimens will be subjected to subcritical crack growth to fracture at room temperature through 650°C. The theoretical and numerical T^* will be compared with its experimentally-determined counterparts generated at the University of Washington under a parallel DOE research project. A simple procedure for determining experimentally, T^* integral of a fracture specimen will be explored.

The large ductility of A533B steel requires the development of a moire interferometry protocol for low density moire grating. We have just succeeded in using a 40 lines/mm diffraction grating on a 2024-T3 aluminum fracture specimen. This procedure, combined with a suitable chemical etching technique, should provide the necessary protocol for high temperature moire interferometry analysis. The loading fixture and oven with optical access is already in place.

Idaho National Engineering Lab

Applied Physics & Optics Unit $485,000
Idaho Falls, ID 83415 06-A
93-3

Fundamentals of Thermal Plasma Processing
J. Fincke

The objective is to fundamentally improve the thermal plasma spray process. Modifications to conventional torches are being examined along with a new generation of high-velocity, high-power (HVHP) plasma torches. These devices offer larger plasma volumes at higher velocities while minimizing power fluctuations due to anode spot movement. Higher particle velocities decrease residence time, an important factor in minimizing oxidation reactions, and generally produce a higher density and more consistent coating. The chemical dynamics of high velocity flow fields is also expected to lead to large departures from equilibrium, significantly increasing ion and dissociated species populations. Since surface recombination increases plasma/particle heat transfer rates, this can be a significant advantage, yielding fully molten particles with less residence time.

Based on the development of a fundamental understanding of the fluid mechanics and thermodynamics of high temperature, nonequilibrium, flowing systems, process improvements are sought. These improvements are: controlled/minimized entrainment of external atmospheres, increased velocities, increased plasma volume, and minimized jet fluctuations. 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, a better understood process will allow improvements in coating adhesion and strength while other characteristics, such as porosity, can be specified and controlled. This ability leads to the possibility of engineering unique new coatings with graded composition, porosity, etc. and enhanced properties for advanced applications.

Idaho National Engineering Lab

Materials Science Division **$249,000**
Idaho Falls, ID 83415 **03-A**
93-3

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

The aim of this project is to show that the productivity of mixed-culture bioprocesses can be greatly increased by applying intelligent systems to the process control problem. Controllers will be developed 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. The culture complexity will then 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 **$233,000**
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 flow and temperature distributions in the plasma plume and of the interactions between the plasma and injected particles. The present research is directed toward the development of a comprehensive computational model capable of providing such information. The model is embodied in the LAVA computer code for two- or three-dimensional transient or steady state thermal plasma simulations. The plasma is represented as a multicomponent ideal gas governed by the compressible Navier-Stokes equations. Multicomponent diffusion is calculated by a self-consistent effective binary diffusion approximation, including a new formulation for ambipolar diffusion of charged species. Subgrid-scale and k-epsilon turbulence models are included. Dissociation, ionization, and plasma chemistry are treated by means of general explicit and implicit chemistry routines for treating slow, fast, and equilibrium chemical reactions. Discrete particles interacting with the plasma are represented by a stochastic particle model which allows for distributions in particle sizes, shapes, temperatures, etc. Departures from local thermodynamic equilibrium are accounted for by a two-temperature model which permits the electron and heavy-particle temperatures to differ. Nonequilibrium populations of excited levels are treated as separate chemical species, with collisional and radiative transitions between levels modeled as kinetic chemical rate processes. Applications of the model to date include realistic simulations of plasma jets and plasma spraying, and detailed studies of excitation nonequilibrium in plasma jets.

Idaho National Engineering Lab

Materials Technology Group **$430,000**
Idaho Falls, ID 83415-2218 **01-A**
93-3

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

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 a structural component. Structural components are being tested and analyzed in collaboration (in-kind contributions) with Lehigh University (funded by the U.S. Coast Guard).

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.

This project is a collaborative program with MIT.

Idaho National Engineering Lab

Materials Technology Group **$530,000**
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 materials processing. 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 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 nine years. Research is being conducted on an extension of the fundamental process physics, application of knowledge-based dynamic controllers and signal/image processors, and development of noncontact sensing techniques. Tasks include analytical modeling of nonlinear aspects of molten metal droplet formation and transfer; developing fundamental ties between knowledge-based controllers (including artificial neural networks and fuzzy logic based connectionist systems) and classical and advanced control methods; and advanced optical and ultrasonic sensing, including the propagation and interaction of ultrasound in metallic solid and liquid media. Results are being transferred to industrial partners through a related ER-LTT 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 **$200,000**
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 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. Recent accomplishments include measurements on silver sheathed tapes and correlation with a new analytic approach to predicting the critical state in geometries utilizing non-uniform applied fields, as are found in most NDE applications. A new integral equation approach has been found that can be solved iteratively to determine the flux-front profile in geometries with azimuthal symmetry. This approach has been applied to configurations involving samples in a uniform field and tapes in the field of an external coil.

University Of Illinois

Coordinated Science Laboratory **$127,000**
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. The main theme is goal-oriented model simplification for control and decision making. 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 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 jump process, and the additive uncertainties in the system dynamics and measurement channels are deterministic and norm-bounded. Another topic of study at the present is robust identification for dynamic systems with (linear) parametric uncertainty, when the system is perturbed by an additional unknown disturbance input. Here the goal is to develop identification schemes that exhibit fast convergence to true parameter values, in spite of the additive unknown disturbances that impact the system dynamics.

University Of Illinois

Dept of Chemical Engineering **$232,000**
Urbana, IL 61801 **01-C**
92-3

Gas-Liquid Flow in Pipelines
T. Hanratty

The long range goal of this research is to describe the macroscopic behavior of gas-liquid flow systems 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 controlled by droplet-droplet interactions, rather than gas-phase turbulence.

Considerable attention has been given to the role of secondary flow in the gas in opposing asymmetries in the liquid film in horizontal annular flows. Gas phase velocity measurements have revealed that strong secondary flows exist at large drop concentrations which actually aid film drainage.

The spatial variation of local rates of oxygen absorption in a wavy stratified flow vary by an order of magnitude - thus suggesting that interfacial turbulence is not controlling.

University Of Illinois

Dept of Mechanical and Industrial Engineering **$66,751**
01-A
Urbana, IL 61801 **93-3**

Stress Induced Phase Transformations
H. Sehitoglu

Understanding stress-induced phase transformations is of paramount importance in modeling the behavior of engineering materials and components. From the material behavior standpoint, transformations generate internal (micro) stresses which alter the constitutive behavior, and from the component standpoint transformation strains may result in dimensional changes and alteration of macroscopic stress fields. The transformation strains are strong functions of the applied stress state since favorably oriented planes transform in the course of loading. Several unique experiments under combined shear stress - hydrostatic pressure are conducted on steels, containing retained austenite, in order to measure and study anisotropic transformation strains. Test specimens are subjected to externally applied pressures in excess of 700 MPa. The compressive hydrostatic stresses would increase the extrinsic ductility of the material, and hence permit high magnitudes of the stress-induced and strain-induced transformations. Based on these experiments, the work will set the background to evaluate the theories proposed, and lay the foundation for new ones with particular emphasis on complex changes in transformation strains. The basic information obtained from the work will generate improved understanding of transformation under contact loadings and transformation toughening phenomenon in metallic and non-metallic materials.

University Of Illinois At Chicago

Energy Resources Center **$ 0**
Chicago, IL 60680 **01-B**
93-1

Heat Transfer to Viscoelastic Fluids
J. Hartnett

For the past decade the fluid mechanical and heat transfer behavior of non-Newtonian fluids, particularly viscoelastic fluids have been studied. These investigations have concentrated on aqueous solutions of high molecular weight polymers in laminar and turbulent flow through circular and non-circular channels. As a result of these studies the pressure drop and heat transfer behavior of most viscoelastic aqueous polymer solutions under turbulent flow conditions can be predicted with reasonable accuracy provided that the basic rheological properties of the fluid are known. It is noteworthy that under turbulent flow conditions nearly all of the viscoelastic solutions show dramatic reductions in the dimensionless friction factor and heat transfer relative to Newtonian values.

In the case of laminar flow in non-circular ducts the presence of normal stress differences results in secondary flows which do not occur in Newtonian fluids. These secondary flows have little effect in the pressure drop but are sufficient to increase the heat transfer by a factor of 2 to 3 relative to the performance predicted for a purely viscous power law fluid. Analytical studies based on the relatively simple Reiner-Rivlin model appear to capture the basic behavior of the flow and heat transfer.

Johns Hopkins University

Mechanical Engineering Dept **$78,568**
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.

In a separate study, the viscous flow around two slip-free spheres (a useful approximation for gas bubbles) has been studied computationally to evaluate the methods currently used to model viscous effects at large Reynolds numbers.

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 **$67,024**
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 information. Both for practicable computation and for physical understanding, it is necessary to extract essential information in compact form. This project explores novel approaches to economical and meaningful description of turbulence. During the past year, important progress has been made in understanding of the turbulent mixing of passive contaminants. For the 1st time in a turbulence problem, the spatial intermittency of the mixed contaminant has been proved from the equations of motion. Simple scaling laws for small scales of the contaminant have been predicted analytically and are being tested by numerical simulations of unprecedented resolution.

Lawrence Berkeley Laboratory

Dept of Physics **$128,000**
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).

The Lovelace Institutes

Institute for Basic and Applied **$51,928**
Medical Research **03-B**
Albuquerque, NM 87108 **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 **$64,875**
College Park, MD 20742 **01-D**
93-3

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

The development of efficient machine tools which produce parts of high quality and require minimum intervention presupposes the capacity to identify precursors of unstable, chatter, states and integrate such identifiers into control system algorithms. The large amplitude oscillations associated with chatter have a detrimental effect on surface finish, dimensional accuracy, tool wear and may lead to tool fracture.

To address the fundamental problems of the identification and control of chatter, this research effort is directed towards i) creating a large data base of carefully controlled measurements of tool motions for critical ranges of cutting parameters; ii) the identification of numerical algorithms capable of detecting the precursors of chatter occurring in the data base found in (i); iii) the optimization and application of such numerical algorithms to the control of the cutting process.

A data base has been formed of sixty cutting experiments comprising $4 \bullet 10^7$ separate measurements for differing values of depth of cut, turning speed and feed rate. All of the data have been subjected to power spectral, bispectral and bicoherence analysis. The methods of false nearest neighbors, mutual information, singular value decomposition, TOR, time-frequency and attractor dimension estimation have been applied to selected data sets.

This analysis has led to an explanation of the relationship between the cutting parameters and the structure of the power spectra, established properties of the characteristic envelope and associated polyspectral behavior with two well known paths to chatter. Precursors of chatter have been suggested through polyspectral data and model analysis.

University Of Maryland

Dept of Electrical Engineering **$87,300**
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 **$84,272**
Baltimore, MD 21228 **03-B**
92-3

Pulse Propagation in Inhomogeneous Optical Waveguides

C. Menyuk

We are presently working on three separate projects. First, we are studying randomly varying birefringence in optical fibers and its impact on both soliton and NRX communication systems. To do that, we are carrying out Monte Carlo simulations of large numbers of fibers. We have already demonstrated that optimal results are obtained for both types of communication system if one operates with the smallest possible amount of randomly varying birefringence and if the scale length for the birefringence fluctuations are on the same scale as the beat length. Second, we are studying passively modelocked fiber laser systems such as the figure-8 laser. These lasers are of potential importance as sources in future, very high bit rate communication and switching systems. Our approach, which is based on using computers to carry out a stability analysis of the laser's operation, is new in this field. Previous studies relied on either complete, *ab initio* simulations or on purely analytical theories. Our approach allows us to accurately explore large regions of parameter space and optimize the laser's operating conditions. Third, we are studying solid state devices. In the last year, we have been exploring the advantages of using Richardson extrapolation to stabilize several well-known schemes, and we have found that it is very beneficial. In the future, we intend to apply this approach to the study of quasi-phase-matched second harmonic generation which is of importance in obtaining sources which can write higher capacity compact disks.

University Of Maryland

Dept of Mechanical Engineering & Inst for Systems Research College Park, MD 20742 — **$75,660** **03-C** **92-3**

The Mechanics of Redundantly Driven Robotic Systems
L. Tsai

The objective of this research is to increase fundamental knowledge regarding the design of robotic mechanisms. The current goals are to develop general methodologies for the synthesis of tendon-driven manipulators and for backlash and friction compensation in geared servomechanisms.

A general theory for the synthesis of tendon-driven manipulators with isotropic transmission characteristics has been derived. It is shown that an n-Degree-of-Freedom manipulator will possess the isotropic transmission characteristics, if it is constructed with n+1 or 2n tendons, and if its structural and Jacobian matrices satisfy two isotropic conditions. It is also shown that manipulators designed with the isotropic transmission characteristics do have more a uniform force distribution among their tendons.

Backlash and friction problems can be compensated by accurate modeling and adaptive non-linear control strategies. As a first step toward this goal, a dynamic model which accounts for both backlash and frictional effects has been developed. The equations of motion consist of a system of differential equations with discontinuous right-hand sides. The existence and uniqueness of a solution for such a system of differential equations and various control strategies for compensating tracking errors caused by backlash and friction are currently being investigated.

University Of Maryland

Dept of Mechanical Engineering College Park, MD 20742 — **$128,039** **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 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 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) had 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.

University Of Massachusetts-Lowell

Dept of Electrical Engineering Lowell, MA 01854 — **$ 0** **01-C** **91-3**

Stability and Heat Transfer in Time-Modulated Flows
C. Thompson

This project represents an analytical/experimental effort directed toward understanding the processes generating boundary layer instabilities in time-modulated flows. In particular, temporal modulations of the basic state by harmonic and free-stream vorticity is considered. The objectives of this work are to: develop an analytical model for development of instability, describe the growth and propagation of unstable disturbances occurring in the viscous region, investigate influence of steady-flow, examine global and local instability resulting from modulation of the free-stream near points of mean-flow stagnation, and categorize results suggestive of possible mechanisms for heat transfer.

It has been shown that for increasing modulation amplitude of a two dimensional oscillatory flow, with zero mean, undergoes a subcritical transition from the 2-D Stokes boundary layer to a state where streamwise oriented vortices appear. The temporal growth of these streamwise vortices is the result of the imbalance between the centrifugal force and the pressure. The most unstable axial position along the channel corresponds to the location where the convex wall curvature is maximum. For a fixed value of the wall curvature, instability ensues above the critical value of the Taylor number. The instability is found to follow a period doubling path to temporal chaos. The threshold Taylor number for temporally chaotic oscillations to ensue is found to be sensitive to the wavenumber content of the initial disturbance field. In fact the presence of subharmonics is found to decrease this threshold value. The instability is also found to exhibit a spatial bifurcation, where a subharmonic of the linearly least stable wavenumber becomes dominant as the Taylor number is increased. However, a correlation between the onset of temporal chaos and spatial bifurcations is not apparent.

The instability resulting from the interaction of a stagnation point steady flow and a transverse oscillatory flow in the presence of boundary curvature is also considered. The instability is again in the form of streamwise oriented vortices. The velocity field characterizing this instability is found to exhibit temporally chaotic oscillations. The presence of a steady flow, however, has a stabilizing influence on the vortical disturbances.

Massachusetts Institute Of Technology

The Energy Laboratory **$128,622**
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. A lumped-parameter mathematical model of a metal gas arc welding electrode has been developed with the goals of it being suitable for real-time control system design, yielding additional physical understanding, and being readily usable by other researchers and engineers.

A novel gas metal arc welding experiment has been designed and constructed which modifies the fundamental way metal is transferred in the new welding process. 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 is being used to explore new modes of metal transfer, to test algorithms for detecting and controlling these modes, and to verify the electrode model.

The electrode model captures the instantaneous dynamics of drop detachment. Hitherto, dynamic electrode melting models have only sought to capture the average of the process. The model developed in this project captures the instantaneous geometric evolution of drops melting on the end of an axially moving electrode. This model has potential uses for droplet systems other than welding.

Massachusetts Institute Of Technology

The Energy Laboratory **$110,000**
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 two 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 process development. A prototype process development methodology has been proposed that exploits modeling technology to explore alternatives and ensure feasibility of the design. These ideas are currently being implemented in the form of a computer-aided design tool.

Massachusetts Institute Of Technology

The Energy Laboratory **$165,870**
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.

To address these problems, we have begun a series of investigations that include both a general exploration of the distributed-parameter heat transfer control problem presented by the general welding process, and the development of a novel welding process (called "stream welding") that seeks to allow better and more independent control of heat and mass transfer.

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. An eigenfunction (i.e., model approximation) approach has been shown to be superior to finite difference or element methods in terms of model efficiency and controller implementation. A simple 2-D experiment has been undertaken using a scanned-arc source to create a controlled distribution in a rectangular solid.

The stream welding process has been developed to the point where a well-defined stream of steel at 2000°C can be produced, and preliminary welds have been made without any preheat. Penetration is quite small, as was predicted by simple heat transfer models, and methods of preheating are now being investigated.

Massachusetts Institute Of Technology

National Magnet Laboratory **$91,800**
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 frictionally 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 **$205,640**
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. Applications include pressurized thermal shock. 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 are being incorporated into line-spring finite elements for surface-cracked plates and shells, providing simple and extraordinarily accurate analysis and simulation of these important engineering flaws.

Massachusetts Institute Of Technology

The Energy Laboratory **$48,741**
Cambridge, MA 02139 **01-A**
94-3

Basic Engineering Sciences of Solids Comminution
C. Peterson, F. McClintock

Comminution to fine particle size ($<20\mu$)is an energy-intensive process, as for deep cleaning of coal or beneficiation of oil shale or other minerals. Retention of fine material within the charge of coarse material to be fractured is a major source of energy loss. This study has investigated both the mechanics of particle fracture within deep beds of particles subjected to external compressive loads and size-dependent particle transport via fluidization as a means of separating fine materials from coarse as they are formed.

The particle fracture studies included both analytical and experimental work; for simplicity, the work was limited largely to spherical particles. Analytical and experimental work with single particles (glass spheres) indicates that spherical particles of brittle material fracture in response to the application of a size-dependent maximum load, independent of the multitude of lesser loads that would be experienced within a compressively-loaded particle bed.

Analytical models were developed to display the behavior of beds of randomly-sized spherical particles subjected to compressive loading, including fracture of individual particles when appropriate critical loads are experienced (for brittle materials). This behavior correlated well with the behavior observed while crushing glass spheres between flat plates.

From the outset, the overall program was guided by a concept that would use fluidization of the bed to preferentially transport small particles from the crushing zone. Transport experiments have been conducted with bidisperse mixtures of glass spheres (50 - 3000 micrometers in diameter) in water with impulsively-started fluidization, within vertical and near-vertical chambers. The work is continuing with construction of an annular test chamber representative of a practical design.

Massachusetts Institute Of Technology

Dept of Mechanical Engineering **$117,874**
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 experiment. The result for the separating particle size showed that the fine fraction is indeed colloidal.

Massachusetts Institute Of Technology

Dept of Chemical Engineering **$151,142**
Cambridge, MA 02139 **06-A**
94-3

Development of Principles and Methodologies of Metabolic Engineering
G. Stephanopoulos

Advances in molecular biology allow genetic modifications which affect the metabolic network of an organism. However little has been done on relating such modifications to the relative impact on useful biosynthetic production. The proposed effort will develop the methods for identifying those critical points in metabolic networks which have the greatest impact on product formation. Ultimately rate controlling reactions in the rate controlling branch of the metabolic network will be identified. The initial organism to be studied will be a microbial system producing aminoacids through fermentation. The key issue is to find the best pathways for the flow of carbon towards the desired product formation. It is expected that such a study will lead to defining the field of metabolic engineering and its application to the production of fuels and more generally biochemicals.

Massachusetts Institute Of Technology[1]

Dept of Chemical Engineering **$ 0**
Cambridge, MA 02139 **06-C**
91-3

Los Alamos National Lab[2]

MEE-9 **$109,000**
Los Alamos, NM 87545 **06-C**
91-4

Sandia National Laboratories[3]

Engineering Sciences Center **$109,000**
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.

Fluctuations in the mean sedimentation velocity of a falling ball though such suspensions were analyzed and successfully interpreted in terms a "hydrodynamic diffusion" model. Diffusivity results agreed well with a theoretical model of the phenomenon, originally developed for dilute systems.

Spinning-ball rheometry in quiescent suspensions is being developed as a useful adjunct to prior falling-ball rheometric studies. This technique provides another experimental benchmark for numerical and analytical studies of microstructural effects in concentrated suspensions.

The pressure 'drop' incurred by a sphere falling through a quiescent neutrally-buoyant suspension, which constitutes another useful dynamical suspension parameter, was measured and found to agree well with theoretical results for the comparable pressure drop in a homogeneous Newtonian liquid.

In collaboration with Lovelace, NMR imaging was used to study the flow-induced migration of neutrally-buoyant suspensions of rods (of aspect ratio up to 20) dispersed in a Newtonian liquid undergoing inhomogeneous shear. Despite their very different geometry, the rod results were similar to those previously observed for spheres.

University Of Minnesota

Dept of Mechanical Engineering **$126,100**
Minneapolis, MN 55455 **01-B**
94-3

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

Separated and jet flows which enhance heat/mass transfer are of interest in the project. Models using perforated plates with circular hole arrays are of particular interest. The project investigates the local heat/mass transfer for different pore (hole) length-to-diameter ratios and spacings. This study will be extended to multiple layers of the perforated plates to better understand the separation and reattachment flows and their influences on heat transfer.

Short pin-fin arrays have been used for duct-flow heat transfer enhancement. However, the gain achieved by enhanced heat transfer is often offset by an increase in pressure loss which results in the need for extra pumping power to maintain the flow. Based on studies of the effect of horseshoe vortices on heat transfer, a stepped pin-fin geometry has been designed. The vortex flows formed from the step will be examined and they may substantially increase mass (heat) transfer from the duct walls without requiring an increase in pumping power. Local mass transfer measurements, together with flow visualization and pressure and velocity measurements, are employed to understand the mechanisms for higher mass (heat) transfer.

Energy separation, connected with the unsteady pressure fluctuations induced by the convective movement of vortices, has been observed in an impinging jet. Free and impinging jets including the effect of acoustic excitation are being studied. The energy separation occurs in a free jet in the vortex structure around the jet periphery, and is greatly affected by acoustic excitation. This study should reveal the fundamentals of flow that affect the energy separation and the influence on impingement heat transfer.

University Of Minnesota

Dept of Aero Eng & Mechanics **$205,000**
Minneapolis, MN 55455 **01-C**
93-5

Lubricated Transport of Viscous Materials
D. Joseph

The focus of the research is studies of lubricated transport of viscous materials: viscous crude oils, concentrated oil/water emulsions, slurries and capsules. We have emphasized problems which arise in pipeline applications. Four categories of study are underway. The first is the study of the fluid dynamics of core flows emphasizing studies of stability and, more recently, problems of start-up, lift-off and eccentric flow when gravity causes the core flow to stratify. We have also correlated all the available data on friction factors and hold-up for core flow and shown good agreements between experimental data and k - ε models in turbulent flow.

A second category of studies treats the problem of fouling of pipe walls with oil, with undesirable increases in pressure gradients and even flocking. We propose to do the first studies of rates of fouling as they depend on the parameters of lubricated pipelining together with remedial strategies based on the manipulation of the materials of wall construction. The remedial strategies may go a long way in relieving the main problems impeding lubricated pipeline technology.

The third category is to gain an understanding of the mechanisms of flow-induced migration of particles leading to lubricated configurations. For this, we do direct numerical simulations in which the particles are moved according to their equations of motion by hydrodynamic forces computed exactly. One goal of this study is to see if lift forces proportional to the square of the velocity are strongly involved in fast flow of slurries, capsules and oils.

The fourth category of problems is the lubricated transport of concentrated oil/water emulsions.

University Of Minnesota

Dept of Mechanical Engineering **$279,602**
Minneapolis, MN 55455 **06-C**
92-4

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

The objectives of this program are the characterizations of various plasma processes in specific plasma reactors which have been developed at the University of Minnesota, using diagnostics and modeling approaches. The specific reactors used for the plasma processes are a triple torch reactor and a counterflow liquid injection reactor. An rf induction plasma unit has been added as a third reactor for process characterization because of increasing interest by industry in such a reactor.

Diamond film deposition using thermal plasma CVD has been investigated in the triple torch reactor where the emphasis has been on large area coverage, and in the counterflow reactor where the use of liquid precursors for the deposition has resulted in some startling observations. The major new diagnostics which have been used in the characterization have been a combination of a tele-microscope with a laser strobe video system allowing detailed observation of spray droplets. Synthesis of ultrafine SiC particles has been pursued in the rf reactor.

The modeling effort concentrates on the description of the reactant mixing in rf induction plasma reactors, and on the derivation of improved values for thermodynamic and transport properties of mixtures which are sorely needed for both efforts to improve the basis for predicting plasma processes.

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

Washington, DC 20418 **$1,559,000**
06-C
Department of Energy Integrated Manufacturing Fellowship Program **92-3**
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. **$84,600**
Washington, DC 20546 **06-C**
94-5
Center for Aerospace Research & Education for Minority Students at Southern University
I. Blankston

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 Center for Manufacturing Sciences

Technology Sourcing **$ 0**
Ann Arbor, MI 48108 **06-C**
93-2
Industrial Liaison Pilot Program
J. Sheridan

The National Center for Manufacturing Sciences has been funded by DOE, Basic Energy Sciences, to direct a program which will place employees of the National Laboratories at industrial sites to work with their corporate colleagues on issues of importance to manufacturing industry. The goals of the program are to evolve expertise in a broad range of manufacturing issues at the National laboratories, identify fundamental DOE research needs, and build a long-range sustained commitment to collaboration on industrial issues both at DOE and within industry. Results from the Liaison Program will strengthen industry's energy efficiency in its operations by enhancing the quality of the total product and developing efficient production and management techniques. This will directly benefit American manufacturing competitiveness and will help DOE Basic Energy Sciences identify fundamental research needs in energy efficient industrial methodologies and technologies.

A pilot program will be conducted to immediately place a limited number of workers and carefully evaluate the effectiveness of a sustained program. The pilot program is important. There are a number of potential risks and blockers which need to be assessed carefully before a large commitment is made. The Industrial Liaison Program (ILP) will place DOE laboratory workers into the industrial environment to focus the attention of the laboratories on industry issues. The worker will remain a full time employee of the Laboratory but the costs of the off-site per diem will be shared by the host company through a formula-based reimbursement.

National Institute Of Standards & Technology

Thermophysics Division **$123,675**
Boulder, CO 80303 **06-A**
94-3

Gelation of Dense Silica Suspensions: Effect of Shear
H.J.M. Hanley

The objective of this work is to understand microstructure changes during gelation of nanometer particulate material. In particular the effect of an applied shear on the gelation mechanism is being investigated. Practical objectives are to understand better the energy efficient sol-gel casting process and to explore the possibility of constructing novel composite materials. The gelation mechanism is studied by small angle neutron scattering (SANS) experiments, supplemented by light scattering measurements. Data are taken from the neutron scattering spectrometers of the NIST Cold Neutron Research Facility (CNRF), and from a light scattering facility under development in the Thermo-physics Division. An automated shearing cell, which was constructed previously under DoE funding and now a user facility at CNRF, is a central component of the work. Candidate systems are colloidal silica in water, or heavy water, and gelation is triggered by changing the pH and salt content of the solvent. Results to date include a determination of structure factors of dense silica gels. It is established that shear has a definite effect on gel structure. Complementary nonequilibrium molecular dynamics simulation studies have modeled the gelation process. A connection between the gelation mechanism and spinodal decomposition to a gas-solid mixture has been established.

National Institute Of Standards & Technology

Thermophysics Division **$573,000**
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 that can be used to measure 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 key systems. The specific measurement capabilities completed (denoted by asterisk) 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 will extend significantly the existing 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. This project also includes benchmark experimental measurements on alternative refrigerants and refrigerant mixtures (completed and ongoing), aqueous solutions, and carefully selected systems consisting of species of diverse size (methane + neopentane) and polarity (methane + ammonia) that are important to the development of predictive models for energy-related fluids.

National Institute Of Standards & Technology

Electromagnetic Technology Div **$108,000**
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 patterning 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 **$ 0**
The Benjamin Levich Institute **06-C**
for Physico-Chemical Hydrodynamics **90-3**
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.

The City University Of New York

The City College **$256,836**
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 due to the central role played by FCC's in modern refineries. 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 FCC is an excellent example of such plants, being both nonlinear and multivariable.

A dynamic simulation model of the FCC has been developed for these studies, submitted for publication and is available on request. Compared to available models, it is based on a more detailed kinetic representation of the FCC operation and more accurately predicts the trends actually observed in the plant.

The work has demonstrated that the performance of FCC's in the region of current operation exhibits not only the expected multiple steady-states but input multiplicities as well. Further, there are preferred choices of dominant variables as well as control structures depending upon the mode of operation (partial versus complete CO combustion). Some long-standing control problems that have puzzled industry have been resolved and a new approach to choosing control structures is being developed.

The City University Of New York

The City College **$101,850**
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.

Northwestern University

Engineering & Applied Science **$90,452**
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 T_c 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 these applications.

Both the film and the substrate are generally anisotropic. A line-focus acoustic microscope, is being used to measure the speed of surface acoustic waves (SAW) 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 SAW data. Recent results include: (1) analytical and numerical techniques for the direct problem and the inverse method, (2) measurements of superlattice film constants, (3) investigation of the effect of surface roughness and (4) measurements of residual stresses in thin films.

Northwestern University

Dept of Chemical Engineering **$155,079**
Evanston, IL 60208 **01-B**
92-3

Stability and Rupture of Thin Fluid Films on Heated Solids Surfaces
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 **$53,230**
Evanston, IL 60208 **01-C**
94-3

Microscopic Interfacial Phenomena During Flow in Porous Media
M. Miksis

The objective of this proposal 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 **$ 0**
Evanston, IL 60208-3120 **06-C**
91-3

Mixing of Immiscible Fluids in Chaotic Flows and Related Issues
J. Ottino

The basic goal of this work is to obtain basic understanding of mixing of immiscible fluids leading to the determination of flow conditions which result in efficient breakup and dispersion of one mass of fluid in the bulk of another. Related issues are the prediction of the morphological structures and drop size distribution for a given set of operating conditions. The primary motivation for these investigations is to produce basic knowledge leading to increased understanding of industrial processes involving blending, agitation, emulsification, and dissolution. Work was carried out in several inter-related areas: (i) stretching and breakup of filaments in chaotic flows, (ii) analysis of details of breakup and sub-satellite formation at small scales, (iii) understanding of the statistics of drop size distributions produced for different viscosity ratios. Work in all these areas has been completed. Current research is proceeding in three directions: mixing of equal volumes of fluids using either the marker and cell technique or the boundary integral element method, investigation of the role of rheology especially shear thinning effects, in chaotic mixing processes, and experimental studies of chaos-enhanced transport. Our most recent studies focus on dispersion of powdered solids in viscous liquids.

Northwestern University

Dept of Eng Sci & App Math **$68,656**
Evanston, IL 60208 **06-C**
92-3

Stability and Dynamics of Spatio-Temporal Structures
H. Riecke

This research will be concerned with a study of physical systems which exhibit a transition from a homogeneous state to a spatial and/or temporal structure when driven sufficiently far from thermodynamic equilibrium. Such non-equilibrium structures are found, for instance, in fluid dynamics - Rayleigh-Benard convection and Taylor vortex flow -- and in solidification -- Mullins-Sekerka instability. They also serve as paradigms for non-equilibrium structures in general which arise in other fields such as chemistry and mechanics.

Specifically, the research focusses on localized waves observed in binary-mixture convection. They have been described theoretically as dissipatively perturbed soliton solutions of the complex Ginzburg-Landau equations. However, it has been found that the resulting predictions qualitatively disagree with certain aspects of the observations. The present work will build on an extension of these equations derived earlier, which incorporates an additional slow time-scale due to the slowness of mass diffusion. The derivation will be considered for more realistic conditions. The velocity of the waves will be calculated in a perturbation around the soliton. The effect on plane waves will be investigated.

In addition, localized structures in the form of domain walls will be studied. Arrays of such walls are related to zig-zag structures as found in isotropic and anisotropic convection.

University Of Notre Dame

Dept of Chemical Engineering **$59,774**
Notre Dame, IN 46556 **01-C**
92-3

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

The objective of this project is to characterize the wave dynamics on a falling film and to analyze its effect on heat/mass transfer efficiencies. Using a combination of numerical computation, experimentation and analysis, the study of wave evolution and its statistics is almost complete and the analysis of transfer mechanisms will begin in the next phase. A mixed spectral/finite-elements method is developed to simulate 3-dimensional, low Reynolds number (< 600) films. The code allows closer scrutiny of interfacial structures than our fluorescence experimental characterization and of the underlying liquid flow field that cannot be easily measured. It was found that the wave evolution near the inlet evolves by a classical convective mechanism that selects a monochromatic 2-dimensional wave. This monochromatic wave then saturates and excites, through subharmonic and oblique wave resonance, certain 2-dimensional and 3-

dimensional waves downstream to generate complex interfacial pattems. The dynamics of those pattems have been classified and analyzed by coupled amplitude equations from a weakly nonlinear theory. Further downstream, however, all the Fourier modes synchronize to form unique near-solitary waves that interact and, sometimes, annihilate each other. The solitary waves are constructed numerically and an inelastic coherent structure theory is developed that is capable of predicting the statistics of the wave dynamics from simple dynamical systems theory.

University Of Notre Dame

Dept of Chemical Engineering **$ 0**
Notre Dame, IN 46556 **01-C**
91-3

Study of Interfacial Behavior in Cocurrent Gas-Liquid Flows
M. McCready

The objectives are to develop a fundamental understanding of how flow instabilities cause waves and slugs that influence important overall properties (e.g., pressure drop, atomization) of gas- liquid flows.

Eigenfunction expansion and center manifold projection have been used as the basis for weakly nonlinear analysis of the Navier- Stokes equations and boundary conditions for two-layer flow. It is found that the transition to waves is usually supercritical for density and viscosity ratios typical of gas-liquid flows. The primary mechanism of stabilization of the unstable fundamental wave can be either a cubic self interaction, or a quadratic interaction with the first overtone -- depending upon the closeness in speed of the fundamental and overtone. This mechanism is critical to developing procedures to predict the entire wave field and to interfacial transport because studies have shown that waves with wavelengths shorter than the fundamental enhance transport.

Exact linear analysis of this problem, which has been previously verified by experiments, has been compared to popular approximate models such as Kelvin-Helmholtz and one-dimensional equations. These approximate models, which form the basis for flow regime transition and atomization prediction procedures, give predictions for neutral stability that are not usually within a factor of 2 in (e.g.) gas Reynolds number. This suggests that they have little theoretical basis and casts doubt on their general applicability.

Oak Ridge National Laboratory

Engineering Physics **$1,373,000**
and Mathematics Division **03-C**
Oak Ridge, TN 37831 **94-3**

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

The objective of CESAR is to develop, demonstrate, evaluate, and provide quantitative performance analysis of methods, algorithms and underlying theories necessary to design and build reliable sensor-based robots capable of executing sets of tasks in unstructured workspaces. Particular research areas are chosen to address the long-term technology-base requirements for DOE missions that rely on the use of intelligent machines and robotics. Current research focusses on mobile manipulation systems, machine learning, multi-sensor systems, cooperating robots, and systems integration. Applications include environmental restoration and waste management, manufacturing systems, transportation systems, and nuclear power stations. CESAR facilities include mobile robots: HERMIES-III, OHP (Omnidirectional Holonomic Platform), OSCAR (Omnidirectional Stably-Controlled Autonomous Robot, a new robot under development, based on the OHP mobility system), a modified TRC Labmate mobile robot, and a commercial mobile robot, Andros, manufactured by Remotec, Inc; a Robotics Research Corporation K1207i manipulator; laser range cameras; custom-built, VME-bus compatible fuzzy logic hardware; a CNAPS neural network processor; and a network of computer workstations with access to high performance parallel computers. CESAR staff collaborate with academia and industry through a number of arrangements, including a Cooperative Research and Development Agreement. Results of CESAR research are published in the refereed literature. CESAR research with the OHP robot was awarded a 1993 RD100 Award.

Oak Ridge National Laboratory

Bioprocessing Research and Development Center **$45,000**
Oak Ridge, TN 37831 **06-A**
94-3

A Study of the Mechanisms of Liuqid-Emulsion Bioreactor Systems
C. Scott, T. Scott

The approach taken in this research is to study the liquid-liquid interphase transport and reaction phenomena important to biphasic bioreactors by using a model enzyme system. The system is comprised of an aqueous-phase horseradish peroxidase (HRP) that is activated by hydrogen peroxide to carry out the oxidation of *p*-cresol that is contained in an immiscible organic phase, toluene. Tasks in the research program involve study of aqueous-phase reaction kinetics, interaction of HRP with the liquid-liquid interface, and modelling of a continuous liquid-liquid contractor that uses high-intensity electric fields to create micron-sized aqueous drops for the enzymatic reaction. Work on this project began in June 1994. Detailed kinetics studies indicate that the presence of toluene in the aqueous phase appears to stabilize the HRP due to an interaction with the active sight of the enzyme. Tests with the electrostatic bioreactor indicate that the electric field does not deactivate the enzyme and that significant portions of *p*-cresol can be removed from the organic phase by a continuous biphasic system. Future work will involve the use of a precision two-phase flow device that will allow investigation of interfacial effects on the enzymatic reaction.

Ohio State University

Mathematics Department **$66,118**
Columbus, OH 43210 **06-C**
92-3

The Evolution of a Hele-Shaw Interface and Related Problems in Dendritic Crystal Growth
S. Tanveer

The ultimate objective is the prediction of complicated noisy time evolving features that are observed in Hele-Shaw experiments or in a dendrite growing in an undercooled liquid for small capillarity. From a mathematical perspective, we like to calculate the effect of a small regularization (capillary effects) to regularize an otherwise ill-posed problem. Such problems are characterized by the appearance of disparate scales both in space and time which make a direct numerical calculation very difficult.

Within certain classes of initial conditions, the first step in our approach consists of imbedding the ill-posed time evolving problem at zero surface tension (or zero regularization in a wider context) as part of a well-posed problem at the expense of studying the initial value problem in the unphysical complex plane. This has been done without resort to any approximations by introduction of a novel numerical method.

Small regularization effects have been introduced in a perturbative manner in the extended domain for many cases. This removes the sensitivity of the dynamics to initial conditions when posed in the complex domain. In our next phase, we will also look into dynamics of random initial singularities in order to connect with statistics of nonlinear noise amplification.

Oregon State University

Dept of Mechanical Engineering **$ 0**
Corvallis, OR 97331-6001 **01-B**
91-3

Radiative Transfer Through an Array of Discrete Surfaces
J. Welty

This project involves experimental measurement and characterization of radiative transfer through arrays of fixed discrete surfaces. It is being carried out in cooperation with Battelle, Pacific Northwest Laboratory.

The objective of this research is to identify basic relationships between array geometry (spacing, packing arrangement, and element shapes), surface properties, and radiative transfer through a two-dimensional array of both regularly-and irregularly-spaced discrete surfaces. The information resulting from this study may also be useful in establishing criteria for the valid application of participating media models to systems of discrete surfaces.

Accomplishments to date include the following: (1) the design, construction and operation of a bidirectional reflectometer, (2) measurements of bidirectional reflectances of several materials, (3) demonstration of the need for full BRDF (bidirectional reflectance distribution function) information for striated surfaces, and (4) installation and operation of an enhanced Monte Carlo code. The two-dimensional Monte Carlo code was used to extend the results of a classic problem originally published by Hottel over 60 years ago, dealing with radiant exchange from an infinite plane to parallel rows of infinitely long tubes.

The reflectometer that has been designed and built locally possesses flexibility of use and precision which are superior to any similar devices described in the literature. The need for such an instrument stems from the direct dependence of Monte Carlo results on the accuracy of surface property information. Measurements have been taken for several materials possessing varying degrees of diffuse and specular reflecting characteristics.

A common assumption made, in analyzing radiant heat transfer among surfaces, is that the reflectance is independent of the azimuthal angle of the incident beam. Our instrument has the capability for complete surface property description which will allow Monte Carlo simulation of surface arrays to be made without the inherent errors resulting from the azimuthal angle assumption.

Pacific Northwest Laboratory

Battelle Memorial Institute **$104,000**
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 **$102,292**
Philadelphia, PA 19104 **01-C**
92-3

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 **$94,142**
University Park, PA 16802 **06-B**
92-3

Experiments on the Gas Dynamics of the HVOF Thermal Spray Process
G. Settles

High Velocity Oxy-Fuel (HVOF) thermal sprays are an important emerging technology for the application of metallic coatings. High-density, low oxide coatings produced with HVOF are an attractive alternative to plasma sprayed coatings, offering comparable performance with the advantages of economy and simplicity.

Because HVOF uses high-speed gaseous products of combustion to heat and accelerate spray particles, the gas dynamics of the process profoundly influences coating performance. However, commercial HVOF equipment has yet to exploit the field of gas dynamics to produce more reproducible coatings with improved properties. The objective of this research is to study HVOF gas dynamics through experiments and modeling and to determine potential improvements to the spray process. The transfer of technology from the fields of rocket propulsion and high-speed aerodynamics is a key element of this project.

Flow visualization of the supersonic HVOF jet reveals rapid turbulent mixing and large amounts of entrained atmosphere. Analysis of sprayed coatings indicates detrimental oxides form principally after particle impact, thus explaining the recent revision of suggested operating parameters for many commercial HVOF systems. The thermal spray industry has been informed of these results with presentations and papers at the last two National Thermal Spray Conferences. In addition, analysis and experiments to optimize the design and operation of the supersonic HVOF spray nozzle are underway. Currently, improved HVOF equipment embodying gas-dynamic principles is being tested.

Physical Sciences Inc.

20 New England Business Center **$ 0**
Andover, MA 01810 **06-A**
92-4

Experimental and Theoretical Studies of Multicomponent Vapor Condensation
G. Wilemski, B. Wyslouzil

This research program comprises experimental and theoretical studies of nucleation and condensation in multicomponent gas mixtures. The program goals are: (1) to improve basic understanding of nucleation and droplet growth, (2) to stringently test theories of nucleation at high nucleation rates and under nonisothermal conditions, (3) to develop improved theories where needed, (4) to enlarge the data base for systems of both fundamental and practical interest, and (5) to provide reliable means for predicting the behavior of mixtures in practical devices and in the atmosphere. Condensible vapors, mixed with a carrier gas, are cooled in a supersonic Laval nozzle to obtain high nucleation rates under steady state conditions. Interferometry and laser light scattering are used to detect the "onset" of condensation and to monitor subsequent droplet growth. Theoretical calculations of the droplet size distribution along the flow axis are performed to assess competing theories of nucleation and droplet growth. A new experimental apparatus is also being constructed to study binary nucleation in mixtures of sulfuric acid and water vapor.

Recent nozzle experiments with a fixed water or ethanol vapor pressure reveal a small increase in the onset temperature of condensation that accompanies a decrease in the carrier gas stagnation pressure from 3 to 0.5 atm. This effect can be quantitatively explained by the changes that occur in the boundary layer displacement thickness and the heat capacity of the flowing gas at different pressures. The results provide no evidence for the role of energy transfer limitations on nucleation under conditions of excess carrier gas in the atmospheric pressure range. Other recent experimental and theoretical studies of ethanol condensation have shown that the relative importance of nucleation and droplet growth at onset changes dramatically depending on the magnitude of the nucleation rate achievable for dfferent experimental conditions. Under conditions yielding lower nucleation rates in the nozzle, the condensate mass occurs overwhelmingly as large (5-25 nm radius) supercritical droplets. This indicates that droplet growth and nucleation are concurrent processes under these conditions. As the temperature and ethanol vapor pressure are lowered, increasingly higher nucleation rates are attained at onset, and the mass of condensate occurs predominantly as small (0.5-1 nm radius) nearly critical droplets. Under these conditions droplet growth contributes substantially to the accumulation of condensate only after nucleation has subsided.

Princeton University

Dept of Mech & Aero Eng **$93,120**
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 steady propagation of the planar premixed flame in the doubly-infinite domain, with chain branching-termination reactions and weak volumetric heat loss, is studied using activation energy asymptotics. The analysis yields the characteristic dual solution, extinction turning point flame response, and shows that the flame propagation speed is reduced to $e^{-1/2}$ of the adiabatic value. The generality of this limit flame speed is noted.

The possibility of stabilizing a Bunsen flame without heat loss to the burner rim is experimentally investigated by examining the temperature of the rim, the temperature gradient between the rim and the flame base, and the standoff distance of the flame base in relation to the flame thickness. Results show that adiabatic flame stabilization and subsequently blowoff are indeed possible for weak flames in parabolic flows. The adiabatically stabilized flame is then modeled by using the scalar field formulation and by allowing for the effects of curvature and aerodynamic straining on the local flame speed. Calculated flame configuration agrees well with the experiment. Results further show that active modification of the flame curvature is the dominant cause for the flame to maintain adiabatic stabilization.

Princeton University

Dept of Civil Engineering **$205,892**
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 and computer-simulation 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.

Purdue University

School of Mechanical Engineering **$93,664**
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 **$251,742**
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 **$120,786**
West Lafayette, IN 47907 **01-B**
93-3

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

The proposed project will target the development of a theoretical model for critical heat flux (CHF) in vertical upflow. Experiments will be performed with the aid of a velocity/interfacial boundary analyzer in order to examine near-wall conditions at heat fluxes approaching and exceeding CHF.

These measurements will determine the trigger mechanism for liquid sublayer dryout beneath the coalescent vapor layer which forms at high heat fluxes. Instability features (e.g. wavelength, amplitude) of the wavy vapor-liquid interface will be measured over heaters of various lengths to determine the frequency and spatial span of interfacial contact with the wall at heat fluxes approaching CHF and explore the mechanism of dryout in the contact regions. This information will be used to construct a validated theoretical model applicable to vertical upflow in long channels and to different fluids and channel configurations.

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 $125,664
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 involves 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 liquid with the continuous vapor. Ensemble averaging concepts are being applied to different interface configurations in order to derive closure conditions for momentum transfer and Reynolds stress. A model for droplet deposition has been developed and work is also continuing on coalescence/break-up models.

Conservation equations for the evolution of interfacial area density, and Gauss and mean curvature are being developed to model the evolution of the interface between the continuous liquid and continuous vapor fields.

Rensselaer Polytechnic Institute

Dept of Chemical Engineering **$89,156**
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. Currently, microscopic image processing equipment, procedures, and related computer programs are being developed to record the two-dimensional thickness profile. The further development, evaluation, and use of a novel ellipsometric technique (Image Scanning Ellipsometry, ISE) is being emphasized. ISE is a full-field imaging technique that can be used to measure the thickness of a thin film with high spatial resolution and thickness sensitivity, i.e., it can measure and map the 2-D film thickness profile. Results obtained using the initial design were presented in Applied Optics, 33, pp1223-1229, 1994.

Rice University

Dept of Civil Engineering **$ 0**
Houston, TX 77251 **01-A**
91-3

Stochastic Quadrization for Probabilistic Analysis of Large Compliant Off-Shore Structures
P. Spanos

The statistical linearization method is often inadequate for estimating spectral properties of random responses of nonlinear systems. This is sometimes due to the fact that the power spectra of responses of linear systems span only the frequency range of the excitation spectrum, whereas significant responses outside this range are possible for nonlinear systems. In this research program, the concept of the statistical "quadratization" method has been introduced to address this shortcoming of the linearization methods. The effectiveness of statistical quadratization has been demonstrated on several single-degree-of-freedom systems. The method has also been generalized to multi-degree-of-freedom systems. The statistical quadratization solution procedure involves replacing the nonlinear system by an "equivalent" system with polynomial nonlinearities up to quadratic order. The nonlinear equivalent system has a form whose solutions can be approximated by using the Volterra series method. The non-Gaussian joint response probability distribution is approximated by a third-order Gram-Charlier expansion. The method has been formulated for systems with general nonlinearities and with nonlinearities of a special form. To demonstrate the usefulness of the method, solutions have been obtained for a specific system. The corresponding results compare well with Monte Carlo simulation data. Further, it has been shown that the quadratization method is notably superior to the linearization method for the considered system. The method has proved especially suitable for systems with "drag" type nonlinearity encountered in a multitude of structural systems in the oil production/distribution cycle.

University Of Rochester

Dept of Physics and Astronomy **$70,519**
Rochester, NY 14627 **06-C**
92-3

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 **$94,090**
Rochester, NY 14627 **06-C**
93-3

Coherence Effects in Radiative Energy Transfer
E. Wolf

The investigations are chiefly aimed at clarifying the foundations of radiometry and the theory of radiative energy transfer and determining the effect of state of coherence of a source on both the spatial and the spectral distributions of energy in the radiated field.

Among the results obtained during the past year was a derivation, on the basis of statistical wave theory, of radiometric expressions for the spectral density and the flux density of fields generated by a broad class of partially coherent sources. A new radiometric law was found for propagation of the spectral degree of coherence from sources of this kind. The law makes it possible to determine the coherence properties of partially coherent fields at arbitrary distances from their sources. The spectral degree of coherence of fields generated by large Lambertian sources was also investigated. Research is continuing on determining the correlation properties of random media from the knowledge of the scattered fields. New conservation law for partially coherent fields were formulated and some of their consequences were studied. Non-interferometric methods for measuring coherence properties of optical fields were also developed.

The Rockefeller University

Department of Physics **$82,922**
1230 York Avenue **06-C**
New York, NY 10021 **92-3**

Some Basic Research Problems Related to Energy
E. Cohen

The present project is concerned with the following problems.

1. The visco-elastic and rheological behavior of concentrated colloidal suspensions have been computed on the basis of the Smoluchowski equation and by scaling from a corresponding dense hard sphere fluid, respectively. These microscopic theories lead to results that agree well with experiment. The connection between the two approaches and their applications is being investigated.

2. The kinetic roughening of an initially flat surface of a solid by impinging ballistic or diffusion limited particles, which remain intact and spread diffusively into the solid, is studied as a function of this diffusion process. Many features of real interfaces, like island and inlets, are observed. The surface width depends both on the diffusion process in the solid and the way the particles reach the surface.

3. The investigation of new types of diffusion, discovered in Lorentz lattice gas cellular automata, is continued. In this gas a point particle moves on a lattice occupied by deterministic scatterers. For randomly placed fixed scatterers from super diffusion to no-diffusion (trapping) is observed, depending on the lattice and the nature of the scatterers. For periodically placed flipping scatterers randomization of the scatterers by the particle as well as particle propagation occur.

Sandia National Laboratories

Combustion Research Facility **$146,000**
Thermofluids Division **06-B**
Livermore, CA 94550 **93-3**

Mixing and Phase Change During Combustion
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 **$100,000**
Livermore, CA 94551-0969 **06-B**
90-3

Structure of Inverse Diffusion Flames in Supercritical Fuel/Water 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 second set of experiments has determined spectroscopically the concentration histories of methane, oxygen, and carbon dioxide in homogeneous mixtures at concentrations lower than the flame ignition conditions. The latter data have yielded high-pressure, global reaction rates for methane as a function of fuel/oxidizer concentrations, temperature, and total pressure (water density). The global rates are an important component of SCWO process design tools and serve as well to calibrate proposed elementary reaction mechanisms. A future goal of the experiments is to measure characteristic temperatures of the hydrothermal flames using a bare junction thermocouple probe built for the reactor.

University Of Southern California

Dept of Mechanical Engineering **$117,926**
Los Angeles, CA 90089-1453 **01-C**
94-1

Particle Pressures in Fluidized Beds
C. Campbell

The particle pressure represents the portion of the momentum transport in a fluidized bed that can be attributed to the the motion of particles and their interactions. Preliminary measurements, in gas-fluidized beds, have shown that the particle pressures exerted on the side walls are primarily due to the presence of bubbles. This work is continuing in a 2-D bed with the goal of trying to measure the particle pressure field around bubbles. These results are very surprising. It was anticipated on beginning this work that the particle pressure field around a bubble would be something like the gas-pressure field in the sense that the particle pressure changes induced by the bubble would be local to the bubble and would disappear far away. Instead, the results show that the largest pressures are observed in the wake behind the bubble. But, instead of being local, the pressures increase as the bubble moves away and reach the maximum when the bubble erupts from the bed. This indicates that the bubble defluidizes the material in its wake; the particle pressures increase in the far wake as more and more defluidized material is piled on top of itself. This observation may have profound implications in chemical processing as there may not be sufficient intermingling of the gas and solid in the large amount of defluidized material in the wake.

Work is also being performed in a liquid fluidized bed to try and understand how particle pressures are generated in the absence of bubbles. These particle pressures are extremely small ande quired a redesign of the particle pressure transducer. The results show that the particle pressures are a tradeoff between the particle agitation and concentration. Thus, as the fluidizing flow is increased, the particle pressures rise immediately after minimum fluidization due to the increased agitation, reach a maximum and then dropoff due to the reduced concentration. Also, the propagation of voidage disturbances in a liquid bed have been studied to infer bed properties by filtering the instabiltities through a "generic" stability model.

University Of Southern California

Dept of Mechanical and Aerospace Engineering **$126,099**
Los Angeles, CA 90089 **01-C**
93-3

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

T. Maxworthy, E. Meiburg

We have been performing an experimental and computational investigation of miscible two-phase flow in capillary tubes. The experimental program concerned with the interface motion has been completed, and a report is being written for publication. The diffusion coefficient between glycerine and various glycerine-water mixtures was laboriously measured and the final plot of film thickness vs. Pe determined. By comparing with the corresponding plot of film thickness vs. Capillary number, we have found that the effective surface tension of the miscible interface for an Atwood number of close to unity is given by ~400 (μ)D/d. For a typical 1mm diameter tube, this gives a value of 0.03 dynes/cm.

Multigrid finite difference simulations of the flow show good agreement with the data. Currently, the simulations are extended to account for different fluid densities as well. We are furthermore constructing the Hele-Shaw cell to be used in the second part of the experiment. We plan to begin experiments and computations on this part of the work in September 1994. Also we have originated a collaboration on problems of miscible interface dynamics with the group of Prof. Wesfried of the Ecole Sup. de Physique et Chimie Industr. de Paris. We anticipate that the combined talents of the two groups will enable us to make significant progress on the problems of mutual interest.

Southwest Research Institute

6220 Culebra Road **$ 0**
San Antonio, TX 78228-0510 **03-B**
91-3

Application of Magnetomechanical Hysteresis Modeling to Magnetic Techniques for Monitoring Neutron Embrittlement and Biaxial Stress

M. Sablik, G. Burkhardt, H. Kwun

The purpose of the project is to investigate magnetic nondestructive evaluation (NDE) procedures which have promise for monitoring (1) neutron embrittlement in nuclear pressure vessels and (2) biaxial stress in oil and gas pipelines. Such monitoring should help in safeguarding against structural failure in critical energy industries.

Neutron embrittlement is presently monitored using quantities defined by the statistical distribution of fracture energies of heated Charpy samples. A procedure has been determined whereby identification can be made between magnetic measurements and Charpy neutron embrittlement parameters. This procedure offers promise for direct magnetic measurement of neutron embrittlement in certain reactor steels (e.g. SA302B).

Also, guided by successful magnetomechanical hysteresis modeling, a procedure has been found which uses magnetic hysteresis parameters, or alternatively, magnetic Barkhausen noise for measurement of the difference of two perpendicular biaxial stresses. Magnetically induced velocity changes (MIVC) in ultrasonic waves additionally have found promising for NDE of the stress difference; furthermore, under compression, it is possible to use MIVC for measuring the stress sum, suggesting that under compression, the individual biaxial stresses themselves can be measured directly.

An additional result of this project has been greatly improved development of basic magnetomechanical hysteresis modeling and Barkhausen noise modeling.

Stanford University

Dept of Mechanical Engineering **$75,054**
Stanford, CA 94305-3030 **01-A**
93-3

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

This is part of a long-range study to develop predictive tools and physical understanding of the effects of mean flow three dimensionality on convective heat transfer. Experiments have been conducted in two different rotating disk facilities, one operating at low speeds in water and the other operating at high speed in air. Two-point correlation measurements in air and visualization in water have shown that longitudinal vortices near the wall are distorted by the radial "crossflow" near the disk surface. This distortion renders the vortices less capable of generating bursts of low speed fluid away from the wall and sweeps of high speed fluid toward the wall. This accounts for the reduction in the turbulent shear stress relative to similar two-dimensional boundary layers. This mechanism should result in a similar reduction in the turbulent heat flux. Measurements of the mean heat transfer rate from a constant heat flux disk are now complete. Detailed profile measurements including the turbulent heat flux measured with coupled hotwire and resistance thermometer probes are underway. Development of a laser Doppler anemometer system designed to measure into the viscous sublayer is progressing in parallel.

Stanford University

Dept of Mechanical Engineering **$174,600**
Stanford, CA 94305-3030 **01-A**
91-4

Energy Changes in Transforming Solids
G. Herrmann, D. Barnett

The objectives of this project are many fold and include: a) the development of a new thermodynamical theory of continuum damage mechanics capable of incorporating nonisothermal processes; b) the implementation of novel approaches to analyze elastic bodies with defects and to study the behavior of advanced multiphase and composite materials; c) the application of the newly proposed Neutral Action method to derive conservation laws for non-homogeneous and dissipative systems.

In the area of continuum damage mechanics, the basic elements of a thermodynamic theory of damage in elastic bodies have been established. To this end, the formulation of classical thermodynamics in the form of the local state approximation is adopted. It is found, for instance, that the response of an elastic bar depends not only on the loading or straining processes, but also on some global geometric parameters as well as on temperature. The predictions of the theory seem to agree in many details with experimental observations.

The methodology of heterogenization has been expanded further and applied to piezoelectric inclusions problems and elastically embedded fibers in composite materials, simulating either imperfect boundary or the stiffness of an intermediate layer between fiber and matrix, such as a coating.

Also, the newly proposed Neutral Action method to derive conservation laws has been applied to non-homogeneous beams, plates and also to thermo- and poro-elasticity.

Stanford University

Edward L. Ginzton Laboratory **$285,000**
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

Dept of Civil Engineering **$ 0**
Stanford, CA 94305-4020 **01-B**
90-3

Fluid Dynamics of Double Diffusive Systems
J. Koseff

A study of mixing processes in doubly diffusive systems is being conducted. In the initial phase of this work continuous gradients of two diffusing components (heat and salinity in our case) were used as initial conditions and forcing was introduced by lateral heating and surface shear. The goals of the work were: (1) quantification of the effects of finite amplitude disturbances on stable, double diffusive systems, particularly with respect to lateral heating, and (2) formulation of a numerical code for such flows. More recently in the second phase of the work the focus has shifted to understanding mixing, evolution, and structure of turbulence in a stratified fluid. The goals of this aspect of the work include (1) determining the effects of stratification and molecular diffusivity on the change of mean potential energy in a stratified flow, and (2) evaluating the small-scale structure of stratified turbulence. The research on mixing includes using towed grid experiments and analytical work to verify results of a sealing analysis which predicts the effect of stratification on the mixing efficiency, and the predictions of a time-scale analysis which suggests when the diffusivity should affect the mixing. The work is being carried out in an experimental facility which is located in the Stanford Environmental Fluid Mechanics Laboratory, and on laboratory workstations.

Stanford University

Mechanical Engineering Dept **$225,880**
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. Results with an induction plasma facility show significant nonequilibrium within a downstream quartz test section, and suggest the possibility of erroneous results when using conventional diagnostics that assuming 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 is also under preliminary investigation as another possible 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 diamond synthesis 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 **$100,077**
Stanford, CA 94305 **06-C**
92-3

Thermodynamics and Stochastic Theory of Hydrodynamics and Power Producing Processes
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 **$195,907**
Stanford, CA 94305 **03-A**
92-4

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

This research pioneers a nonlinear technique, called degenerate four-wave mixing (DFWM), as a means to provide high sensitivity and spatial resolution of species in a high-pressure plasma. We have succeeded in carrying out *in situ* DFWM measurements of the trace species CH and C_2 in an atmospheric-pressure diamond synthesis reactor. DFWM measurements of the CH radicals in the boundary layer of an rf inductively coupled plasma deposition reactor are compared to a computational model of the deposition environment. Although the agreement is not perfect the match suggests that this environment can be closely modeled by a one-dimensional stagnation point simulation with coupled gas-phase and surface chemistry using an equilibrium chemical composition at a measured free stream temperature.

The research includes investigating how to extract relative internal state populations from the DFWM signal for different excitation-detection geometries and as a function of the polarization characteristics of the four beams, the three input beams and the signal output beam. The results to date include a determination of the conditions under which thermal gratings are important and how they can be used to advantage, and that saturation effects do not significantly impair the quantitative information contained in the DFWM spectra.

Stevens Institute Of Technology

Dept of Physics & Eng Physcis **$67,589**
Hoboken, NJ 07030 **06-C**
92-3

Investigation of Transitions From Order to Chaos in Dynamical Systems
G. Schmidt, A. Chernikov

Basic properties and applications of chaotic dynamical systems are studied, analytically as well as computationally.

1. A fast dynamo is a highly conductive fluid in stationary chaotic motion that enhances a small seed magnetic field exponentially. It has been conjectured that solar and stellar magnetic fields are generated by such a process. Recently we have identified the first realistic candidate for fast dynamo action. A convective cell (fluid heated from below) has been studied analytically and computationally, and exponential growth of a seed magnetic field over several orders of magnitude has been detected on the computer model. A new numerical scheme, the fractal grid method, has been developed to measure the magnetic flux reliably. In this model the fluid had infinite conductivity. To measure the effect of finite (but very large) conductivity a new numerical method has been developed, and future work will concentrate on the computation of this model with finite conductivity. One expect a slower flux growth with this more realistic model, and the aim is to find the growth rate as a function of conductivity.

2. Charged particle beams are often afflicted by a process called emittance growth, reducing beam quality. We intend to study this process on the basis of chaotic motion of beam particles. Cylindrical beams will be studied, moving in a confining field as well as the self consistent field produced by the charged particles. Preliminary studies indicate emittance growth due to chaotic effects once cylindrical sheets cross.

Texas A&M University

Petroleum Engineering Dept **$144,517**
College Station, TX 77843 **06-C**
93-2

Hydrocarbon/CO_2/Water Multiphase Equilibrium Separations
***C. Wu, P. Eubank,* M. Barrufet**

The objectives of this project are: (1) to obtain the basic laboratory multiphase equilibrium separation data of hydrocarbon (C_1-C_{12}; naphthenes and aromatics; pseudo-components of crude oil)/CO_2/water systems at temperatures up to 500°F and pressures to 10,000 psi, and (2) to *develop an equation of state computer simulator* (EOSS) based on the Area Method (a rigorous Gibbs' energy minimization technique) to accurately describe the multiphase equilibrium separation.

The laboratory measurements are from two separate apparatus: (1) a new distillation cell for three-phase measurements to 10,000 psi and 500°F and (2) a Hg-free windowed cell for measurement of both density and composition of the three phases to 350°F and 10,000 psi. The methodology for achieving the second objective continues to use the Area Method to predict phase splitting with the landmark development of the new Wong-Sandler mixing rules in EOSS allowing superior prediction of phase equilibria for VL, LL and VLL systems. A new Gibbs Equal Area Rule (GEAR) is also developed which is simpler and faster than previous methods. Two technical manuscripts, one for the experiment work and one for the new computer simulator have been submitted to recognized journals. Some details of the experimental method and completed experimental results are given in a manuscript accepted for publication in Fluid Phase Equilibria and in SPE 27873 in the proceeding for SPE Western Regional Meeting, Long Beach, CA, March 23-25, 1994.

University Of Texas At Austin

Ctr for Studies in Statistical Mech **$200,001**
and Complex Systems **06-C**
Austin, TX 78712 **94-3**

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

Non-integrable Poincare systems with continuous spectrum (so-called Large Poincare Systems, LPS) lead to the appearance of diffusive terms in the frame of dynamics. These terms break time symmetry. They lead, therefore, to limitations to classical trajectory dynamics and wave mechanics. These diffusive terms correspond to well-defined classes of dynamical processes, as is the case in statistical mechanics and also generally in interacting fields. The diffusive effects are amplified in situations corresponding to persistent interactions; as a result, the two aspects, *probability and irreversibility, must be included in* the fundamental dynamical description. Both classical and quantum mechanics are formulated on the Liouville level of probability distributions for density matrices). For integrable systems, the usual formulations of classical or quantum mechanics are recovered. Instead of being irreducible concepts, which cannot be further analyzed, trajectories and wave functions appear as special solutions of the Liouville-von Neumann equations. This extension of classical and quantum dynamics permits the unification of the two concepts of nature, based on dynamical time-reversible laws, and on an evolutionary view associated with entropy. It leads also to a unified formulation of quantum theory avoiding conventional dual structure based on equations on the one hand, and on the "collapse" of the wave Schrodinger's 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 functions exist. In both cases, a generalized formulation of dynamics in terms of probability distribution functions or density matrices is needed.

University Of Texas At Austin

Dept of Physics **$178,067**
Austin, TX 78712 **06-C**
93-5

Complex Spatiotemporal Patterns in Nonequilibrium Systems
H. Swinney

The formation of spatiotemporal patterns is being studied in chemical and physical systems maintained far from equilibrium. The goal is to understand what features are common in diverse pattern-forming systems. When does a pattern emerge spontaneously in an initially homogenous system as the external stress is varied? What kinds of bifurcations between different patterns are allowed? Such questions are being addressed for several different systems. Experiments on a reaction-diffusion system reveal striking dynamic patterns of spots of high pH in a low pH background. The spots grow and replicate in a continuous process, but a spot overcrowded by its neighbors dies; simulations of models with two species yield similar behavior. An experiment on a vertically oscillated granular layer in a circular container yields, at a critical acceleration, a well-defined transition from a flat surface to standing wave patterns that are either squares or stripes, depending on the driving frequency. A study of double diffusive convection in a novel apparatus reveals an abrupt yet continuous bifurcation to convection; this observation is consistent with a stability analysis. The comparison of experiment and theory for different systems should provide general insights into the formation of spatiotemporal patterns.

Tufts University

Dept of Mechanical Engineering **$60,324**
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.

United Technologies Res Center

Process Diagnostics Lab **$ 0**
Silver Lane **03-A**
East Hartford, CT 06108 **92-1**

Investigation of PACVD Protective Coating Processes Using Advanced Diagnostic Techniques

W. Roman, S. Hay

The objective of this research program is the comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process as applied to hard face coatings (e.g. TiB_2 or diamond). Non-intrusive laser diagnostics (e.g. laser induced fluorescence (LIF) and coherent anti-Stokes Raman spectroscopy (CARS) are being used to probe gas phase species, concentrations and rotational temperatures *in situ*. Detailed coating characterization is accomplished using Auger, Ion Scattering and secondary ion mass spectroscopies (AES, ISS and SIMS) and complimentary techniques. In addition, coating characteristics such as smoothness, adhesion (with UTRC custom built pin-on-disk apparatus) and hardness (using state-of-the-art nanoindenter apparatus) are measured. Gas phase spectroscopy is interpreted through chemical kinetic modeling and will be correlated to coating characteristics, thus providing a predictive capability that is severely lacking in the present science base of advanced protective coatings. These techniques are also applicable to other process such as PVD, CVD, combustion and thermal plasma deposition. Results to date include:

1) fabrication of a reactor system
2)) initial characterization of TiB_2 and diamond coatings
3)) *in situ* axial concentration and temperature profiles of key species (diborane and H_2)
4)) formulation of chemical kinetic models to account for spectral observations
5) comparison with experimental results indicate thermal pyrolosis is not the mechanism for chemical initiation
6) *in situ* axial concentration and temperature profiles of diborane in the 1-10 torr pressure range in a diborane/Ar plasma
7) emission spectroscopy applied to diborane/Ar and diborane/He plasmas, results indicate chemistry is not photoinitiated
8) possible surface species are evaluated and a heterogeneous reaction mechanism is proposed for the PACVD of boron from a diborane/Ar plasma
9) hydrogen axial concentration and temperature profiles obtained in a diborane/$TiCl_4$/Ar plasma

University of Washington

Dept of Mechanical Engineering **$69,282**
Seattle, WA 98195 **01-A**
94-3

3-D Experimental Fracture Analysis at High Temperatures

A. Kobayashi

The objective of this research project is to assess experimentally, the validity of T^* integral and its applicability to quasi-static and dynamic ductile fracture analyses. The surface displacement fields, which will be determined by moire interferometry, of two- and three-dimension fracture specimens will be used to compare directly the T^* integral for various contours surrounding the crack tip. Single-edge notched and surface flawed, A533B steel specimens will be subjected to subcritical crack growth to fracture at room temperature through 650°C. The experimentally-determined T^* will be compared with its theoretical and numerical counterparts generated at the Georgia Institute of Technology under a parallel DOE research project. A simple procedure for determining experimentally, T^* integral of a fracture specimen will be explored.

The large ductility of A533B steel requires the development of a moire interferometry protocol for low density moire grating. We have just succeeded in using a 40 lines/mm diffraction grating on a 2024-T3 aluminum fracture specimen. This procedure, combined with a suitable chemical etching technique, should provide the necessary protocol for high temperature moire interferometry analysis. The loading fixture and oven with optical access is already in place.

Washington University

Department of Systems Science and Mathematics **$76,667**
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 **$73,683**
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 understanding conceming 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 will employ time dependent experimental and numerical techniques to provide information concerning the particulate dispersion process caused by three dimensional vortex structures. The free shear flows to be investigated will include modified plane mixing layers, and modified plane wakes. The modifications to these flows will involve slight perturbations to the initiation boundary conditions such that three-dimensional vortex structures will be rapidly generated by the experimental and numerical flow fields. The particulate dispersion process associated with these three-dimensional structures will then 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 **$231,878**
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 **$115,003**
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-D

03-A

03-A (cont'd)

03-B

03-C

06-A

06-B

06-C

Principal Investigators

Principal Investigators (cont'd - pg. 2)

H. Smartt	Phone: (208) 526-8333; Fax: (208) 526-0690; e-mail: hbs@inel.gov	16
K. Telschow	Phone: (208) 526-1264; Fax: (208) 526-0690; e-mail: telsch@inel.gov	16
T. Basar	Phone: (217) 333-3607; Fax: (217) 244-1653; e-mail: tbasar@bllack.csl.uiuc.edu	17
T. Hanratty	Phone: (217) 333-1318; Fax: (217) 244-8068;	17
H. Sehitoglu	Phone: (217) 333-4112; Fax: (217) 244-6534;	17
J. Hartnett	Phone: (312) 996-4490; Fax: (312) 996-5620;	18
A. Prosperetti	Phone: (410) 516-8534; Fax: (410) 516-7254; e-mail: prosper@polaris.me.jhu.edu	18
R. Kraichnan	Phone: (505) 986-3979; Fax: (505) 989-4737; e-mail: rhk@lanl.gov	18
R. Littlejohn	Phone: (510) 486-4763; e-mail: rglittlejohn@lbl.gov	19
A. Kaufman	Phone: (510) 486-4763;	19
E. Fukushima	Phone: (505) 262-7155; Fax: (505) 262-7043; e-mail: eiichi@lucy.tli.org	19
S. Altobellli	Phone: (505) 262-7155; Fax: (505) 262-7043;	19
A. Caprihan	Phone: (505) 262-7155; Fax: (505) 262-7043;	19
B. Berger	Phone: (301) 405-5283; Fax: (301) 314-9477; e-mail: berger@eng.umd.edu	19
I. Minis	Phone: (301) 405-5283; Fax: (301) 314-9477; e-mail: minis@src.umd.edu	19
J. Mayergoyz	Phone: (301) 405-3657; Fax: (301) 314-9281; e-mail: isaak@eng.umd.edu	20
C. Menyuk	Phone: (410) 455-3501; Fax: (410) 455-1048;	20
L. Tsai	Phone: (301) 405-6629; Fax: (301) 405-6707; e-mail: lwtsai@src.umd.edu	21
J. Wallace	Phone: (301) 405-5271; e-mail: wallace@eng.umd.edu	21
P. Bernard	Phone: (301) 405-5272; e-mail: bernard@eng.umd.edu	21
L. Ong	Phone: (301) 405-5343; e-mail: kuching@eng.umd.edu	21
C. Thompson	Phone: (508) 934-3360; Fax: (508) 458-8289; e-mail: thompson@dragon.cpe.uml.edu	21
T. Eagar	Phone: (617) 253-3229; Fax: (617) 258-6118; e-mail: tweagar@mit.edu	22
J. Lang	Phone: (617) 253-4687; Fax: (617) 258-6774; e-mail: lang@mit.edu	22
L. Evans	Phone: (617) 577-0100; Fax: (617) 577-0722; e-mail: evans@aspentec.com	23
P. Barton	Phone: (617) 253-6526; Fax: (617) 258-5042; e-mail: pib@mit.edu	23
D. Hardt	Phone: (617) 253-2252; Fax: (617) 252-1399; e-mail: hardt@mit.edu	23
Y. Iwasa	Phone: (617) 253-5548; Fax: (617) 253-5405; e-mail: iwasa@jokaku.pfc.mit.edu	24
D. Parks	Phone: (617) 253-0033; Fax: (617) 258-8742;	24
F. McClintock	Phone: (617) 253-2219; Fax: (617) 258-8742;	24
C. Peterson	Phone: (617) 253-5373; Fax: (617) 258-6149; e-mail: peterson@mit.edu	24
R. Probstein	Phone: (617) 253-2240; Fax: (617) 258-8559; e-mail: rfprobst@mit.edu	25
G. Stephanopoulos	Phone: (617) 253-4583; Fax: (617) 253-3122	25
H. Brenner	Phone: (617) 253-6687; Fax: (617) 258-8224; e-mail: hbrenner@mit.edu	26
A. Graham	Phone: (505) 665-5259: Fax: (505) 667-0600; e-mail: graham@lanl.gov	26
L. Mondy	Phone: (505) 844-1755; Fax: (505) 844-8251; e-mail: lamondy@sandia.gov	26
R. Goldstein	Phone: (612) 625-5552; Fax: (612) 625-3434;	26
D. Joseph	Phone: (612) 625-0309; Fax: (612) 626-1558	27
E. Pfender	Phone: (612) 625-6012; Fax: (612) 624-1398; e-mail: pfender@maroon.tc.umn.edu	27
J. Heberlein	Phone: (612) 625-4538; Fax: (612) 624-1398; e-mail: jvrh@maroon.tc.umn.edu	27
T. Rozzell	Phone: (202) 334-2908; Fax: (202) 334-2753; e-mail: trozzell@nas.edu	28
I. Blankston	Phone: (202) 358-4610;	28
J. Sheridan	Phone: (313) 995-0300; Fax: (313) 995-4004:	28
H.J.M. Hanley	Phone: (303) 497-3320; Fax: (303) 497-5224; e-mail: hanley@central.bldrdoc.gov	29
R. Kayser	Phone: (301) 975-2483; Fax: (301) 869-4020; e-mail: kayser@micf.nist.gov	29
W. Haynes	Phone: (303) 497-3247;	29
M. Moldover	Phone: (301) 975-2459;	29
J. Levelt-Sengers	Phone: (301) 975-2463;	29
J. Moreland	Phone: (303) 497-3641; e-mail: moreland@boulder.nist.gov	30
S. Russek	Phone: (303) 497-5097; e-mail: russek@boulder.nist.gov	30

Principal Investigators (cont'd - pg. 3)

S. Sanders	Phone: (303) 497-5096; e-mail: sanders@boulder.nist.gov	30
J. Ekin	Phone: (303) 497-5448; e-mail: ekin@boulder.nist.gov	30
A. Acrivos	Phone: (212) 650-8159; Fax: (212) 650-6835; e-mail: cheaa@ccnyme	30
R. Shinnar	Phone: (212) 650-6679; Fax: (212) 650-6686; e-mail: shinnar@che-mail.engr.ccny.cuny.edu	31
I. Rinard	Phone: (212) 650-7135; Fax: (212) 650-6686; e-mail: rinard@che-mail.engr.ccny.cuny.edu	31
G. Sivashinsky	Phone: (212) 650-8157; Fax: (212) 650-6835; e-mail: chemw@ccnyme	31
J. Achenbach	Phone: (708) 491-5527; Fax: (708) 491-5227; e-mail: achenbach@nwu.edu	31
S. Bankoff	Phone: (708) 491-5267; Fax: (708) 491-3728; e-mail: gbankoff@casbah.acns.nwu.edu	32
S. Davis	Phone: (708) 491-5397; Fax: (708) 491-2178; e-mail: sdavis@nwu.edu	32
M. Miksis	Phone: (708) 491-5585: Fax: (708) 491-2178; e-mail: miksis@nwu.edu	32
J. Ottino	Phone: (708) 491-3558; Fax: (708) 491-3728; e-mail: ottino@bart.chem-eng.nwu.edu	33
H. Riecke	Phone: (708) 491-3345; Fax: (708) 491-2178; e-mail: h-riecke@nwu.edu	33
H. Chang	Phone: (219) 531-5697; Fax: (219) 631-8366; e-mail: hsueh-chia.chang.2@nd.edu	33
M. McCready	Phone: (219) 631-7146	34
R. Mann	Phone: (615) 574-0834; Fax: (615) 574-7860; e-mail: mannrc@ornl.gov	34
E. Oblow	Phone: (615) 574-6187; Fax: (615) 574-7860; e-mail: oblowem@ornl.gov	34
L. Parker	Phone: (615) 241-4959; Fax: (615) 574-7860; e-mail: parkerle@ornl.gov	34
N.S.V. Rao	Phone: (615) 574-7517; Fax: (615) 574-7860; e-mail: raons@ornl.gov	34
C. Scott	Phone: (615) 574-6775; Fax: (615) 574-6442; e-mail: scottc@ctdvx5.priv.ornl.gov	35
T. Scott	Phone: (615) 574-5962; Fax: (615) 574-6442; e-mail: tcs@ornl.gov	35
S. Tanveer	Phone: (614) 292-5710; Fax: (614) 292-1479;	35
J. Welty	Phone: (503) 737-3441: Fax: (503) 737-2600;	35
K. Drost	Phone: (509) 375-2017;	36
H. Bau	Phone: (215) 898-8363; Fax: (215) 573-2065; e-mail: bau@eniac.seas.upenn.edu	36
G. Settles	Phone: (814) 865-6961; Fax: (814) 863-4848; e-mail: gss@ecl.psu.edu	37
G. Wilemski	Phone: (508) 689-0003; Fax: (508) 689-3232;	37
B. Wyslouzil	Phone: (508) 831-5250; Fax: (508) 831-5853;	37
C. Law	Phone: (609) 258-5271; Fax: (609) 258-6233; e-mail: cklaw@pucc.princeton.edu	38
S. Torquato	Phone: (609) 258-1309; Fax: (609) 258-1270;	38
F. Incropera	Phone: (317) 494-5688; Fax: (317) 494-0539; e-mail: incroper@mn.ecn.purdue.edu	39
M. Ishii	Phone: (317) 494-4587; Fax: (317) 494-9570;	39
I. Mudawar	Phone: (317) 494-5705; Fax: (317) 494-0539	39
E. Krempl	Phone: (518) 276-6351; Fax: (518) 276-6025; e-mail: krempe@rpi.edu	40
T. Lahey	Phone: (518) 276-8579; Fax: (518) 276-3055; e-mail: laheyr@rpit.edu	40
D. Drew	Phone: (518) 276-6903; Fax: (518) 276-4824; e-mail: drewd@rpi.edu	40
P. Wayner	Phone: (518) 276-6199; Fax: (518) 276-4030; e-mail: wayner@rpi.edu	41
J. Plawsky	Phone: (518) 276-6049; Fax: (518) 276-4030; e-mail: plawsj@rpi.edu	41
R. Spanos	Phone: (713) 527-4909; Fax: (713) 285-5191;	41
S. Teitel	Phone: (716) 275-4039; Fax: (716) 275-8527; e-mail: stte@pas.rochester.edu	41
E. Wolf	Phone: (716) 275-4397: Fax: (716) 473-0687;	42
E.G.D. Cohen	Phone: (212) 327-8855: Fax: (212) 327-8507; e-mail: rhyne@rockvax.rockefeller.edu	42
A. Kerstein	Phone: (510) 294-2390; Fax: (510) 294-1004; e-mail: kerstein@ca.sandia.gov	43
R. Steeper	Phone: (510) 294-2618; Fax: (510) 294-1004; e-mail: steeper@ca.sandia.gov	43
C. Campbell	Phone: (213) 740-0498; Fax: (213) 740-8071; e-mail: campbell@ian.usc.edu	43
T. Maxworthy	Phone: (213) 740-0481; Fax: (213) 740-7774; e-mail: maxworth@mizar.usc.edu	44
E. Meiburg	Phone: (213) 740-5376; Fax: (213) 740-7774; e-mail: eckart@spock.usc.edu	44
M. Sablik	Phone: (210) 522-3342; Fax: (210) 647-4325; e-mail: mjsablik[marty@swri.space.swri.edu	44
G. Burkhardt	Phone: (210) 522-2705; Fax: (210) 684-4822;	44
H. Kwun	Phone: (210) 522-3359; Fax: (210) 684-4822;	44

Principal Investigators (cont'd - pg. 4)

J. Eaton	Phone: (415) 723-1971; Fax: (415) 723-4548; e-mail: eaton@sierra.stanford.edu	45
D. Barnett	Phone: (415) 723-4143; Fax: (415) 725-4034; e-mail: barnett@leland.stanford.edu	45
G. Herrmann	Phone: (415) 723-4134: Fax: (415) 723-1778;	45
G. Kino	Phone: (415) 723-0205; Fax: (415) 725-7509; e-mail: kino@sierra.stanford.edu	46
J. Koseff	Phone: (415) 723-9032; Fax: (415) 725-8662; e-mail: koseff@cive.stanford.edu	46
C. Kruger	Phone: (415) 723-0977; Fax: (415) 725-6847; e-mail: kruger@sierra.stanford.edu	46
T. Owano	Phone: (415) 723-1295; Fax: (415) 723-1748; e-mail: owano@saha.stanford.edu	46
J. Ross	Phone: (415) 723-9203; Fax: (415) 723-4817; e-mail: ross@chemistry.stanford.edu	47
R. Zare	Phone: (415) 723-3062; Fax: (415) 723-9262; e-mail: zare@stanford	47
G. Scmidt	Phone: (201) 216-5643; Fax: (201) 216-5638; e-mail: gschmidt@vaxc.stevens-tech.edu	47
A. Chernikov	Phone: (201) 216-8358; Fax: (201) 216-5638; e-mail: achernik@vaxc.stevens-tech.edu	47
C. Wu	Phone: (409) 845-8401; Fax: (409) 845-1307; e-mail: wu@spindletop.tamu.edu	48
P. Eubank	Phone: (409) 845-3339; Fax: (409) 845-6446;	48
M. Barrufet	Phone: (409) 845-0314; Fax: (409) 845-1307; e-mail: barrufet@spindletop.tamu.edu	48
I. Prigogine	Phone: (512) 471-7253; Fax: (512) 471-9621; e-mail: statmech@order.ph.utexas.edu	48
T. Petrosky	Phone: (512) 471-7253; Fax: (512) 471-9621; e-mail: statmech@order.ph.utexas.edu	48
H. Swinney	Phone: (512) 471-4619; Fax: (512) 471-1558; e-mail: swinney@chaos.utexas.edu	49
M. Kachanov	Phone: (617) 627-3318; Fax: (617) 627-3819;	49
W. Roman	Phone: (203) 727-7950; Fax: (203) 727-7911; e-mail: war@utrc.utc.com	50
S. Hay	Phone: (203) 727-7198; Fax: (203) 727-7911; e-mail: soh@utrc.utc.com	50
A. Kobayashi	Phone: (206) 543-5488; Fax: (206) 685-8047; e-mail: ask@u.washington.ed	50
B. Ghosh	Phone: (314) 935-6039; Fax: (314) 935-6121;	51
T. Troutt	Phone: (509) 335-4375; Fax: (509) 335-4662; e-mail: troutt@mme.wsu.edu	51
G. Kojasoy	Phone: (414) 229-5191; Fax: (414) 229-6958;	51
W. Ray	Phone: (608) 263-4732; Fax: (608) 262-0832; e-mail: ray@chewi.che.wisc.edu	52

United States
Department of Energy
Washington, D.C. 20585

Official Business