DOE/ER-0601P

Summaries of FY 1993 Engineering Research

September 1993

U.S. Department of Energy

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

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831; prices available from (615) 576-8401,

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.

Printed with soy ink on recycled paper

DOE/ER-0601P
UC-402

Summaries of FY 1993 Engineering Research

September 1993

U.S. Department of Energy

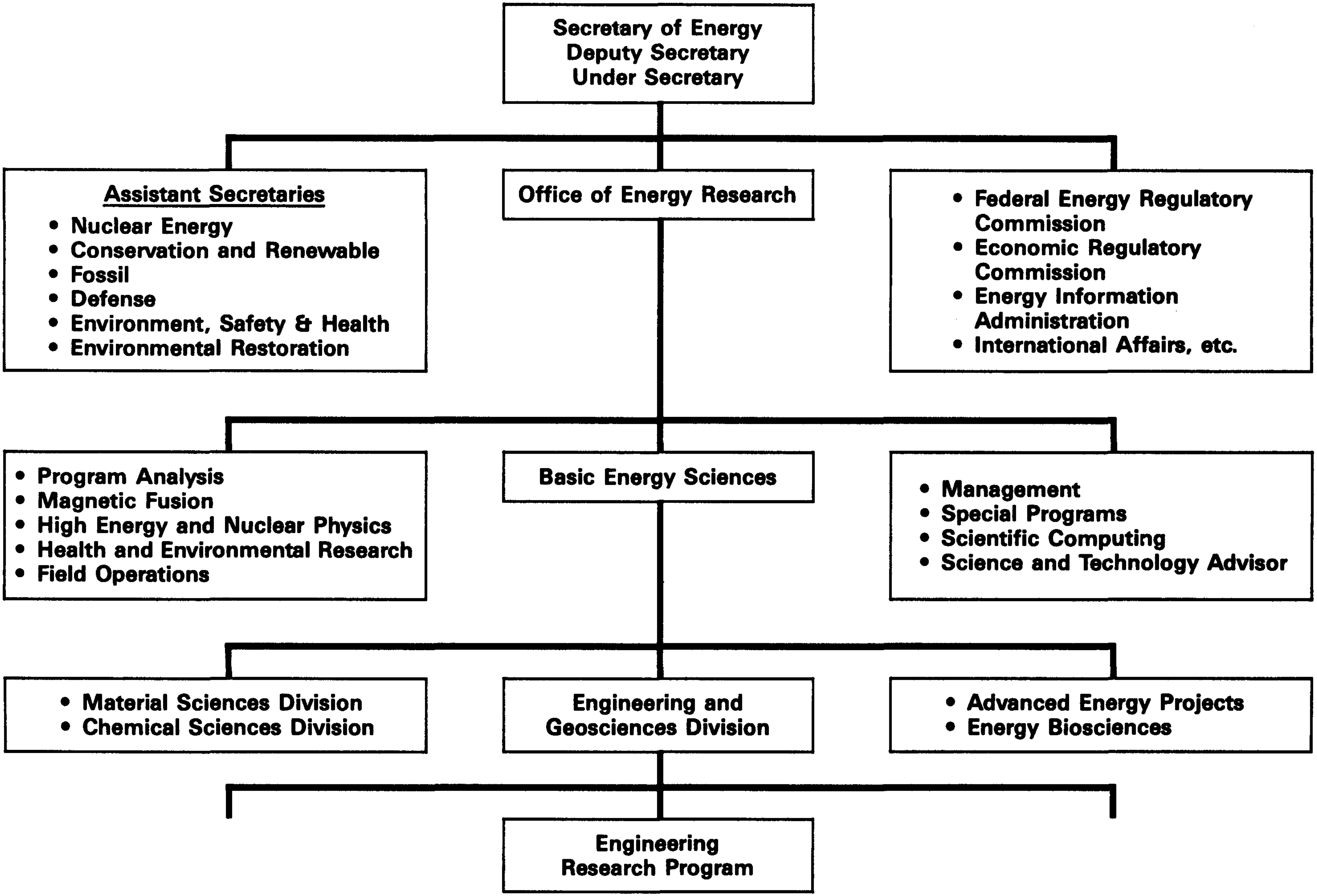
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences
Washington, DC 20585

Foreword

This report documents the BES Engineering Research Program for fiscal year 1993; it provides a summary for each of the program projects in addition to a brief program overview. The report is intended to provide staff of Congressional committees, other executive departments, and other DOE offices with substantive program information so as to facilitate governmental overview and coordination of Federal research programs. Of equal importance, its availability facilitates communication of program information to interested research engineers and scientists. The organizational chart for the DOE Office of Energy Research (OER) on the next page delineates the six Divisions within the OER Office of Basic Energy Sciences (BES). Each BES Division administers basic, mission oriented research programs in the area indicated by its title. The BES Engineering Research Program is one such program; it is administered by the Engineering and Geosciences Division of BES. Dr. Oscar P. Manley is technical manager of the Engineering Research Program; inquiries concerning the program may be addressed to him, in writing or by phone at (301) 903-5822.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1993. 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 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 1993.

The projects are numbered sequentially for individual identification in the indexes. 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 1993 appears to the right of title; it is followed by the budget activity number (e.g., 01-A). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The 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., 90-3). 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).

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, two 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.

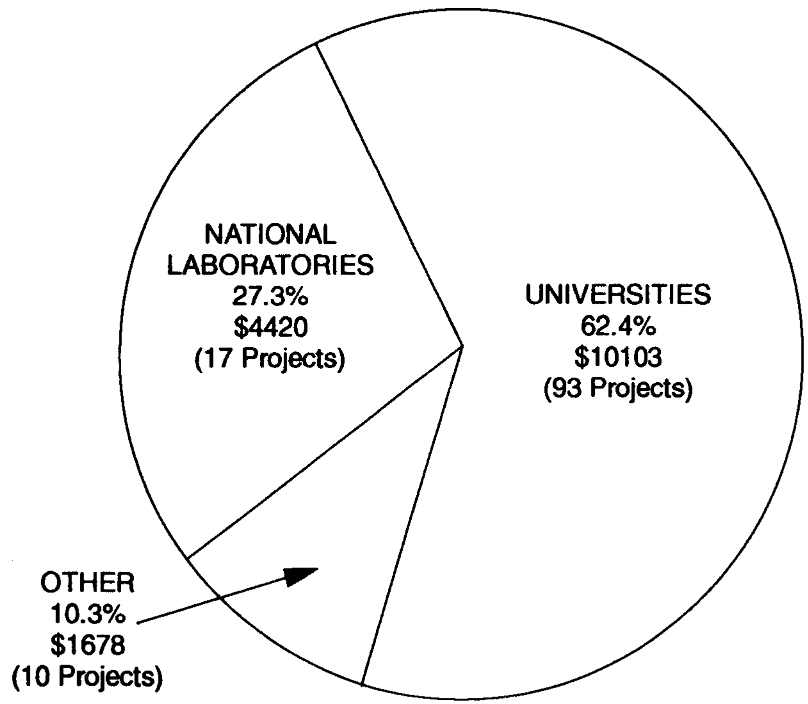
Another workshop aimed at identifying research opportunities to mitigate the effects of aging in energy production and distribution systems took place in October 1992. The proceedings have appeared in Applied Mechanics Reviews.

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 24 three-year doctoral fellowships administered by National Academy of Science 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 1993 the available program operating funds available amounted to about $16.2 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 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 '93 BUDGET ($000's) BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM

FY '93 BUDGET BY TECHNICAL AREAS

	($000's)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	**5329**	**32.9**	**51**
SYSTEMS SCIENCES	**4573**	**28.2**	**22**
ENGINEERING ANALYSIS	**6300**	**38.9**	**47**

Table of Contents

Table of Contents (continued)

University Of Alabama

Dept of Mathematics **$54,123**
Tuscaloosa, AL 35487 **01-C**
91-3

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**
90-3

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 Cornell 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**
90-3

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.

University of Arizona

Aerospace & Mechanical Eng **$136,301**
Tucson, AZ 85721 **01-B**
93-3

Film Cooling in a Pulsating Stream
I. Wygnanski

This project will deal with heat transfer to or from *an isothermal surface whose temperature will be either hotter or colder than the jet temperature. The jet temperature, on the other hand, might be equal to or different from the ambient temperature.* This will help us to separate the coherent structures which are affected by the heat flux from the surface from the coherent structures which are affected by the heat flux occurring between the jet and the ambient stream (i.e. in the outer mixing layer). The wall jet will flow over a thick conducting plate placed above a constant temperature reservoir which might be either hotter or colder than either the jet or the ambient fluid. Measurements of turbulent heat flux in the direction normal to the plate will be accomplished with a combination of hot-wire anemometers and miniature thermocouple sensors (effective diameters 0.003 in.), or by a combination of cold-wire (resistance) anemometers and PIV (Particle Image Velocimeter).

We shall start the study with the unheated jet flowing over a heated surface thus the flow will never attain a thermal equilibrium with the surface. Whenever the wall and the ambient stream are at the same temperature but the jet emerges from the nozzle at a different temperature the flow might approach an equilibrium far downstream due to the finite heat flux from the nozzle. We propose to initiate an investigation in the absence of an external stream and we shall add a relatively weak external stream soon thereafter. Forcing the flow uniformly across the span at a single frequency will provide a well-defined correlation between the large spanwise eddies and heat transfer.

The first step in each investigation will cover the Reynolds averaged quantities for the unperturbed flow. This will include temperature ranges which will alter the mean flow characteristics through the nonlinear coupling between velocity and temperature fluctuations while keeping the boundary conditions at the wall and at infinity well defined (i.e. constant). It will enable us to validate our experimental techniques and our numerical codes as well as some of the conventional models used. We may also consider the major instability mechanisms of such flows in order to establish the forcing parameters needed as inputs to the second stage (the main stage) of the investigation. It will be useful to consider the relative significance of the secondary instabilities and the non planar modes as their relevance may be altered by the addition of heat. (We only recently discovered that the plain, unforced, turbulent incompressible wall-jet contains two, nonlinearly coupled modes of instability. Both must be considered in any attempts to understand and control the wall jet). We will then force the flow by providing velocity oscillations emanating from the plenum chamber and later we may attempt to force the flow by using oscillatory heating thus altering the forcing between velocity and temperature fluctuations.

Arizona State University

Mechanical & Aerospace Eng **$50,000**
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 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 is 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 **$94,027**
Columbus, OH 43201-2693 **01-A**
90-3

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

The goal of this research is to study the high-temperature damage and failure processes and to further develop a method for predicting this behavior in an effort to increase structural life. In particular, we focus on time-dependent damage which occurs under history-dependent loading conditions, i.e. transient conditions.

The approach taken here is to combine experimental studies of both sustained-load and variable-load creep with careful analytical studies. To date, eight crack-growth tests on both a stainless steel and a 9CRMo steel have been performed. These time dependent crack-growth specimens were subjected to carefully chosen load-history spectrums so that different crack-growth histories were obtained. The implications of using classical creep constitutive theories (Norton, strain hardening) to predict the behavior were ascertained. In addition, the use of various integral parameters to characterize the crack tip phenomena were developed and evaluated.

It was clearly shown that constitutive laws such as Murakami-Ohno Krempl-type laws must be used in order to adequately predict the response. Most importantly, recently it has been shown that new energy-based integral parameters can characterize the crack- growth behavior of the test specimens subjected to complex history-dependent loading. In addition, they can predict crack nucleation. Classical methods based upon rate-type asymptotic parameters developed from simple constitutive theories break down.

University Of California/B

Dept of Electrical Engineering & Computer Sciences
Berkeley, CA 94720

$184,369
06-C
93-3

Dynamics of Electronegative Plasmas for Materials Processing

A. Lichtenberg, M. Lieberman

The purpose of this project is to study electron heating mechanisms in radio frequency (r.f.) discharges. These discharges are used extensively by industry for surface modification of electronic and mechanical materials. In addition to the usual r.f. ohmic heating in the plasma interior, it has been found theoretically that stochastic heating at the plasma surface arising from successive decorrelated reflections of electrons with the oscillating sheath plays a major role. The efficiency of stochastic heating depends on the detailed sheath dynamics.

The sheath dynamics have been measured and related to the predicted stochastic heating for a plane parallel argon discharge. The measured results, together with related plasma simulations, have been used to construct better predictive models of discharge behavior and parameter scaling. It has been found for a low pressure discharge at 3 mTorr, power of 100 watts, and frequency of 13 MHz,95% of the electron heating is predicted to occur stochastically.

Stochastic heating can be enhanced with a resonant helical discharge structure. This geometry is of importance for materials processing applications in that it may be operable at very low pressure (<1 mTorr). Studies of stochastic heating and determination of equilibrium plasma parameters have been made in argon and nitrogen, with good agreement between theory and experiment.

University Of California/B

Dept of Mechanical Engineering
Berkeley, CA 94720

$120,603
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. Specifically, the program includes investigations of radiative heat transfer in thin films, conductive heat transfer in quantum well laser, and short-pulse laser-material interactions.

A combined analytical and experimental research program on radiative interactions with microstructures has been directed to characterize (1) the partially coherent radiative properties of thin films and (2) the strong coupling between electromagnetic wave propagation and the radiation absorption thermal field. The findings are useful for optical characterization of thin films, design and operation of optical bistability devices, and localized processing of film structures.

Allium arsenide based quantum well lasers represent a rapidly expanding area of research and development. A new measurement technique that determines thermal diffusion of thin films in both parallel and perpendicular directions has been developed, and the experimental results agree with those of the concurrent theoretical study. With knowledge of the anisotropic thermal diffusivity in semiconducting quantum well lasers, the temperature rise and heat generation mechanisms at the facets were further investigated.

Pulse durations in modern short-pulse lasers have been reduced from microseconds to femtoseconds, greatly increasing the time resolution of optical observations and the spatial controllability of laser processing. A general macroscopic model based on microscopic electron-lattice interaction and electron transport was developed to describe short-pulse laser heating of metals. Femtosecond laser heating experiments were conducted for single and multi-layer metal films. The knowledge gained in this research program is useful for the thermal design of high-power laser components and for a better control of short-pulse laser microfabrication as well as short-pulse laser diagnostics.

University Of California/LA

Mech, Aero & Nuclear Eng Dept **$90,024**
School of Eng & Applied Science **01-C**
Los Angeles, CA 90024-1597 **92-3**

Basic Studies of Transport Processes in Porous Media
I. Catton, V. Travkin, L. Gratton

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 **$112,850**
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 **$79,000**
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 **$165,000**
La Jolla, CA 92093-0402 **06-C**
90-4

Nonperiodic, 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 this 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 **$126,000**
La Jolla, CA 92093 **06-B**
93-3

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

This research involves a combined experimental and theoretical effort related to the behavior of fuel droplets in well defined but nonuniform flows. Our current research concerns 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 opposed and impinging flows has been put into operation. By installing an appropriate grid in one or both ducts sprays in turbulent streams can be studied. Initial results involve the structure and extinction characteristics of laminar flames using a phase doppler particle analyzer which permits measurement of two velocity components, droplet diameter and number density. Several publications on this research have appeared. One interesting observation from these laminar studies is that under some flow conditions larger droplets from the spray pass through the stagnation plane into the opposing gas stream and oscillate about that plane. This phenomenon has been studied experimentally in terms of single droplets and in sprays. Related theoretical studies identify the parameters of droplet and flow determining whether or not oscillations occur. An interesting manifestation of such oscillations in sprays is that the probability density of the axial velocity of droplets on the axis of the flow at points above the stagnation plane can be bimodal with both positive and negative velocities. A theoretical treatment of this phenomenon is underway. Initial experiments on a turbulent spray impinging on a wall without combustion with the aim of determining the relative velocity between gas and droplets of various sizes has been completed. Data analysis and interpretation are underway.

University Of California/SD

Department of Chemistry, 0340 **$183,512**
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. The asymptotic behavior is well established, but sets in only after extremely long times. The hierarchy of kinetic regimes for all times has now been determined under a variety of conditions. This work continues with a broader set of reactions and geometries.

Transport on certain quasi-random fractals has been determined analytically. One aim is to extend the approach to more complex fractals. Another is to investigate transport on structures that in one extreme parameter regime are Euclidean but in another are fractal. This is done by replacing holes or disallowed pathways on fractals with appropriate barriers. At short times a walk on such a structure is indistinguishable from that on the associated fractal; at long times it should appear Euclidean. The crossover time should be determined by a tunable parameter such as the temperature. Preliminary results have been obtained.

Systems subject to deterministic and/or stochastic forces exhibit interesting behavior caused by the interplay of nonlinearity, noise and deterministic forces. A path integral approach has been successful for the analysis of the response of nonlinear systems to colored noise; developments in this area continue. A difference equation approach has provided the response of a linear system to a coin-toss square wave, leading to unexpected non-monotonic response. The response of nonlinear systems to combinations of deterministic and stochastic forces is under investigation.

University Of California/SD

Department of Mathematics **$98,000**
La Jolla, CA 92093 **06-C**
93-1

Knot Invariants and the Thermodynamics of Lattice Gas Automata
D. Meyer

Some discrete models for dynamical systems (like lattice gas hydrodynamics) exhibit approximately thermodynamic behavior despite the presence of conserved quantities other than the energy/momenta and even for small system size (e.g., the lattice gas models for two phase flow through porous media). The goal of this project is to build on the understanding of the connections between knot invariants, exactly solvable statistical mechanics models and discrete dynamical systems gained in earlier work (appearing in Physica D and Knots 90) toward an answer to the question of how this early and robust thermodynamic behavior occurs in lattice gas automata.

The basis of the approach is exemplified by the result that one specific reversible cellular automaton model with a conserved quantity is equivalent, in the sense that the ensemble of 1 + 1 dimensional spacetime evolutions is the same as the equilibrium ensemble of 2 dimensional configurations, to a solvable statistical mechanics model at a critical point. In addition to the association between the critical limit of solvable models and knot invariants, the physical characteristics of the critical point are consistent with the canonical distribution observed in simulations.

Current work includes the application of this approach to a family of 1 dimensional lattice gas automata based on a model of 't Hooft. The intention is also to study the relation between the lattice gas analysis of this model and 't Hooft's defect/curvature interpretation. Recent developments (Vassiliev knot invariants) are expected to lead to a better understanding of the connection between the usual perturbative analysis and global topological properties of these nonlinear systems. Investigation of higher dimensional models, *via* solutions of the tetrahedron equation, has also begun.

University Of California/SD

Inst for Nonlinear Science, R-002 **$95,145**
La Jolla, CA 92093 **06-C**
93-3

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

The direct numerical simulations (DNS) of turbulent flows with high Reynolds numbers (which are encountered in many engineering enterprises), are impossible now and in the foreseeable future. The major goal of this project is to advance the knowledge of the structure of turbulence, aiming it at a subgrid-scale modelling for the large-eddy simulations (LES). Among the tools being developed for achievement of this goal are: 1) conditional averaging of Navier-Stokes (NS) equations; 2) use of Markov processes with dependent increments, consistent with NS equations, 3) description of intermittency in terms of breakdown coefficients and associated infinitely divisible probability distributions; and 4) incorporation of experimentally observed coherent structures into the statistical description of turbulence.

A number of new results was obtained by using these tools, in particular, probability distribution for three-dimensional vectors of velocity increments, which has an unusual form. A hierarchy of subgrid-scale models was obtained and preliminary testing was done by DNS (for moderate Reynolds numbers) and by LES for isotropic, shear-flow and free-surface turbulence. Numerical simulations are performed in cooperation with workers at Stanford University and Science Applications International Corporation. Corresponding laboratory experiments (in particular, for free-surface turbulence) are performed in cooperation with Caltech. The obtained analytical, numerical and experimental results open a new perspective for more detailed studies of the structure of turbulence and subgrid-scale modelling.

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 wife variety of potentially important phenomena. Examples of practical interest include solar ponds and atmospheric and oceanographic flows.

Experiments involving an annular geometry have been used to confine the convective rolls to a quasi one-dimensional pattern which facilitates a simplified theoretical analysis. As a result of this work, there is now a basic understanding of the dynamics of uniform and confined states of traveling waves, including an understanding of the role that the concentration field plays in these dynamics. Recent work in this one-dimensional geometry bs focused on the instability of uniform traveling waves to wavelength perturbations (i.e., the "Eckhaus" instability). Experiments in progress focus on the nature of traveling-wave convection in a large aspect ratio, two-dimensional geometry. Important issues to be addressed include two-dimensional wavelength instabilities and the dynamics of defects.

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 tire 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, G. Hetsroni

Experiments have been completed to visualize wave turbulence interactions near shear-free gas-liquid interfaces. Mechanically generated waves of different lengths and amplitudes were imposed on the flow and the effects on the turbulence structure determined. It was found that the nearwall structure was affected by interfacial waves in the relatively shallow stream studied. In particular, the wall region was found to couple with waves in frequency ranges of about the same magnitude as bursts/ejections. A paper has been published in Physics of Fluids ("Wave-Turbulence Interactions in Free-Surf ace Channel Flows", M. Rashidi, G. Hetsroni and S. Banerjee, 1992).

In addition, work using laser Doppler anemometry has continued in parallel with flow visualization. It has been found that wall region coherent structures, which are normally thought of as streaks, burst/ejections and in-sweeps, as well as relatively short quasi-streamwise vortices, may actually be one funnel-shaped structure in which the fluid motion is initially in the form of relatively tight quasi-streamwise vortices, later on expanding to trace the surface of a funnel laid sideways in the flow. The phenomenon, to some extent, is reminiscent of vortex breakdown. Ejections and in-sweeps are then the rising and falling portions of fluid that trace the surface of the funnel. Work is continuing to establish whether these are in reality the determining structures in boundary layer flows and whether simple models can be constructed on their basis. To support these efforts, three-dimensional velocity fluctuations are being measured in conjunction with visualization of small oxygen microbubble tracers.

So far as the effect of interfacial waves is concerned, a new wavemaker has been constructed and is in the process of being commissioned. The wavemaker is placed in the tank from which the fluid enters the test section, and care is being taken to suppress vortex shedding which may give rise to nontypical and persistent flow structures.

The thrust of the work has now turned to the effect of interfacial waves on the streamwise funnel-shaped structures described in the previous paragraphs. Direct numerical simulation in support of these experiments has continued. It has been found that if fluid tracer particles are injected into numerical simulations, then they do trace a path similar to the streamwise funnel-shaped vortices seen in the experiments.

Direct simulation of the effect of interfacial waves will be initiated, again, when the wall region structures have been better identified in order to understand the interactions between waves and such structures.

California Institute Of Technology

Chemical Engineering 210-41 **$125,728**
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. For example Partial Least Squares (PLS) has been highly regarded by practitioners although the relationship between PLS and other established regression methods has been incomplete. A firm mathematical link has been developed between PLS and statistical significance testing. Based on these new results, PLS has been extended to deal with outliers (robust estimation) and more general statistical models, e.g. the measurement error model.

Carnegie Mellon University

Chemical Eng Dept & Graduate **$ 0**
School of Indus Admin **03-A**
Pittsburgh, PA 15213 **89-4**

Integration of Redesign Methodologies for Chemical Processes
L. Biegler, I. Grossmann, G. Thompson, A. Westerberg

Process redesign, commonly known as retrofit, is a major task in the chemical industries. However, most systematic design strategies have been developed for new process and often do not apply. This project addresses the development of systematic design methodologies for the redesign of chemical processes. This integrated approach deals with a broad range of problems in process redesign. Here we discuss progress in the following areas:

1) Development of Efficient Optimization Algorithms for Discrete and Continuous Variables. Efficient decomposition strategies for nonlinear programming have been developed for large-scale process optimization. These are currently being tailored to various problem types including optimization problems in flowsheet optimization, parameter estimation and data reconciliation. The work also includes the solution of several large scale combinatorial optimization problems that frequently occur in chemical engineering applications, namely, traveling salesman, and set covering set packing, and set partitioning problems. These algorithms have also been developed on various sequential and parallel computers such as the CRAY YMP, the Alliant FX/8 and the CMU Nectar network.

2) Redesign of multicomponent separation sequences. Our goal is an approach to redesign separation processes where the species display azeotropic behavior. These processes are complex, requiring recycles in principle. Mixing

can often be used to improve separation. For homogeneous azeotropic ternary mixtures, we have two analysis results: (1) a technique to determine all possible products which can be obtained in a single feed, two product distillation columns whether at total or finite reflux and (2) an approach to determine if an extractive agent will allow separation of a binary mixture into desired products.

We are testing a new method to compute minimum flows in any column. We have a methodology to produce automatically alternative process configurations for such processes and have tested it on many examples, including a mixture of methanol, water, n-pentane and acetone. We are also studying retrofit design for such processes involving trace species - i.e., for waste recovery systems.

(3) Redesign of energy management systems. Mixed-integer nonlinear programming (MINLP) models have been developed for grassroots and the redesign problems. The unique feature of these models is the fact that the level of energy recovery and selection of matches is optimized simultaneously without fixing temperature approaches. We have recently developed a new global optimization algorithm for networks with fixed topology. The basic idea relies on a rigorous nonlinear convex NLP underestimator that provides tight lower bounds, and that is coupled with a spatial branch and bound method. Typically not more than five NLP optimizations are required to find the global optimum. Work is under way to extend this method for the optimization of topologies in which we intend to use as a basis a recent LP/NLP based branch and bound method for MINLP optimization. Finally, the interactive program SYNHEAT is under development for the implementation of these models.

(4) Redesign for flexibility and reliability. The expected stochastic flexibility, a new measure that integrates the two operability characteristics, has been developed. The proposed measure can be used to evaluate the probability of feasible operation, given uncertainties in process parameters and operational states. We have recently developed an NLP optimization model for optimizating the stochastic flexibility in nonlinear process models. This formulation, which embeds the integration of multiple integrals using Gaussian quadrature, is solved with the Generalized Benders decomposition method. The application of this method has been illustrated in bi-criterion optimization problems for maximizing flexibility and minimizing investment cost. Also, an interesting relationship of our metric with Taguchi's quadratic loss function has been established.

(5) Optimization-based Methods for Process Identification and Control. Optimization-based algorithms are being developed for the control of constrained, nonlinear processes; these are also being used to control open loop unstable processes. An extended stability theory has been developed and demonstrated, both for constrained and unconstrained systems. In addition, both exterior and exact penalty function strategies have been developed and analyzed for constrained model-predictive control algorithms. Finally, tailored nonlinear and quadratic programming algorithms are being developed for more efficient solution of these problems. These have been illustrated on a number of process examples.

Carnegie Mellon University

Dept of Elec & Comp Eng **$100,860**
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 of 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 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 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. And the dynamic task requirements are translated to obtain the sizes and rating of the actuators or joints.

University Of Chicago

Dept of Chemistry **$ 0**
Chicago, IL 60637 **06-C**
92-1

Finite-Time Thermodynamics and Effective Energy Use
S. Berry

The period 1992-93 was fruitful. The work followed two lines, the principal objectives of the current work. One is the development of methods of optimizing engines and processes by optimal control methods for distributed systems and averaged systems. The other is the development of a self -consistent thermo-hydro-mechanics for nonequilibrium systems. The two publications from the former illustrate that approach[1,2]: the first continues our earlier work[3] by applying constraints of finite-time operation and by developing a computational algorithm for cases with no analytic solutions. The second analyzes the internal combustion engine and exposes ways to improve its efficiency or power delivery, in some cases by heating the system rather than cooling it, for part of the cycle. This work is being continued with a postdoctoral, Vladimir Kazakov, and Professor Anatoly M. Tsirlin, visiting in Fall, 1993. Both are from the Institute for Optimization and Control Theory, Pereslavl-Zalessky, Russia.

The other line is also represented by two recent publications[4,5]: the first overcomes the traditional limitation of neglect of the finite heat propagation rate and develops a finite-time formalism based on hyperbolic differential equations. The, second develops a Lagrangian treatment in which canonical variables are introduced for nonequilibrium thermodynamics.

---

1. V. N. Orlov and R. S. Berry, "Analytical and numerical estimates of efficiency for an irreversible heat engine with distributed working fluid," Phys. Rev. A 45, 7202 (1992).

2. V. N. Orlov and R. S. Berry, "Power and efficiency limits for internal combustion engines via methods of finite-time thermodynamics," J. Appl. Physics (in press, 1993).

3. V. N. Orlov and R. S. Berry, "Power output from an irreversible heat engine with a nonuniform working fluid," Phys. Rev. A 45, 7230 (1990).

4. S. Sieniutycz and R. S. Berry, "Least-entropy generation: Variational principle of Onsager's type for transient hyperbolic heat and mass transfer," Phys. Rev. A 46, 6359 (1992).

5. S. Sieniutycz and R. S. Berry, "Canonical formalism, fundamental equation and generalized thermomechanics for irreversible fluids with heat transfer," Phys. Rev. E 47, 1765 (1993).

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.

Clarkson University

Dept of Chemical Engineering **$62,000**
Potsdam, NY 13676 **01-C**
91-3

Lift and Drag Forces on Droplets and Particles in Wall-Bounded Flows
J. McLaughlin

The goal of this research is to obtain quantitative information about the lift and drag forces that act on small droplets or particles that translate through shear flows. Such forces affect the motion of droplets or particles near a rigid wall. Thus, a knowledge of the forces is needed to describe processes such as the deposition of aerosols on solid surfaces.

The approach used in the research involves a combination of analytical, numerical, and laboratory work. Asymptotic expressions have been derived for the lift and drag forces in the regime of small Reynolds numbers. In most situations of practical importance, however, the droplet or particle Reynolds numbers are not small compared to unity. At finite Reynolds numbers, direct numerical simulations of the three-dimensional flow field around a sphere in a shear flow have provided the forces. The experiments involve measurements of particle migration velocities in a vertical homogeneous shear flow apparatus. The results provide checks of the numerical and theoretical work.

The asymptotic and experimental portions of the project are done. The numerical study is still under way. The numerical results to date are in good agreement with the asymptotic and experimental findings when the particle Reynolds numbers are smaller than unity.

University Of Connecticut

Dept of Mechanical Engineering **$50,000**
Storrs, CT 06268 **01-A**
92-3

Engineering Science Software

Smithfield, RI 02917 **$48,000**
01-A
92-3

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

In the first part of the program a model that allowed polycrystalline elastic and viscoplastic constitutive behavior to be predicted from crystallographic slip in single crystals was developed and verified in high temperature biaxial polycrystal experiments.

In the ongoing research the goal is to predict the degree of heterogeneity of deformation and verify these predictions experimentally. Two types of theoretical models have been used to predict heterogeneity. The first model involves averaging the effect of neighboring grains while the second model using a unique Green's function method, allows arrays of grains to be modeled explicitly. Calculations done to date show that the self-consistent model significantly underestimates the heterogeneity compared to the more realistic explicit model. The most extreme heterogeneity found in studying 50,000 grains was not nearly as great as in a pair of artificially constructed arrays designed to produce extreme heterogeneity.

The strain in individual grains was recorded in a coarse grained sample using the Moire' interferometry apparatus at INEL. Reduction of this raw data to strain fields is now ongoing. Preliminary results show that the inelastic response is extremely heterogeneous. The modeling software is now being enhanced to include constitutive model with an appropriate abrupt yield behavior to see if the observed extreme heterogeneity can be modeled. Neutron diffraction experiments are to commence on July 22, 1993 at Argonne National Labs. In these experiments elastic strains will be measured for both surface and interior grains. Thus data will nicely complement the Moire' data which reveals the total strain of surface grains only. Developing models to predict grain to grain heterogeneity and verifying these models is a basic element in modeling mechanical behavior. Such heterogeneity is important in fatigue which starts in the most unfavorably oriented grain, in modeling stress induced phase transformation and in grinding where heterogeneity may influence surface finish.

Cornell University

Mechanical & Aerospace Engineering $62,988
Ithaca, NY 14853 01-A
91-3

Chaos in 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, 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 multifractals 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 later 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 motions 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 walk 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 **$105,818**
Ithaca, NY 14853 **01-C**
91-3

Experiments in Turbulent Mixing
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.

The jet experiment, in which a fine circular heated wire is placed close to the jet exit and concentric with it, is an analogue of a heated line source in grid turbulence, a much studied subject. The motivation in both cases is to determine the rate at which a scalar contaminant mixes disperses when it is introduced at a scale much smaller than that of the velocity field. Our results show that in the jet, mixing is faster due to the shear and that by about 20 jet diameters downstream complete mixing has occurred. Examination of various quantities such as the probability density function (pdf) and conditional statistics provides insight into the dynamical details of the mixing process.

Our work on grid turbulence has concentrated on the behavior of temperature spectra and the scalar pdf. We have shown that the pdf, under certain circumstances, has tails much broader than would be expected from a Gaussian distribution and that the temperature spectra obey Obukhov-Corrsin-Kolmogorov scaling even at very low Peclet numbers and without local isotropy in the scalar field.

Dartmouth College

Thayer School of Engineering **$ 0**
Hanover, NH 03755 **06-C**
91-2

Mixing and Settling in Continuous Metal Production
H. Richter

In modern metallurgical processes metal is produced continuously and directly from ore in single converters operated in horizontal mode using submerged gas injection into the liquid metal-slag bath. These reactors promise substantial fuel savings and much better control of pollutants than common practice. The injected gas must create sufficient turbulence to provide excellent gas-liquid contact in order to maximize heat and mass transfer in the bath, but this turbulence must be selectively localized to provide adequate phase separation zones of metal and slag between active turbulent zones.

Knowledge of liquid entrainment into the bubble plume created by submerged gas injection, and of liquids separation are of fundamental value in designing reactors, however these phenomena are also of generic interest to other processes, such as the current major DOE-AISI direct steelmaking process or severe accident analysis of nuclear reactors.

In this work mixing caused by submerged gas injection into a bath and subsequent phase separation of two immiscible liquids representing slag and metal are being studied experimentally and analytically. Novel instrumentation for local measurement of volume fractions of gas and liquids has been developed. First experimental results of liquid flow velocities induced by gas injection and volume fractions of gases and liquids in and around the gas plume as well as complementing numerical results are available.

Dartmouth College

Thayer School of Engineering **$120,600**
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 Bernoulli 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 Bernoulli 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

Department of Physics **$60,000**
Durham, NC 27706 **01-C**
93-3

Experimental and Analytical Investigations of Flows in Porous Media
R. Behringer

Research objectives for this project include the development and application of two novel techniques for studying flow in porous media. These techniques are: 1) magnetic Resonance Imaging (MRI), and 2) a novel shadowgraph technique, to be referred to as MST (Modified Shadowgraph Technique). The primary goals are to use these techniques to characterize and understand convective flows in porous media, including pattern selection, secondary instabilities, and time dependence. MRI provides both local velocity and local fluid density information. MST provides pattern information easily and efficiently. Both techniques are fully operational. An important finding is that the geometric structure of the medium plays a fundamental role in pattern selection. Media constructed from periodic arrays of bars show a well defined transition to convection and sharply defined parallel convection rolls with orientation determined by the symmetry of the array. Media consisting of a random array of holes show disordered patterns and an imperfect bifurcation to convection. Numerical studies are underway to probe the role of media structure on the pattern. Studies where the median is constructed from semi-ordered and well ordered arrays of spheres show patterns near onset with more symmetry than the random-hole media but less symmetry than the periodic bar media.

Idaho National Engineering Lab

Bioprocess & Environ Assessment **$109,000**
Idaho Falls, ID 83415 **06-A**
89-3

Three Phase System Modelling
G. Andrews

The behavior of bubbles of gas in liquids containing surface-active solutes is critical to the performance of processes like floatation, fermentation, and gas/liquid reaction. These bubbles are usually in the millimeter size range, ellipsoidal or cap-shaped rather than spherical and rise with a Reynolds number, Re, of several hundred. This project is developing a theoretical model for such bubbles. It includes mass transfer of surfactants between the liquid and the bubble interface, the effect of the absorbed surfactant on the interface force balance and thus on the mobility of the interface and the hydrodynamics in the boundary layer around the bubble. The objective is to predict gas/liquid mass transfer rates, particle capture rates by the rising bubble and ultimately bubble shape as a function of surfactant concentration. New forms of integral boundary layer theory have been developed to predict the behavior of boundary layers on a moving spherical interface at Re of a few hundred.

Results are significantly different from previous theories based on creeping flow ($Re<1$) hydrodynamics. Experiments on the capture of latex particles are being conducted for comparison with the theory.

Idaho National Engineering Lab

Applied Physics & Optics $493,000
Idaho Falls, ID 83415 06-A
90-3

In-Flight Measurement of the Temperature of Small, High Velocity Particles
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 $250,000
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 will be demonstrated in the laboratory using the oxidation of ferrous iron by Leptospirillum ferrooxidans as a model system. A controller will be 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 Leptospirillum, 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 **$232,000**
Idaho Falls, ID 83415 **06-A**
90-3

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 electon 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**
90-3

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

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. Presently, compact tension and bend specimens are being used to develop state-of-the-art fracture toughness results. Specimens containing surface cracks are used to simulate the fracture process (crack growth initiation, subcritical crack growth, and catastrophic failure) that may occur in a structural component.

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 a structure 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 the Massachusetts Institute of Technology.

Idaho National Engineering Lab

Materials Technology Group **$530,000**
Idaho Falls, ID 83415 **03-A**
90-3

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. 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 eight 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.

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**
90-3

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. Microstructural and, particularly, superconducting properties, need to be measured non-invasively and spatially in order to aid the fabrication process.

Past work has concentrated on developing a noncontacting AC induced current measurement technique that can determine critical currents on a local scale with high resolution. 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. With the aid of the "critical state" model for flux pinning, local critical current values have been determined empirically without any connections to the sample.

Current research is concentrated on silver sheathed tape geometries and the development of an analytic approach to predicting the critical state in geometries utilizing non-uniform applied fields, as are found in most NDE applications. An integral equation has been found that can be solved iteratively to determine the flux front profile in the tape geometry. This approach shows promise for application to other geometries involving the critical state with demagnetization effects.

University Of Illinois

Coordinated Science Laboratory **$127,000**
Urbana, IL 61801 **03-A**
91-3

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

This program involves fundamental research on the modeling, control, and optimization of large scale systems. The main theme is model simplification for control and decision making. It encompasses both linear and nonlinear models, and deterministic and stochastic systems with regular and/or singular perturbations. Research issues addressed are in modelling, optimization, stabilization and coordination, as well as in the development of implementable control policies. Their common goal is to broaden the applicability of the concept of multimodeling as a systematic approach to model simplification through decomposition/aggregation of linear and nonlinear large scale systems.

One area of current research is the *robustness* of a controller, designed based on a nominal linear or nonlinear system, to unmodeled fast dynamics and external norm-bounded disturbances. The issue here is not only the robustness analysis of a given controller, but also the design of *optimally robust* controllers that are least sensitive to such structural and external perturbations. Another topic of study at the present is the relationship between deterministic and stochastic formulations for uncertain systems, from the point of view of model simplification, and robustness to unmodeled dynamics and nonlinear perturbations.

University Of Illinois

Dept of Chemical Engineering **$232,000**
Urbana, IL 61801 **01-C**
82-3

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. Specific goals are (1) to obtain measurements of drop sizes in vertical annular flow in order to provide an understanding of the rate processes that govern entrainment, (2) to study the role of gravity in causing an asymmetric distribution of the liquid and of the flow field in horizontal annular flow, (3) to use new results on the formation of slugs to develop an understanding of the frequency of appearance of slugs in horizontal slug flow, and (4) to study 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. This is being interpreted with direct photographic measurements. A mapping of the gas phase velocity shows the existence of secondary flows both for horizontal stratified flow and for horizontal annular flow. Of particular interest is the discovery that spatial variations of drop concentration can induce these flows.

University Of Illinois

Dept of Mechanical and Industrial Engineering **$66,169**
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 **$79,980**
Chicago, IL 60680 **01-B**
93-1

Heat Transfer to Viscoelastic Fluids
J. Hartnett

Numerical studies of the steady laminar flow heat transfer behavior of non-Newtonian fluids through rectangular ducts have been carried out. The

Reiner-Rivlin model which gives rise to secondary flows in non-circular ducts is used to investigate the influence of elasticity on the flow. Finite difference methods are developed to obtain the heat transfer results for the H2 thermal boundary condition for difference combinations of heated and adiabatic walls.

The influence of the second normal stress coefficient, the Reynolds number, the Peclet Number, and the aspect ratio on the heat transfer are considered. It is found that the secondary flow has a relatively weak influence on the pressure drop but the effect on heat transfer is increased by a factor of 2 to 3 as compared to the case of a purely viscous fluid. The predicted behavior of the Nusselt number for the Reiner-Rivlin fluid is found to be in good agreement with experimental results.

Johns Hopkins University

Mechanical Engineering Dept **$149,980**
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 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.

A study has also been carried out of the accuracy of the singularity method for the direct numerical simulation of the potential flow motion of many particles in a liquid.

Current efforts center on the simulation of suspensions of non-spherical particles in the potential- and Stokes-flow limits.

Robert H. Kraichnan, Inc.

303 Potrillo Drive **$66,440**
Los Alamos, NM 87544 **01-C**
93-3

Turbulence Theory
R. Kraichnan

Turbulent fluid motion plays an essential role in atmospheric and oceanic dynamics, in aerodynamics, and in chemical and other industrial processes. Turbulence is so complicated in detail that apt statistical description is essential, and there is strong motivation for new theoretical approaches that extract essentials of the dynamics in a compact fashion. The present project is devoted to these objectives. One part of the work has been collaboration in the design and interpretation of unprecedented high-resolution computer simulations of turbulence at Los Alamos National Laboratory. This has led to some clarification of the strongly- intermittent very-small-scale structure of turbulence; the data are consistent with some earlier theoretical predictions. Another accomplishment with the simulation data has been verification of fundamental similarity hypotheses made years ago by Kolmogorov and recently challenged. On the theoretical side, work has continued on methods of approximating turbulent flow-field statistics by simple nonlinear transformation, or mapping, of fields with known statistics ("mapping closure"). Progress has been made thereby in understanding some key probability distributions that have been measured in turbulence simulations and in the laboratory. An additional project, involving both computational and theoretical work, has been the study of Lagrangian turbulence statistics (statistics measured while moving the flow).

Lawrence Berkeley Laboratory

Accelerator & Fusion Res Div **$132,000**
University of California **06-C**
Berkeley, CA 94720 **90-3**

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).

Lovelace Medical Foundation

Bioengineering Research **$51,475**
Albuquerque, NM 87108 **03-B**
93-3

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

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

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

University Of Maryland

Dept of Mechanical Engineering **$70,896**
College Park, MD 20742 **01-D**
93-3

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

The dynamics of metal cutting significantly affects the quality of machined parts and the productivity of the machining operation. Cutting instabilities for large material removal rates result in substantial annual losses of productivity, energy and material. The goal of this research project is to contribute towards efficient machine tools that require minimum human intervention. This will be accomplished through the intelligent control of the cutting process.

The first objective of this study is the verification of the following three conclusions reached by the PI's from the analysis of experimental measurements of tool work piece relative acceleration: i) The dimensions of attractors associated with noisy turning data can be successfully estimated with existing algorithms; ii) Pre- and mild chatter are characterized by attractors of low dimension; iii) Qualitative properties of the dimension function discriminate between steady and pre-chatter cases.

The second objective is the determination of the applicability of other measures of attractor structure, and asymptotic behavior to the analysis of cutting data.

The third objective is the use of dimension, Lyapunov exponents and other measures of dynamic behavior in characterizing pre-chatter states thus providing a rule base for controlling the cutting process.

Based on the patterns of change of the fundamental descriptors of dynamical behavior, a rule base will be developed to be used for chatter avoidance. The rule base will be integrated into a system to control speed and feedrate in response to changes in the dynamic measures that signify the imminence of chatter.

Currently computer programs for the computation of the dimension function, D(γ), Lyapunov exponents, noise reduction, singular spectrum, noise floor, and attractor construction with singular vectors have been implemented. A machine tool has been instrumented and verification testing is under way.

University Of Maryland

Dept of Electrical Engineering — $86,033
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 — $83,537
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 & Systems Research Inst College Park, MD 20742

$75,000
03-C
92-3

The Mechanics of Redundantly Driven Robotic Systems

L. Tsai

Gear backlash introduces rattling and position uncertainty in robotic systems. To overcome these difficulties, an innovative concept utilizing redundant drives to ensure positive coupling of gear meshes has been conceived. The objective of this research is to gain further understanding of the mechanics associated with such manipulating systems. Such systems can also be found in tendon-driven manipulators, wherein the redundant drives are used to maintain positive tension in tendons.

Force transmission characteristics associated with n-DOF manipulators controlled by n+l actuators has been investigated. It is shown that actuator torques required to act against externally applied forces are functions of the structure matrix, its null vector, and the Jacobian matrix. Design equations for synthesizing a manipulator to possess isotropic transmission characteristics have been derived. The theory will be extended to n-DOF manipulators controlled by more than n+l actuators.

A two-DOF wrist with three unidirectional drives has been designed to illustrate the principle. Actuators and gears are carefully sized to achieve the isotropic transmission characteristics. Driveline flexibility is included in the model as a primary concern. To make sure that backlash has been eliminated, reaction forces in the meshing gears are carefully monitored. Preliminary simulation results indicate that driveline flexibility does have significant effects on the system stability. Backlash can be out of control, if the controller is not properly designed.

University Of Maryland

Dept of Mechanical Engineering College Park, MD 20742

$132,000
01-C
91-3

Lagrangian Analysis of Contaminant Dispersal in Bounded Turbulent Shear Flows

J. Wallace, P. Bernard, J. Balint

The objective of this project is to study the physical processes associated with turbulent scalar transport in shear flows with a view towards developing novel techniques for predicting contaminant dispersal in the environment. A closely coordinated experimental and theoretical research program is followed combining wind tunnel experiments using hot- and cold-wire probes, smoke visualizations and image processing, with numerical simulations. Temperature and concentration contours of point and line source diffusion in the boundary layer obtained from visualization data and from a numerical simulation of channel flow are being compared in order to verify the accuracy of the two techniques. A Lagrangian decomposition of the scalar transport correlation into fundamental physical processes is being carried out using ensembles of particle paths computed in the simulation of turbulent channel flow. This provides insight into the physical mechanisms underlying transport and how they may be modeled.

Images from the boundary layer flow visualization, at $R_\theta \approx 1070$, of the line source of smoke have been digitized and analyzed. It has been determined that there is a strong correlation between the momentum and mass fluxes and the vortical structures of the boundary layer wall region. In addition, temperature measurements have been carried out for comparison to the numerical simulation. Turbulent plumes emanating from line sources have been computed using a direct numerical simulation of channel flows. The mean scalar field and higher order statistics have been compared with the physical experiments as well as a series of computations we have performed using turbulent closures and random flight models.

University Of Massachusetts

Chemical Engineering Department **$ 0**
Goessmann Laboratory **03-A**
Amherst, MA 01003-0011 **90-3**

A General Procedure for the Synthesis of Process Flowsheets
J. Douglas, M. Malone

The goal of this project is to develop systematic procedures for the synthesis of processes for chemical manufacturing. The current aims are to develop general procedures for separation systems and multiproduct batch processes.

Douglas (AIChE J, 31, 353, 1985) developed a hierarchical procedure for continuous, single-product processes containing vapor-liquid mixtures. However, mixtures of vapors, organic liquids, aqueous liquids, and solids are common; fortunately, the material flows entering and leaving the process, the reactor, and the separation systems can be determined with minor extensions of the original procedure. The new procedure isolates vapors using a flash, removes solids in a filter or centrifuge, and separates the organic from aqueous liquids in a decanter. New synthesis methods have been developed for the solid and liquid recovery systems. The complete procedure appears to describe most flowsheets that appear in the literature as well as many new alternatives.

Multiproduct batch processes are treated by optimization of costs for raw materials, energy, late production, early production, and investment.

Simulated annealing has proven effective for (approximate) optimizations in the scheduling, design, retrofit, lot-sizing and parts of the process synthesis, for processes producing hundreds of products in dozens of units.

University Of Massachusetts-Lowell

Department of Electrical Engineering **$61,753**
Lowell, MA 01854 **01-C**
91-3

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

This project represents a 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 the stabilizing 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 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 most unstable of these wavenumbers or primary mode persists through amplitude saturation and chaos. It has been found that this mode undergoes successive period-doubling temporal bifurcations to chaotic motion. However, if subharmonic spatial wavenumbers are initially present in the disturbance spatial bifurcation can also occur.

Massachusetts Institute Of Technology

The Energy Laboratory **$122,300**
Cambridge, MA 02139 **03-B**
91-3

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 the system is being developed with the goals of being suitable for real-time control system design, yielding additional physical understanding, and being readily usable by researchers and engineers.

A novel gas metal arc welding experiment, which modifies the fundamental way metal is transferred in the welding process, has been designed and constructed. The experiment uses mechanical energy as a new control input to the welding process. The metal electrode is vibrated axially during 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 and for testing algorithms for detecting and controlling these modes.

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

Massachusetts Institute Of Technology

Energy Laboratory **$105,000**
Cambridge, MA 02139 **03-A**
91-3

Synthesis and Optimization of Integrated 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 US, 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 is culminating with an investigation of the simultaneous synthesis and optimization of the chemical process, its heat exchange network, and the utility system. Secondly, a new initiative is addressing the need for process design and optimization technologies for batch/semi-continuous processes. Such processes are of increasing industrial importance for the manufacture of high-value added specialty products and pharmaceuticals, which have relatively short product life cycles. Research is therefore focusing on the development of computer-aided design tools for rapid and efficient process development.

Massachusetts Institute Of Technology

Lab for Manufacturing & Product **$158,000**
Cambridge, MA 02139 **03-B**
91-3

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

In previous work, a basic approach to the problem of control of welding processes using multivariable adaptive control theory was established and a set of non-stationary process transfer functions for both the thermal and geometric aspects of the process, capturing the non-linear dynamics and statics, were developed. In addition, depth estimators based on real-time inverse heat transfer solutions and surface temperature measurements have been developed.

However, it has become increasingly apparent through the modeling and experiments, that the process has insufficient latitude to respond to realistic disturbances in a multivariable fashion. In particular, the heat and mass transfer processes involved are far too coupled to allow independent regulation of weld geometry or thermal properties. Accordingly, process modifications to enhance the "reachability" of the process, including transverse and longitudinal high frequency weaving of the heat source to vary the input heat distribution, are being developed.

In current work, this problem of three-dimensional heat distribution control is being generalized using both a distributed parameter control theory and a novel heat source design. While many simplistic inverse heat transfer and distributed parameter control research efforts have been reported, none deal with the problem in the face of variable geometries and high degrees of model uncertainty. Efforts in this area are focused on just such uncertainties and on realistic geometries.

Finally, a new welding process that seeks to decouple heat and mass transfer by using a stream of superheated filler material to both heat and fill the joint has been developed. This "stream welding" process relies upon very precise control of the temperature and flow rate of the metal stream. This control is achieved by a novel continuous-flow arc furnace that has a small thermal mass, thereby allowing rapid temperature changes in the filler material. Preliminary tests with this apparatus are now underway.

Massachusetts Institute Of Technology

National Magnet Laboratory **$91,000**
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 nobel 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

Dept of Mechanical Engineering **$196,000**
Cambridge, MA 02139 **01-A**
91-3

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 constants 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 **$133,000**
Cambridge, MA 02139 **01-A**
91-3

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

Comminution of energy materials is energy intensive; one of the principal sources of inefficiency in many classes of devices is the presence of excessive fines within the coarse medium. The fines cause an unwanted shielding of the coarse medium and impose multiple passes on the feed (e.g. roller tables, ball mills) resulting in frictional losses. This study investigates the mechanics of rapid fines removal to provide design criteria for a new generation of comminution machines with a significantly elevated comminution efficiency.

It is well known that dense, size distributed particulate media have a natural tendency to segregate in the presence of flow and gravity, although these effects remain poorly characterized and are typically viewed as a hindrance. Here, the aim is to understand and incorporate these phenomena to improve comminution efficiency. Using a cylindrical rotary crusher, the research studies particle segregation by means of unsteady fluidization in vertical and near vertical configurations. In the conceptual device, the time scale of the unsteadiness is the period of rotation. The goal is to achieve full separation in minimal time to accommodate a large and efficient comminution throughput.

Experiments have been conducted with bidisperse mixtures of silica spheres (50-3000 micrometers in diameter) in water with impulsively started fluidization. The results of numerous experiments are summarized with the following observations:

- segregation of bidisperse mixtures can be achieved with impulsive fluidization, even for systems in which the fines are sufficiently large to prevent their percolation through the coarse matrix. It has been found that separation critically depends on the initial formation of an upward propagating pocket within which segregation occurs: coarse particles rain down through it while fines remain fluidized, leaving a fines-free bed of coarse particles below. Segregation is markedly reduced in the absence of this structure.

- the limiting factor to the speed of segregation and hence fines through-put is the speed of the leading edge of the pocket. This interfacial speed is directly linked with the rate at which coarse particles can become detached from the above binary dense-pack. The present work is addressing the mechanics of this process theoretically and experimentally.

The program aims to develop the theoretical base of understanding for particulate segregation phenomena in a variety of configurations to help improve processes in which segregation is either desired, as it is here, or unwanted, as in mixers for example.

Massachusetts Institute Of Technology

Dept of Mechanical Engineering **$116,846**
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 Inst Of Tech[1]

Dept of Chemical Engineering **$60,855**
Cambridge, MA 02139 **06-C**
91-3

Los Alamos National Lab[2]

MEE-9 **$108,000**
Los Alamos, NM 87545 **06-C**
91-3

Sandia National Laboratories[3]

Division 1512 **$98,000**
Albuquerque, NM 87185 **06-C**
91-3

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

This research combines theory, experiments and numerical calculations to focus on slow flows of suspensions in which colloidal and inertial effects are negligibly small (Macrostatistical Hydrodynamics). We conduct nuclear magnetic resonance imaging experiments to quantitatively measure particle migration occurring in concentrated suspensions undergoing a flow with a nonuniform shear rate. These experiments address the issue of how the flow field affects the microstructure of suspensions. In order to understand the local viscosity in a suspension with such a flow-induced, spatially varying concentration, one must know how the viscosity of a homogeneous suspension depends on such variables as solids concentration and particle orientation. We employ the technique of falling-ball viscometry, using small balls, as a method to determine the effective viscosity of a suspension without affecting the original microstructure significantly. We also obtain data. from dispersivity experiments in which the detailed fluctuations of a falling ball's velocity indicate the noncontinuum nature of the suspension and may lead to more insights into the effects of suspension microstructure on macroscopic properties. Finally, we are beginning to perform other experiments in quiescent suspensions, measuring the slip on a rotating sphere and the pressure drop caused by a falling ball (in contrast to the use of conventional rotational viscometers which impose a macroscopic shear on the suspension) in order to learn more about the microstructure and boundary effects in concentrated suspensions.

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 - E 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 **$141,904**
Minneapolis, MN 55455 **06-C**
92-4

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

The objective of this research project is to study analytically and experimentally specific thermal plasma processes for materials treatment. Processes of interest include the synthesis of ultrafine ceramic powders and of diamond films.

During the past year, we have concentrated on (a) characterizing the deposition process of diamond films over larger areas, and (b) studying the TiO_2 submicron powder synthesis process experimentally and theoretically.

The deposition of diamond films over a larger area required tailoring the substrate cooling such that a uniform substrate temperature was obtained in spite of strongly non-uniform heating by the plasma jet. Modeling of the heat flux distribution in the substrate holder led to specific substrate holder designs resulting in a temperature variation of only +/-20°C over a 50 mm diameter substrate, and a uniform film growth over this region at growth rates of 200 μm/hr.

The submicron TiO_2 powder synthesis required several apparatus modifications-for maximizing the rutile phase in the product. At present, we are modeling the temperature and species distribution in an induction plasma reactor for optimization of the reactor design for obtaining a single phase product.

National Academy of Sciences/ National Research Council

Washington, DC 20418 **$1,064,701**
06-C
Department of Energy Integrated Manufacturing Fellowship Program **92-3**
B. Kuhn

Twelve three-year predoctoral fellowships in integrated manufacturing have been awarded by the National Research Council, under the aegis of the National Academy of Engineering following a national competition. The winners were selected from a pool of 144 applicants by a panel of 15 engineering scholars and industrial experts. The objective of the program is 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 for the loss of competitiveness of the United States in manufacturing. Recent studies of manufacturing in the United States showed a need for a more integrated approach to manufacturing than that prevailing in industry today. 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 Center for Manufacturing Sciences

Technology Sourcing **$45,500**
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 **$551,000**
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 **$ 0**
Boulder, CO 80303 **06-C**
89-3

Low Resistivity Ohmic Contacts Between Semiconductors and High-T_c Superconductors
J. Moreland, J. Ekin

The purpose of this project is to fabricate and characterize contacts between high-T_c superconductors (HTS) and semiconductors. Developing a method for optimizing the current capacity of such contacts will extend the application of HTS materials to semiconductor hybrid technologies that have HTS interconnects (both on-chip and package) and proximity HTS/ semiconductor/HTS SNS Josephson Junctions. Presently, these are some of the most promising HTS applications, but an essential first step is the development of stable ohmic contacts between semiconductors and HTS materials.

The project is now focused on $YB_2Cu_3O_x$ (YBCO) thin-films grown on Si wafers. Recent discoveries have shown that it is possible to grow high quality HTS films on Si using laser ablation deposition and a yttria stabilized zirconia buffer layer between the YBCO film and the Si. Processing steps are being optimized for depositing and patterning YBCO films on Si to form contact vias to the Si substrate. The goal is to minimize the specific resistance of the contacts using techniques that are compatible with standard Si processing.

The City University Of New York

The City College **$89,804**
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. 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.

Viscous resuspension was studied both theoretically and experimentally in various unidirectional flows, e.g. a 2-D Hagen-Poiseuille flow, as well as a Taylor-Couette system, and excellent agreement has been found to-date between the experimental results and the theoretical predictions even though the latter do not entail the use of adjustable parameters. In addition, the stability of the resulting stratified two-phase flows was investigated theoretically on the basis of a small disturbance stability analysis, and again good agreement was found between the theoretically predicted conditions for the onset of growing disturbances and experimental observations regarding the appearance of interfacial waves.

The City University Of New York

The City College **$126,528**
Department of Chemical Engineering **03-A**
New York, NY 10031 **91-3**

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. The FCC control problem is rich enough to contain many of the nonlinear features found in such plants.

A dynamic simulation model of the FCC has been developed for these studies. It is based on a recently published model but contains many enhancements which insure that its behavior is representative of current FCC operation.

The work has demonstrated that the performance of FCC's in the region of current operation exhibits five multiple steady-states as well as input multiplicities of some of the important manipulatable variables. This size of the region of five steady-states can be greatly reduced by the use of a combustion promoter. This helps explain why the use of a promoter is so popular in the industry even though its use has little economic benefit other than better controllability.

The City University Of New York

The City College **$102,500**
The Benjamin Levich Institute **06-C**
of Physico-Chemical Hydrodynamics **91-3**
New York, NY 10031

Studies in Premixed Combustion
G. Sivashinsky

The objective of this research is a combined analytical and numerical study of the influence of various hydrodynamic, thermal-diffusive and reaction rate factors on speed, shape, stability and the extinction limits of premixed gas flames. Different modelling techniques will be employed to reduce the study of the pertinent combustion systems to simple approximate problems tractable either analytically or numerically. Specifically, the project is concerned with (1) the dynamics of premixed flames spreading through a one- and multiple-scale system of eddies and with the further development and refinement of the associated cascade-renormalization concept of turbulent flame speed; (2) the intrinsic dynamics and the pattern formation in premixed flames sustained by the thermal-diffusive and thermal expansion induced mechanisms of flame instability; (3) the hydrodynamical aspects of combustion limits with particular attention to the phenomena of flame extinction by one- and multiple-scale periodic flow fields and extinction in upward and downward propagation flames in tubes; and (4) the development of new numerical methods especially assigned for the free-boundary problems of flame-flow interaction and spontaneous pattern formation in premixed flames.

Northwestern University

Engineering & Applied Science **$89,450**
Evanston, IL 60208 **03-B**
93-3

Thin-Film Characterization and Flow 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 **$235,036**
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. The analysis has been extended to stratified flow of two thin incompressible, immiscible layers between stationary parallel walls, subject to body forces and surface tension. A long-wave generalized evolution equation of the Benney type is derived, which reduces for special cases to previously derived results. Upon linearization, four different stability diagrams are found in wavenumber/flow rate space, representing the competition of different physical effects. A small-amplitude analysis yields an extended Kuramoto-Sivashinsky (KS) equation containing both quadratic and cubic nonlinearities. It is found that the symmetry-breaking bifurcation of the KS equation is now imperfect. Modulated travelling waves of large amplitude may bifurcate from the traveling wave solutions, and hysteresis loops may be formed, which may be pertinent to the flooding phenomenon in countercurrent parallel flows.

The experimental program is designed to confirm the range of validity of the theoretical analysis, and to determine its practical limits. By operation under conditions of extreme quiet, the classical linear stability theory for long waves on a falling film was fully confirmed for the first time. A mirror system allows a complete 360° view of the tube to be obtained in a single frame. This allows the measurement, using image digitization, of the development of circumferential secondary waves from the primary ring waves. As predicted, this development is rapid when the tube is heated, owing to thermocapillary effects.

A numerical investigation is under way to examine nonlinear spatially growing or decaying waves on a falling film.

Northwestern University

Dept of Eng Sci & App Math **$53,000**
Evanston, IL 60208 **01-C**
91-3

Effects of Capillarity of Macroscopic Flow in Porous Media
M. Miksis

The objective of this project is to study the effects of capillarity on the motion of a fluid in a porous material. The primary concern will be the micromechanics of the fluid motion when interfaces are present and its effect on the macroscopic flow. These interfaces could exist as a liquid moves into an unsaturated porous material or when there are two phases within the porous material; e.g., liquid/gas or liquid/liquid. Attention will be directed to understanding and modeling the dynamics of these interfaces and then relating their dynamics to the macroscopic behavior of the material.

Part of our attention is directed to foam flow in porous media. A foam is generated when, for example, a gas is injected into a fluid saturated porous media. We have studied this generation process by considering the dynamics of a gas bubble as it is driven past a constriction; e.g., in a capillary tube. Here we have observed that under certain conditions, the bubble snaps into two parts; hence forming the building blocks of a foam. These new smaller bubbles are separated by a thin liquid film, a lamella, which controls the stability of the foam. The stability of this lamella has also been studied.

Northwestern University

Dept of Chemical Engineering **$111,422**
Evanston, IL 60208-3120 **06-C**
91-3

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

The goal of our work is to provide a general understanding of the mixing of viscous fluids. The problem is of importance in the chemical and processing industries. We have nearly completed the original objectives under this grant and we are now actively engaged in pursuing avenues suggested in the course of our investigation. We have completed our studies of stretching, breakup, and dispersion of viscous droplets in chaotic flows. As a result of these studies we developed a method to measure the interface between two liquids based on the complete surface tension-driven time evolution of a stretched filament, including satellite and sub-satellite formations, in terms of Boundary Integral Equation Methods. Two important extensions are also being pursued: Mixing of non-Newtonian fluids and chaos-enhanced transport. The non-Newtonian area consists of two sub-projects: (i) mixing of viscoelastic fluids (Boger fluids), and (ii) mixing of shear thinning fluids. Area (i) involves both experiments and computations whereas (ii) is exclusively computational. The chaos-enhanced transport focuses on transport to and from cavities, the flow within the cavity being modulated by a wavy flow and the cavity itself possessing, possibly, a multicellular structure. These two last areas will comprise the bulk of our efforts for the next year and beyond.

Northwestern University

Dept of Eng Sci & App Math $68,058
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

Department of Chemical Engineering $60,246
Notre Dame, IN 46556 01-C
92-3

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

Wave formation on a falling liquid film can be a desirable phenomenon since the waves enhance interphase heat or mass transfer in many industrial gas-effluent cleaning devices (scrubbers) and in some solar energy collectors. In paper and optical fiber coating processes, however, waves tend to reduce the coating quality and lower the production rate. This project is to investigate how the waves are formed, how they can be removed and how they can enhance heat/mass transfer. Our approach is to combine theoretical techniques from Dynamical Systems theory, numerical simulation, and experiments to achieve these goals. With the first two techniques, we have been able to understand the primary, secondary and tertiary transitions of waves from nearly sinusoidal waves at the inlet to the solitary waves downstream. It is the only hydrodynamic instability that is understood beyond the primary inception. Our nonlinear analysis allows us to associate drop formation during fiber coating to a blow-up solution. We are currently developing the wavelet numerical method for wave evolution, finalizing an experiment for falling film and using renormalization group theory to predict interphase transfer from the predicted wave spectra. Feedback control to stabilize the waves will soon be attempted.

University Of Notre Dame

Department of Chemical Engineering $54,000
Notre Dame, IN 46556 01-C
91-3

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

The objectives of this work are to develop a mechanistic and mathematical understanding of various types of small-scale (e.g., waves) and large scale (e.g., slugs) disturbances that are observed in cocurrent gas-liquid flows.

Measurements of wave properties (e.g., speed, wavelength, amplitude and rates of evolution) are used to verify linear and nonlinear theoretical approaches that are based on simplifications of the Navier-Stokes equations. Most of this work is done at conditions close to neutral stability where definite comparisons of theory and experiments are possible.

Currently, several important secondary wave transitions are being studied. These are:(1) formation of waves with twice the wavelength of the fundamental (i.e., subharmonics); (2) initiation of very long wavelength modes that can grow into roll waves or slugs; (3) formation of transverse modes which lead to greater dissipation and a degree of stabilization of the flow. It is found that weakly-nonlinear theory gives insight into these secondary transition mechanisms that cannot be understood using only linear theory. An additional topic of current interest is determination of the features of turbulence that must be incorporated into linear and nonlinear theories to accurately describe the generation and evolution of waves.

Oak Ridge National Laboratory

Engineering Physics $1,250,000
and Mathematics Division 03-C
Oak Ridge, TN 37831 87-5

Center for Engineering Systems Advanced Research (CESAR)
R. Mann, F. Pin

The Center for Engineering Systems Advanced Research [CESAR] is established at Oak Ridge National Laboratory to address long-range, energy-related research in intelligent machine systems. These systems are intended to plan and perform a variety of tasks in incompletely known environments, given only qualitatively specified goals. The Center provides a focal point for interdisciplinary research in machine intelligence, cognitive systems, advanced control, and systems engineering. Research objectives are chosen to address the technology-base requirements for DOE missions that rely on the use of robotics and intelligent machines. In particular, research concentrates on issues related to autonomous systems, unstructured dynamic work environments, and multiple cooperating robotic systems. Results from CESAR research in automation-related technologies and intelligent machines can increase productivity and safety in the development and operations of DOE-sponsored systems. Potential and actual applications include emergency situations, remote operations, resource exploration, transportation systems, advanced power generation systems, and environmental restoration and waste management.

CESAR is intended to be a national resource, and a major objective is to disseminate R&D accomplishments freely and comprehensively. Results and technology advancements are distributed through publications in the scientific literature, through organization of workshops on selected topics, and through the development of prototype systems that demonstrate concepts and new methodologies. CESAR cooperates with universities, laboratories and industry, serving as a collaborative research facility to provide guests with access to state-of-the-art and often unique equipment in a stimulating research environment.

Ohio State University

Physics Department $69,000
Columbus, OH 43210 06-C
91-3

Turbulence and Spatio-Temporal Chaos
C. Jayaprakash, F. Hayot

This program deals with the dynamics of extended (with many degrees of freedom), dissipative, non-linear systems.

An important issue in this area concerns the existence of effective stochastic equations to describe the long wavelength properties of partial differential equations that exhibit deterministic chaos. We are currently studying the Kuramoto-

Sivashinsky (K-S) equation and its variants. This is done numerically(using spectral codes) by explicit elimination of short wavelength modes with an emphasis on interpreting the physical basis of the parameters in the effective equations. For the K-S equation in one and two spatial dimensions, the effective equation is the Kardar-Parisi-Zhang equation that is a generic model for stochastic growth of interfaces although the crossover length scale beyond which this applies is very large. We have also been studying the complex Ginzburg-Landau equations from this point of view.

Extensive numerical simulations of coupled map lattice models and resistively shunted junction models of Josephson junction array's are being carried out to elucidate features of spatio-temporal chaos in extended systems. We have found that these systems exhibit non-Gaussian probability distribution functions for local variables, a phenomenon that occurs in fluid systems. This has led us to suggest a new mechanism for such behavior.

A focus of current research in the field is generic scale invariance (algebraic decay of spatial correlations without tuning external parameters). The aims of projects underway include understanding how a conserved mode can induce scale invariance in non-conserved modes, and elucidating different mechanisms that can lead to generic scale invariance by studying model systems.

Ohio State University

Mathematics Department **$66,143**
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 **$102,142**
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 aim of this research is directed at identifying basic relationships between array geometry (spacing, packing arrangement, and element shapes), surface properties, and radiative transfer through a two-dimensional array. The information resulting from this study may also be useful in establishing criteria for the valid application of participating media models to arrays of fixed 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 reflectometer 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. Measurements of BRDF for striated surfaces indicate that, for a broad class of surfaces, this assumption can lead to significant error. 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**
91-3

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 1993 accomplishments consist of: 1) the Monte Carlo code has been completed and validated against other Monte Carlo results, 2) simulation of a range of array geometries showed, that radiation heat transfer in most arrays of practical interest can not be predicted solely on the scattering properties of an individual element but, also depend on the geometric arrangement of the elements. Accurate modeling of radiation heat transfer in arrays will, in most cases, require that the array is modeled as discrete surfaces rather then as a homogeneous media, 3) parametric studies have shown that the inclusion of polarity in Monte Carlo modeling can have a significant effect on the results of the Monte Carlo simulations and needs to be considered by other researchers, and 4) one technical paper was published in FY 93 and two journal articles were submitted to journals for publication in 1993.

University Of Pennsylvania

Mechanical Engineering Dept **$101,400**
Philadelphia, PA 19104 **01-C**
92-3

Active Control of Convection
H. Bau

Active, feedback control strategies to alter the structure of convection in a fluid layer heated from below and cooled from above (the Rayleigh-Benard problem) are studied experimentally and theoretically. The 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, chaotic convection. This work is a continuation of an effort in which it was successfully demonstrated that feedback control can be used in a thermal convection loop to tame chaos. The results of this work may be of importance, among other things, to materials processing and crystal growth applications in which it is desirable to eliminate convective currents or suppress oscillatory convection. What is learned during this research may also be useful for devising control strategies for other non-linear flow phenomena. 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 can be significantly delayed. An apparatus for experimental verification of theoretical predictions is under construction and a computer code to study time-dependent flows is under development.

Pennsylvania State University

Mechanical Engineering Dept **$95,793**
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 spray technology has grown in a decade to become second only to plasma spraying in the application of metallic coatings. HVOF coatings have desirable high densities and other potential advantages of economy and simplicity.

Because HVOF uses high-speed gaseous combustion products to heat and accelerate metal particles, the gas dynamics of the process exerts a profound influence on its performance. However, commercial HVOF equipment has yet to exploit this potential. The objective of this research is to conduct experiments and modeling of HVOF gas dynamics, thus to improve the process.

Schlieren visualizations reveal that the supersonic HVOF jet undergoes very rapid turbulent mixing with the atmosphere. Planned experiments will examine and attempt to reduce this mixing, using analysis of the oxide content of sprayed coatings as a measure of success. Analysis and experiments are also being performed to optimize the design and operation of the supersonic HVOF spray nozzle. The heat and momentum transfer between the gas and sprayed particles are also being examined.

Ultimately, an improved HVOF apparatus embodying gas-dynamic principles will be designed and tested. Technology transfer from rocket propulsion and supersonic aerodynamics is a key element of this project.

Physical Sciences Inc.

20 New England Business Center **$130,000**
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 different 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 **$96,000**
Princeton, NJ 08544 **06-B**
93-3

Mechanisms and Enhancements of Flame Stabilization

C. Law

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

A comprehensive study has been conducted for the structure of the adiabatic, equidiffusive, and freely-propagating premixed methane/air flame situated in a counter flow. The velocity, temperature, and major species concentration profiles were experimentally mapped through laser-based instrumentation and computationally determined with detailed reaction mechanisms and transport properties. These results agree closely with each other, and demonstrate that the structure of such flames remain basically invariant to strain rate variations. The results are of relevance to the modelling of turbulent flames.

The geometry and dynamics of stretched, wrinkled flames have also been analytically studied. The analysis successfully describes the geometry of the experimentally-observed configuration of the Bunsen flame tip at the state of opening, and demonstrates that the flame temperature and flame speed remain finite at such a state. Analysis of flame propagation in periodic flows shows that the average flame speed increases with either increasing fluctuation amplitude or increasing wavelength of the imposed flow, that the flame surface can locally extinguish for sufficiently large fluctuation amplitudes of the imposed flow, and that the structure of the flame cusps resembles that of the Bunsen flame.

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 ben investigated and computed. This has led to accurate predictions of transport properties of realistic models of isotropic as well as anisotropic heterogeneous media. An efficient Brownian motion computer-simulation methodology has been employed to yield exactly effective diffusion parameters for a host of useful models. Rigorous relations which link the fluid permeability to length scales obtainable from Nuclear Magnetic Resonance experiments and the effective electrical conductivity have been derived.

Purdue University

School of Mechanical Engineering **$92,888**
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 objectives of the proposed research program are to develop instrumentation methods, experimental data base and analysis leading to predictive 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, 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 of the interfacial velocity, wave characteristics, fluid particle coalescence and disintegration. These will be characterized by the collision frequency, interfacial energy and turbulence dissipation in liquid.

The five-sensor resistivity probe is developed for the measurement of the local interfacial area, void fraction and three-dimensional components of interfacial velocity. This five-sensor probe is intended to be used for general two-phase flow except annular flow. By combining the capability of a double-sensor probe for the measurement of small bubble characteristics and that of a four-sensor probe for the measurement of large slug bubbles or irregular large bubbles, it can be applied to a wide range of flow regimes. Furthermore by separately measuring the contributions from these two different groups of bubbles, the gradual changes in the interfacial structures associated with flow regime transition can be quantified. Such an instrumentation method has never been developed previously. The double-sensor and multi-sensor probes are used for vertical two-phase flow to obtain detailed data on the interfacial structure and its axial development from the entrance to the exit. The combination of these probes will give information on the local void fraction, interfacial area, interface velocity, bubble size and turbulent characteristics of the bubble motion in bubbly, slug and churn-turbulent flow. The changes in these parameters quantitatively characterize the flow regime transitions from bubble to slug and slug to churn-turbulent flow. Then this information will be used to understand the dynamics of fluid particle coalescence and disintegration as well as the interfacial instability and their relation to the global changes in the interfacial structure or flow regime. Finally, the long term goal is to develop an interfacial area transport equation by mechanistically modeling the contributions from the particle coalescence, disintegration and convection. The phase change, coalescence and disintegration effects appear as source and sink terms in the transport equation. The major mechanisms for the coalescence of fluid particles are particle collisions, wake entrainment and bubble crowding into a form similar to a Taylor bubble, whereas the fluid particles disintegrate due to turbulent effects. These different mechanisms are modeled separately using a simple physical model and data obtained under Tasks 2 and 3.

Purdue University

School of Mechanical Engineering **$119,733**
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 feature (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 Eng, **$ 0**
Aeronautical Eng Mechanics **01-B**
Troy, NY 12180-3590 **89-4**

Ultimate Limits of Boiling Heat Fluxes
A. Bergles, M. Jensen

This study is directed toward the thermal-hydraulic behavior of water and aqueous mixtures, flowing in plain tubes and in tubes with enhancement devices, at very high heat fluxes. The mode of heat transfer is subcooled nucleate boiling, and the limiting phenomenon is the critical heat flux (CHF). Very large heat fluxes can be accommodated on a steady basis with pure water by use of large subcoolings, high velocities, small tube diameters, and short tubes. It is expected that simultaneous use of several enhancement techniques will extend the maximum heat flux to at least $5x10^8 W/m^2$, which would be higher than that reported in any study to date. The wall temperature characteristics and pressure drops are unknown at such high heat fluxes. Particular emphasis is placed on the pressure drop, as the CHF in many practical applications is determined by the pressure drop characteristics.

An experimental program is systematically investigating the effects of subcooling, velocity, tube geometry, and enhancement techniques on CHF, the boiling curve, and the pressure drop. The CHF without enhancement has been correlated as a function of flow and geometrical variables using the present data base of over 200 points as well as data obtained by other investigators. The correlation describes well other data recently published.

A thesis (C.L. Vandervort, Ph.D.) and interim report (HTL-9) describe the progress to date.

Rensselaer Polytechnic Institute

Dept of Mechanical Engineering, **$134,000**
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 equations which are ultimately intended for use in inelastic stress analysis and life prediction.

The modeling of effects of recovery of state observed in strain rate change and relaxation tests at 538°C on modified 9Cr-1Mo Steel has been completed. The Viscoplasticity Theory Based on Overstress (VBO) with a recovery of state term is capable of reproducing the observed behavior. Finite deformation formulations of VBO include a modification of the growth law for the equilibrium stress and a rationale for choosing objective derivatives of stress-like state variables. Numerical simulations are in progress.

Seven biaxial low-cycle fatigue tests with stainless steel tubular specimens at 538°C have been completed. During these tests, the voltage drop was monitored using a reversing DC potential drop measuring apparatus. A new method of data analysis and smoothing was developed which showed a significant increase in voltage drop in the area of crack formation. Analysis of the theoretical solution for the voltage drop for a semi-elliptical crack in an infinite medium showed similar shapes. Testing and analysis are continuing.

Rensselaer Polytechnic Institute

Dept of Nuc Eng & Eng Physics **$ 0**
Troy, NY 12180-3590 **06-C**
89-4

The Continuum Modeling of Two-Phase Systems
R. Lahey, Jr., D. Drew

This research is concerned with the development of a physically-based, well-posed multidimensional two-fluid model which can be used for the prediction of a wide variety of commercially important multiphase flows.

Significant progress has been made in the modeling of bubbly two-phase flows. The approach taken was to analytically derive the various interfacial closure laws using cell-model, ensemble averaging techniques. In particular, it was assumed that the continuous (liquid) phase was inviscid and irrotational.

The resultant two-fluid model has been numerically evaluated using PHOENICS, a computational fluid dynamic (CFD) solver, and these results have been found to agree very well with a wide range of phase distribution data. Moreover, the dispersion relation of this two-fluid model has shown that it is capable of predicting both sonic and void wave propagation phenomenon and the bubbly/slug flow regime transition.

Further research is expected to focus on heat transfer phenomena, the effect of bubble distortion on lateral lift, the modeling of other flow regimes and the modeling of two-phase turbulence (particularly intermittency and the coherent structures).

Rensselaer Polytechnic Institute

Dept of Chemical Engineering **$88,379**
Troy, NY 12180-3590 **01-C**
93-4

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

The physicochemical phenomena associated with fluid flow and change-of-phase heat transfer in ultra-thin (thickness less than 10^{-5} m) liquid films are being studied. Microscopic image processing equipment, procedures, and related computer programs are being developed to improve data resolution and automate data acquisition. First, the image processing equipments are being developed and used in conjunction with an interferometer designed to study the transient film thickness in draining and evaporating films. The glass cell is designed to optimize temperature control, cleanliness and simplicity. The optical data is obtained using a video camera attached to a microscope through which the interference fringes are recorded. Transport processes in various fluids, with and without heat transfer, are being experimentally studied and analyzed. Using the results of these studies, an image processing ellipsometer (which can measure thinner films with thicknesses down to a nanometer) has been designed, constructed and used. The long term objectives are to measure and model transport processes in thin films. The near term objective is to develop microscopic image processing equipment and a complementary experimental cell.

Rice University

Dept of Civil Engineering **$87,560**
Houston, TX 77251 **01-A**
91-3

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

Nonlinear wave forces acting upon offshore structures have been examined from a system identification perspective. The nonlinearities are induced by the wave-structure interaction effect, and may become non-negligible in many situations, especially for large energy producing systems. They are not necessarily in Morison's form in terms of squared relative velocities or they are not calculated by diffraction theory. Various wave force models have been examined. A particular force function which is adopted for a given class of problems has been expanded in terms of the wave and structural kinematics. The resulting nonlinear system has been decomposed into a number of parallel no-memory nonlinear systems, each followed by a finite-memory linear system. For such multi-input linear sub-systems, a cross-spectrum technique involving Wiener-Volterra kernels has been applied to identify the linear transfer functions, from which the structural properties and the force transfer parameters have been obtained by a least squares approximation. The developed method provides a versatile and non-iterative approach for dealing with the nonlinear interaction problems encountered in offshore structural engineering. Current studies aim to further establish the versatility and the reliability of this method.

University Of Rochester

Dept of Physics and Astronomy **$69,500**
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 **$93,500**
Rochester, NY 14627 **06-C**
93-3

Coherence Effects in Radiative Energy Transfer
E. Wolf

This research is mainly concerned with the elucidation of the foundations of radiometry and radiative energy transfer and with the influence of source correlations on the energy distribution throughout the radiated field.

In the early stages of these investigations the relationship of radiometry to statistical wave theory for fields produced by a certain class of globally incoherent sources was clarified. The present research is concerned with extending this work to fields generated by sources of a broader class. Frequency shifts in spontaneous emission from two interacting atoms, was also investigated. This effect may be considered to be analogous, in some respects, to the Lamb shift.

The possibility of determining spatial correlation functions of random media from the knowledge of the correlation functions of the scattered field in the far zone is also being studied.

The Rockefeller University

Department of Physics **$85,487**
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 investigation of new types of diffusion, discovered in Lorentz lattice gas cellular automata, is continued. In this gas point particles move on a lattice occupied by deterministic scatterers. For randomly placed scatterers this gas can be considered as a dynamical system in a random environment. A beginning has been made to investigate the case of periodically placed scatterers. 2. A relation between the transport coefficients (viscosity, diffusion) of a fluid in a nonequilibrium stationary state and its two maximal Lyapunov exponents is further pursued. This relation is based on the symmetry of the Lyapunov spectrum of the fluid. The class of systems for which this symmetry holds is being investigated. In addition, computer studies are made of the diffusion coefficient of particles in a periodic triangular Lorentz gas in equilibrium. Since this transport coefficient can also be expressed in terms of two Lyapunov exponents, the connection between the two cases is being studied. 3. An analogy has been discovered between the structural relaxation of atomic liquids and monodisperse concentrated colloidal suspensions, consisting of spherical particles. This analogy can be understood via the kinetic theory of a hard sphere model of both fluid systems. Applications to the visco-elastic and rheological behavior of concentrated colloidal suspensions are made providing a microscopic approach to these properties.

Sandia National Laboratories

Combustion Research Facility **$150,000**
Thermofluids Division **06-B**
Livermore, CA 94550 **90-3**

Mixing and Phase Change During Combustion
A. Kerstein

This project involves analytical and computational study of the effect of random advection on two interrelated processes, molecular mixing and front propagation. Some fundamental aspects of advective effects are not well understood even for simple flows involving a limited range of advection length scales. These aspects include the species concentration distribution in statistically steady mixing configurations and, for propagation processes, the dependence of front surface area on stirring intensity. In turbulent flow, involving a wide range of length scales, a key problem is the coupling between flow and mixing in cases for which mixing modifies flow energetics, as in buoyant stratified turbulence.

The methodology employed in this project involves analogies between physical processes subject to random disturbances and stochastic processes. In particular, a novel computational model of turbulent mixing has been formulated in which turbulent stirring is represented by non-linear mappings on a line, iterated according to a stochastic rule that incorporates turbulence scaling laws. Comparisons to experimental results demonstrate substantial gains in predictive capability relative to other methods.

In future work, this and other models will be used to simulate and analyze the effect of random advection, especially turbulent advection, on mixing and propagation processes in combustion and geophysical flows. Propagation processes of interest include flame fronts in fuel-air mixtures and acoustic fronts perturbed by ocean currents.

Sandia National Laboratories

Combustion Research Facility **$ 0**
Livermore, CA 94551-0969 **06-B**
90-3

Structure of Inverse Diffusion Flames in Supercritical Fuel/Water Mixtures
R. Steeper

This project investigates the structure of diffusion flames in high-density fuel-water-oxidizer mixtures. These *hydrothermal flames* are of practical concern in the development of supercritical water oxidation as a waste destruction process. Yet 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 exhibit characteristics distinct from atmospheric-pressure flames. One unique characteristic of the high-density flames is a wide range of possible flame temperatures; another is an insensitivity of flame height to fuel fraction. The research program investigates this unexpected behavior by performing experiments with densities ranging from atmospheric to supercritical. 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 conditions that leads to the ignition of methane-water-oxygen and methanol-water-oxygen flames has been measured. A future goal of the experiments is to map temperature, species, and velocity fields in the hydrothermal flame reactor. Both analytical and numerical models of laminar diffusion flames are available to support the experimental efforts. These models will be modified to include a supercritical fluid equation of state, an appropriate reaction mechanism, and high-pressure transport properties.

University Of Southern California

Dept of Mechanical Engineering **$106,536**
Los Angeles, CA 90089-1453 **01-C**
91-3

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 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 and that the magnitude of the average particle pressure scale with the bubble size. 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. There is some evidence that the material is refluidizing in the far wake, but that is a very slow process. This observation may have profound implications in chemical processing as their 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 and required 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 drop off due to the reduced concentration.

University Of Southern California

Dept of Mechanical and Aerospace Engineering
Los Angeles, CA 90089

$124,999
01-C
93-3

A Combined Experimental and Numerical Investigation of Multiphase Porous Media Flow Dynamics
T. Maxworthy, E. Meiburg

This investigation of multiphase porous media flows addresses two related issues: Part one of the study deals with the question of the proper interfacial boundary conditions to be applied in the interfacial region between two *miscible* fluids moving in a Hele-Shaw cell or, by analogy, in a porous medium. We hope to accurately determine the characteristics of these interfaces by comparing experiments carried out in a Hele-Shaw cell and a circular tube with numerical calculations of the full problem, based on the Stokes equations. By measuring the amount of viscous fluid left behind during *miscible displacement* by a less viscous fluid, we hope to establish the spatial dependence of the gap-averaged concentration profile as a function of the Peclet number. By comparison with the numerical calculations as well as with *immiscible* displacement results, we will attempt to determine if the process can be described in terms of an effective capillary number, in which the concentration-gradient stresses at the interface zone might, possibly, give rise to an effective surface tension. The Hele-Shaw cell geometry will also be used to study the *stability of miscible interfaces* over a wide range of conditions including the effect of a tangential velocity jump across the interface. In part two of the investigation, we will explore the nonlinear dynamics of *immiscible* displacements under the influence of gravity on the basis of the recent linear stability results.

The apparatus has been built to study *miscible displacement* in circular tube as a function of both Peclet and Atwood numbers. Results show a strong dependence of the flow on the latter parameter. A two-dimensional code has been developed for studying the Peclet number influence on *miscible displacements*. The code is currently being tested.

Southwest Research Institute

6220 Culebra Road
San Antonio, TX 78228-0510

$99,979
03-B
91-3

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

The approach was to study the effects of neutron embrittlement and biaxial stress on signals from various magnetic measurement techniques in steels. The purpose was to determine which procedures have promise for use in monitoring neutron embrittlement and biaxial stress.

For neutron embrittlement, six sets of broken Charpy samples were examined from two reactors. In each set, the samples all corresponded to the same number of full power years, but each sample was positioned slightly differently in the containment capsule and so received a different amount of irradiation. Each set nevertheless was characterized by one value for each embrittlement parameter, regardless of the differing amounts of irradiation. Since a true measure of embrittlement was not available for each sample, the magnetic measurements exhibited a large statistical spread. The best correlation occurred for nonlinear harmonic amplitudes, with R^2 of the order of 0.7 (rather than 1).

On the other hand, guided by magnetomechanical hysteresis modeling, a procedure has been experimentally identified for measurement of the difference σ_2-σ_1 of two biaxial stresses. Experiment and modeling exhibit agreement thus far in the case where hysteresis parameters are used in stress monitoring. Other magnetic techniques are now being tried for the stress measurement.

Stanford University

Dept of Mechanical Engineering **$80,500**
Stanford, CA 94305-3030 **01-A**
93-3

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

The objectives of this research are to identify, understand, and model the effects of mean flow three dimensionality on turbulent boundary layer heat transfer. The present experiments are examining the heat transfer and turbulence structure on a large disk rotating in a quiescent environment. Single point measurements show that the vertical mixing of momentum and heat is suppressed by the three dimensionality. Two-point velocity correlations in an air flow apparatus indicated that crossflow weakens the sweeps and bursts which account for most of the production of turbulent shear stress. During the past year, a large water flow apparatus was developed duplicating the airflow geometry. Laser Doppler anemometer measurements confirmed that the flow accurately replicated the air flow. Flow visualization using high speed filming of hydrogen bubbles confirmed our qualitative interpretation of the two-point correlations showing conclusively that the crossflow reduces the vertical motion during a significant fraction of bursting events.

Construction and qualification of a heat-transfer disk for the airflow apparatus were completed and measurements were obtained for tip Reynolds numbers up to 850,000. A two-dimensional finite element code was required to correct for back losses due to the relatively large temperature variation on the constant heat flux surface. This year, the emphasis will be on higher Reynolds numbers and measurements of the turbulent heat flux.

Stanford University

Division of Applied Mechanics **$96,665**
Stanford, CA 94305-3030 **01-A**
91-3

Stability and Stress Analyses of Surface Morphology of Elastic and Piezoelectric Materials
H. Gao

The goal of this research is to investigate the mechanical effects of surface morphology of elastic and piezoelectric materials. In particular, the project will study the stability of material surfaces against diffusional perturbations and the stress concentration caused by surface roughness.

Besides work on piezoelectric surfaces, the most important progress of this project has been the discovery that a cycloid-cusped microscopic rough surface is capable of generating crack-like stress singularities in the form of Dirac-singular strain energy pulses. A cusped cycloid surface induces a crack-like singular stress field and is the most efficient stress concentrator at a fixed wavelength. An important difference is also noted. Cracks are active only under tensile stresses because of crack face contact under compression. In contrast, cusps work both ways: they admit a positive value of mode I stress intensity factor under tension and a negative value under compression. Thin films in semiconductor devices are often under compression due to lattice misfit, in which case the cusp provides a unique mechanism for stress concentration leading to mechanical failure.

A computer algorithm is being developed to simulate the evolution of a rough surface under stress corrosion leading to the formation of stress singularities.

Stanford University

Dept of Mechanical Engineering — $175,000
Stanford, CA 94305-3030 — 01-A
91-4

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

In solid mechanics defects such as inclusions, holes, cracks, and dislocations may undergo rearrangement as well as changes of size and form. The energy changes associated with such rearrangements provide thermodynamic driving forces which help characterize the response of solids under loads to these "transformations", and it is the determination and calculation of these driving forces which a portion of our research has as its aim. In the past year we have extended our methodology of heterogenization to treat certain problems in 3-D elasticity, plane thermoelasticity, and antiplane piezoelectricity; the results obtained are of significance in the areas of advanced composites and smart materials. In addition the Neutral Action Method we have recently developed has been applied to thermoelasticity, piezoelectricity, and porous media, and has yielded much insight into analyses of defects and fracture in these systems. We have continued to extend the thermodynamic theory of elastic solids prone to damage using a formalism based on the local state approximation.

Another portion of our work has as its objective the development of further understanding of subsonic and supersonic surface waves and of bulk and interfacial waves in anisotropic elastic and piezoelectric media. Such waves can serve as useful probes in the non-destructive evaluation of matter, provided sufficient details about them are well-understood. In the past year we have studied the existence of so-called "spaces of simple reflection" (within which are to be found supersonic surface wave solutions) in media with **no symmetry** (triclinic symmetry). In particular, we have found the extension of the space of simple reflection in the neighborhood of a supersonic one-component Rayleigh wave in such a solid (a space that had eluded earlier investigations), and we are now studying where and how such a space terminates with respect to slowness surfaces. The latter is a delicate computing problem that involves finding numerically generalized eigenvectors of non-semisimple matrices, which is a non-trivial computational problem. We are also examining reflection and refraction of plane waves in anisotropic bimaterials. During the coming year we intend to return to an unresolved problem in dislocation mechanics, namely the determination of equilibrated dislocation distributions in elastic solids under zero applied stresses; this critical problem must be solved if modern micromechanics is to prove capable of studying elastoplastic solids allowing for **unloading**.

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, R. Street, S. Schladow

A study of mixing processes in doubly diffusive systems is being Conducted. Continuous gradients of two diffusing Components (heat and salinity in our case) are being used as initial conditions, and forcing is introduced by lateral heating and grid stirring. The goals of the proposed work include: (1) quantification of the effects of finite amplitude disturbances on stable, double diffusive systems. particularly with respect to lateral heating, (2) understanding the role of Prandtl/Schmidt number on the mixing efficiency, evolution, and structure of turbulence in a stratified fluid, and (3) increasing our knowledge-base on turbulent flow in stratified environments and how to represent it. The work is being carried out in an experimental facility which is located in the Stanford Environmental Fluid Mechanics Laboratory. Our current research ideas are centered around the fact that while fluids are stirred by turbulence they are not mixed until molecular diffusion occurs. By stretching and folding surfaces of constant concentration and reducing the distance between them the turbulence sharpens the gradients and increases the diffusive flux. Thus turbulence enhances mixing but only molecular diffusion can perform the actual mixing. The research we are planning includes defining a parameter that measures efficiency of mixing and not just stirring, developing linear theory and extending a time scale analysis to predict the effects of molecular diffusion on mixing efficiency, and measuring the efficiency over a range of stratifications in a system stratified by salt, heat, and/or both.

Stanford University

Mechanical Engineering Dept **$441,508**
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. 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.

Results with an induction plasma facility show significant nonequilibrium within a downstream quartz test section, and suggest errors in conventional diagnostics assuming local thermodynamic equilibrium. Measurements of radiation source strength in argon indicate an order-of-magnitude difference from values reported earlier at temperatures of interest in plasma processing.

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. Growth rate of diamond films in these environments has been demonstrated to be 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 **$194,828**
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 viscus 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. Concurrent Research is done on systems with multiple stationary states and limit cycles. Work is planned on the formulation of thermodynamics of nonlinear (autocatalytic) chemical reactions which produce work or on which external work is done; and a similar formulation for systems with more than one temperature.

Stanford University

Dept of Chemistry **$95,328**
Stanford, CA 94305 **03-A**
92-4

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

This research project concerns the development of degenerate four-wave mixing (DFWM) for *in situ* diagnostics of the boundary-layer region in atmospheric-pressure reactive plasmas. The emphasis is on nonintrusive and state-specific techniques for monitoring the concentration, temperature and spatial distribution of transient radical species during plasma processing. DFWM is a highly sensitive laser-based nonlinear spectroscopy yielding a coherent signal beam that can be detected remotely, free from the interferences of background luminescence.

Recent experiments using DFWM to probe CH and C_2 during the plasma synthesis of diamond thin films have demonstrated the ability to provide parts-per-million-level detection with submillimeter spatial resolution in the measurement of rotational temperatures, vibrational temperatures, and species concentration. These experiments are conducted in an industrial-scale 50 kW inductive plasma reactor operating with argon, hydrogen and methane. The critical region is a narrow (less than 1 cm thick) boundary layer at the gas-surface interface. The CH temperature is found to fall monotonically from nearly 4000 K in the free-stream to 1200 K at the surface. Simultaneously the mole fraction of CH and C_2 rises and falls, with a maximum 200 microns above the surface. Excellent agreement is found between measured profiles and those predicted with a one-dimension computational model.

Stevens Institute Of Technology

Dept of Physics and Engineering **$67,000**
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 **$143,257**
College Station, TX 77843 **06-C**
93-2

Hydrocarbon/CO_2/Water Multiphase Equilibrium Separations
C. Wu

The objectives of this research project are: (1) conducting experimental measurements of phase equilibria for mixtures of selected hydrocarbons with CO_2 and water at pressures up to 10,000 psia and at temperatures up to 500°F and (2) developing a rigorous computer simulator (EOSS) using the Wong-Sandler mixture combining rules and "Area Method" for laboratory data analysis and general applications.

Two existing laboratory apparatus will be modified for the experimental work. A high-pressure mercury-free window cell will be upgraded to conduct the laboratory experiments to 400°F. A high-temperature distillation cell will be modified for experimental tests to 500°F. The experiments will use n-alkanes having carbon numbers from C_1 to C_{12}, naphthenes and aromatics, $C0_2$ and crude oils. Sufficient basic laboratory data will be collected and analyzed to determine three-phase K-Va!ues and phase properties using empirical correlations and the rigorous equation of state approach.

Existing phase-behavior computer simulators will be upgraded concurrently with the experimental work to describe the multiphase equilibrium separations. multiphase computer simulators will be verified with the experimental data for practical applications in compositional reservoir engineering and enhanced oil recovery, and for process design and chemical separation in chemical industry.

University Of Texas At Austin

Ctr for Studies in Statistical Mech and Complex Systems **$100,003**
06-C
Austin, TX 78712 **91-3**

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

A significant development has been achieved in the fundamental aspects of non-equilibrium dynamics. For unstable dynamical systems, there are different classes; this includes dynamical maps. Recent work by this group shows that the evolution operator of the probability distribution admits an irreducible spectral representation with complex eigenvalues related to the Lyapounov exponents. This representation is in generalized spaces (so-called "rigged" Hilbert spaces). The eigenfunctions are distributions (which are, in general, fractals) that have to be used in conjunction with test functions. This excludes the consideration of individual trajectories and implies therefore an irreducible statistical description. The existence of such irreducible representation can be considered as the very definition of chaos.

These representations also can be constructed for an important class of classical and quantum systems, called "Large Poincare Systems" (LPS), characterized by a continuous set of resonances. Most systems in nature are LPS. As a simple example, potential scatterings have been studied in detail. It has been shown that the usual spectral representations of the Hamiltonian or of the Liouville operator fail for persistent scattering; moreover, these are the first examples that show the limit of trajectory dynamics in classical systems and also the limit of quantum mechanics based on wave functions. The results have been verified by numerical simulations. For the persistent scattering, new spectral representation that is irreducible has been constructed in generalized spaces (it cannot be expressed in terms of wave functions). This representation incorporates into dynamics dissipativity, as well as approach to equilibrium.

Several applications of the new spectral representation are in progress. These are matter-field coupled systems (quantum optics), field-field coupled systems, evaluation of genuine three-body scattering cross section, causal behavior of the Lorentz gas, and so on.

University Of Texas At Austin

Dept of Physics **$182,883**
Austin, TX 78712 **06-C**
93-5

Complex Spatiotemporal Patterns in Nonequilibrium Systems
H. Swinney

The formation and evolution 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 ranging from fluid flows to chemical systems. When does a spatial pattern spontaneously emerge in an initially homogenous system as the external stress is varied, and what kinds of bifurcations between different patterns are allowed? How can concepts from dynamical systems theory elucidate the dynamics of nonequilibrium systems? Experiments and analyses are addressing these questions for convecting fluids, electrodeposition, and chemical systems. Experiments on reaction-diffusion systems have revealed a variety of spatiotemporal patterns that arise solely from competition between chemical kinetics and mass diffusion (convection is prevented by using novel gel-filled reactors). A traveling front type pattern has been found that differs from previously studied chemical patterns, but the experiments and simulations indicate that such patterns could often arise in spatially extended nonequilibrium systems. The comparison of experiment and theory for different types of systems should provide general insights into the formation of spatial and temporal patterns in nonequilibrium systems.

Tufts University

Dept of Mechanical Engineering **$59,798**
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 analysed.

(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, F. Otter, A. Eckbreth

The research objective 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). Nonintrusive 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 complementary techniques. In addition, coating characteristics such as smoothness, adhesion (UTRC custom built pin-on-disc apparatus) and hardness (state-of-the-art nanoindenter apparatus) are measured. Gas phase spectroscopy is interpreted through chemical kinetic modelling 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 processes such as PVD, CVD, combustion and thermal plasma deposition. Results to date include:

1) fabrication of a 5 kW rf PACVD reactor system
2) exploratory spectral emission studies
3) development of substrate preparation technology and characterization
4) implementation of a ultramicrohardness tester and adhesion test apparatus and analysis of coating hardness and elastic modulus
5) coating durability testing using UTRC erosion test facility
6) initial characterization of TiB_2 and diamond coatings
7) first time CARS observation of diborane (B_2H_6) in a PACVD process
8) *in situ* axial concentration and temperature profiles of key species (diborane and H_2) in 2 - 5 torr pressure range in a diborane/Ar plasma
9) formulation of chemical kinetic models for diborane pyrolysis
10) comparison with experimental results indicate thermal pyrolysis is not the mechanism for chemical initiation
11) proposal of surface species and heterogeneous reaction mechanism for the growth of boron from diborane plasma
12) extension of *in situ* laser diagnostics to diborane/Ar plasma in the 1-10 torr pressure range
13) *in situ* axial concentration and temperature profiles of diborane in the 1-10 torr pressure range in a diborane/$TiCl_4$/Ar plasma
14) observation of emission spectra of diborane/Ar and diborane/He plasmas indicate chemistry is initiated by electron impact dissociation of diborane and is not photoinitiated
15) surface chemical kinetics incorporated into analytical model

Washington University

Department of Systems Science and Mathematics **$75,999**
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 dynaically moving objects in an environment. It also introduces new challenges in System Theory, wherein feedback control is generated by visual sensors based onthe theory of nonlinear regulation and nonlinear optimal control. The proposed project undoubtedly broadens the technology and conceptual base while introducing some new promising appraoches to visually guided control systems.

Washington State University

Dept of Mech & Matls Engineering **$ 0**
Pullman, WA 99164-2920 **01-B**
91-2

Mass and Energy Coupling Effects in Multiphase Free Shear Flows
T. Troutt

The primary goal of this research program is to examine the effects of two-way multiphase coupling on the development of organized vortex structures in free shear flows and the resultant multiphase dispersion. Previous research studies have determined that one-way coupled particle dispersion in free shear flows is strongly dependent on the vortex structures present in these flows and their interactions as well as the ratio of the particle aerodynamic response time to the time scale of the dominant vortex structures.

Current research efforts are directed towards exploring the effects that two-way momentum, mass and energy coupling have on the multiphase free shear flow dispersion processes previously uncovered. These efforts involve analytical, numerical and experimental investigations. Recent results indicate that momentum coupling effects can change the linear stability characteristics of multiphase mixing layers and wakes. In addition numerical results demonstrate that the large scale vortex structure development can be significantly altered in two-phase mixing layers and wakes through two-way mass and momentum coupling interactions. These multiphase coupling effects may have significant importance with regard to predicting and controlling the performance of 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 **$114,000**
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

03-B

03-C

06-A

06-B

06-C

Principal Investigators

UNITED STATES DEPARTMENT OF ENERGY

WASHINGTON, DC 20585

OFFICIAL BUSINESS
PENALTY FOR PRIVATE USE, $300

FIRST-CLASS MAIL
POSTAGE & FEES PAID
U.S. DEPT. OF ENERGY

PERMIT NO. G20