DOE/ER-0580T

Summaries of FY 1992 Engineering Research

November 1992

U.S. Department of Energy

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

DOE/ER-0580T

Summaries of FY 1992 Engineering Research

November 1992

U.S. Department of Energy

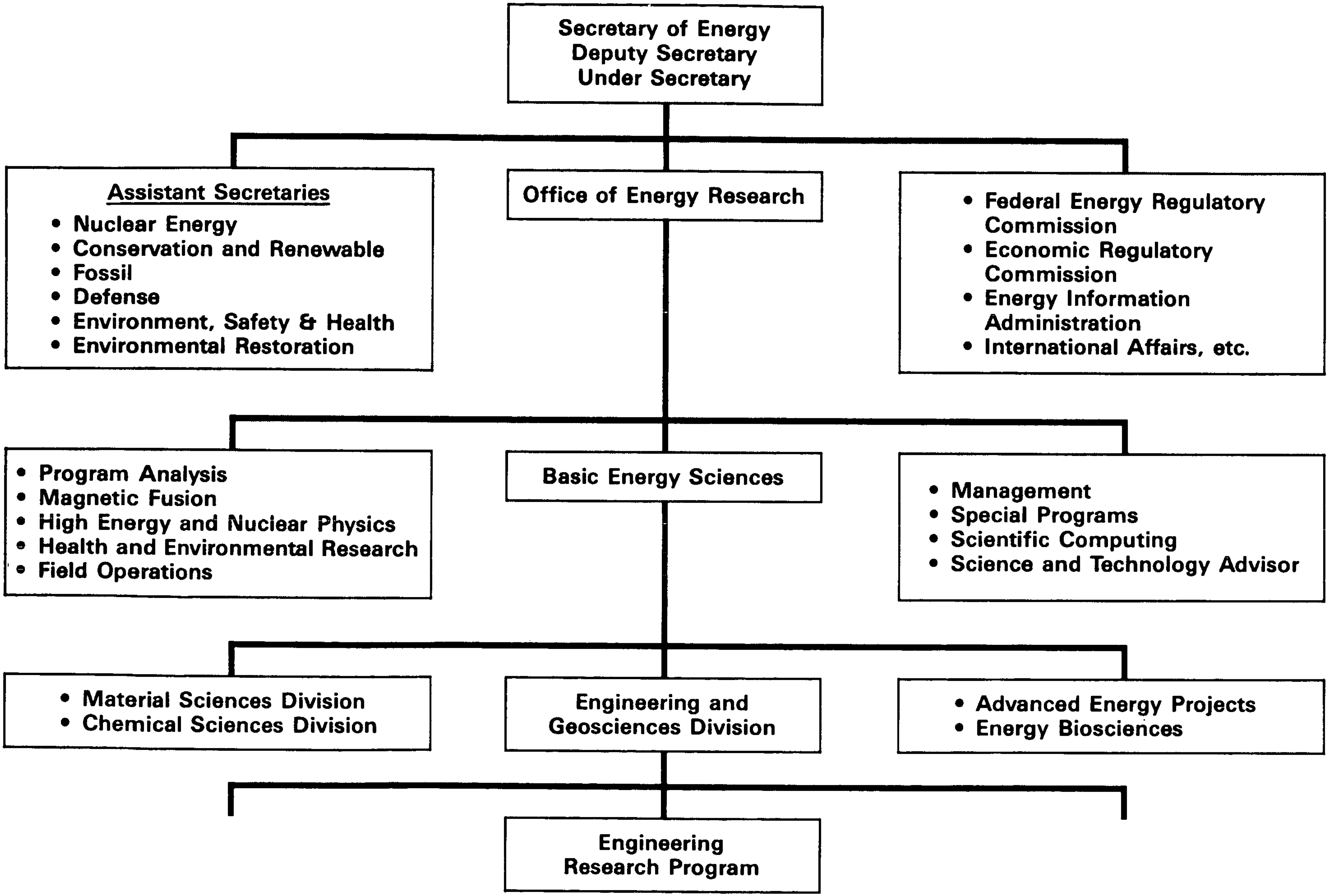
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences

Foreword

This report documents the BES Engineering Research Program for fiscal year 1992; 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 1992. 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 1992.

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 1992 appears to the right of title; it is followed by the budget activity number (e.g.,01A). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The 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.

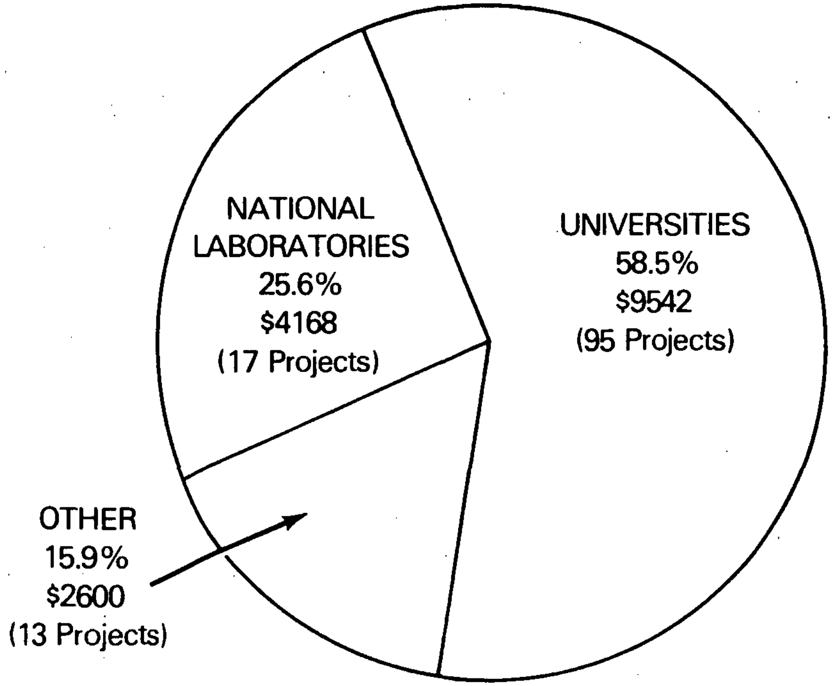
Another workshop aimed at identifying research opportunities to mitigate the effects of aging in energy production and distribution systems took place in October 1992. The proceedings will appear in Applied Mechanics Reviews.

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 twelve 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 1992 the available program operating funds available amounted to about $16.4 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 '92 BUDGET ($000's) BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM

FY '92 BUDGET BY TECHNICAL AREAS

	($000 s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	**4975**	**30.5**	**49**
SYSTEMS SCIENCES	**5160**	**31.6**	**28**
ENGINEERING ANALYSIS	**6176**	**37.9**	**48**

Table of Contents

Table of Contents (continued)

University Of Alabama

Dept of Mathematics **$54,126**
Tuscaloosa, AL 35487 **01-C**
91-3

Hydrodynamic Instabilities and Coherent Structures
A. Frenkel

The objective of this project is to advance the understanding of instabilities of several fluid systems relevant to energy engineering sciences. Some problems, approaches to their solution, and results follow.

For the problem of coherent structures and the inverse energy cascade in turbulent flows, both statistical ensembles and deterministic periodic flows are considered.

It is found that an isotropic turbulent flow is stable to the mean-flow perturbations. This suggests that some statistical anisotropy is necessary for the growth of the coherent structures.

The same techniques, based on mathematical insights into the properties of functionals of Gaussian processes, yields a new description of the diffusion of a passive scalar - such as the temperature - in a turbulent flow.

For a deterministic unidirectional flow with a sinusoidal profile of velocity, it is shown rigorously - by using continued fractions - that some perturbations which do not have the same periodicity as the basic flow, can nevertheless grow. The much more complicated case when the flow is, in addition, sinusoidal in time is reduced to an infinite algebraic eigenvalue problem. Its Galerkin approximation results are not restricted to large scales, in contrast to earlier results. An exact solution of a generalized Orr-Sommerfeld equation in the inviscid case is found and compared to the Galerkin-based results.

For the core-annular flow - important in the lubricated pipelining of heavy oils - a new nonlinear interface equation is derived. It reflects the dynamics of the core in addition to the dynamics of the lubricating film. Several domains of basic parameters are indicated in which the instability cannot break up the flow. The finite but small oscillations of the interface can have the character of either deterministic chaos or else a nonlinear propagating wave.

Argonne National Laboratory

Materials & Components Tech Div **$139,800**
Argonne, IL 60439 **01-A**
90-3

Chaos in Fluid-Structure Systems
S. Chen, T. Mulcahy

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 joint project 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 rows in crossflow is being studied in detail. A tube row with a motion-limiting stop configuration is 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 will also be investigated.

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. The understanding of dynamic characteristics, including periodic oscillations, random vibration, and chaotic motion, will impact the design and reliability of these systems in both the near and long term. In addition, fluid-structure systems are classical examples of autonomous systems that can exhibit chaotic behavior. Knowledge of the fluid-structure systems may provide some insights into the chaotic behavior of other energy system components.

Argonne National Laboratory

Materials & Components Tech Div **$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.

The dynamic plastic deformation of some basic structural configurations are being analyzed for loadings which vary both in magnitude and region of application with time. Mode approximation methods and load correlation parameters are hypothesized and their usefulness in predicting final plastic deformation is determined. The methods, based initially on a rigid, perfectly plastic material model and small deformation response, are extended to include strain hardening, an initial elastic response period, and large deformation interactions.

Arizona State University

Mechanical & Aerospace Eng **$60,000**
Tempe, AZ 85287 **01-A**
92-4

Continuous Damage Mechanics - Critical States
D. Krajcinovic

The research during the fourth, and last, year of the research was focused almost entirely on the two tasks: (a) response of microcrack weakened solids in the vicinity of the critical state, and (b) initial exploration of the use of Preisach model in fatigue analyses.

The studies of critical states were concentrated on fundamental issues such as the determination of the proximity parameter, universal parameters, order parameter and differences between the elastic and traditional (conduction) percolation problems. It was demonstrated that the second order phase (connectivity) transition takes place only in stress (load) controlled conditions. In contrast, localization (emergence of shear bands) of the deformation occurs in the strain (displacement) controlled tests. It was shown that the proximity parameters can in fact be formulated in terms of the Budiansky, O'Connell damage parameter.

Initial exploration of the Preisach model were focused on ductile behavior using parallel bar models. Important conclusions were related to the thermodynamics of the process, including differences between locked-in and dissipated work. It seems that the Preisach model may be very suitable for studies of the fatigue problem. This work will require significant modifications of the original model.

Battelle Memorial Institute

Mechanics Dept **$94,027**
Columbus, OH 43201-2693 **01-A**
90-3

An Investigation of the Effects of History Dependent Damage in Time Dependent Fracture Mechanics
F. Brust, Jr.

The demands for structural systems to perform reliably under severe operating conditions continue to increase. Modern energy production facilities experience degradation and damage because they operate in a severe high-temperature environment where time dependent straining and damage may lead to structural failures. 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 types of time dependent (creep) damage considered in this program include: sustained load creep, variable load creep, and variable load creep with thermal gradients. During the first year of this study, the implications of using Norton's creep law on various integral parameters used to characterize crack tip phenomena were evaluated as a function of time. Other constitutive laws for time dependent materials such as those of Murakami and Ohno are being implemented into the finite element code. In addition, constitutive property data and high temperature creep crack growth data are being obtained on stainless steel. These experiments will be used to verify analytical predictions and characterize time and history dependent damage during crack nucleation and growth.

The results from this work will be used during the design phase by practicing engineers to enhance the life of high temperature structural systems.

University Of California/B

Dept of Electrical Engineering & Computer Sciences **$97,000**
Berkeley, CA 94720 **06-C**
90-3

Self-Generated Stochastic Heating In an RF Discharge
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 plays a major role. The stochastic electron heating arises from successive decorrelated reflections of electrons with the oscillating sheath near the surface of the discharge. Power is also transferred directly to the ions by acceleration in the sheaths. The efficiency of stochastic heating depends on the detailed sheath dynamics. For a low pressure discharge at a pressure of 3 mTorr, power of 100 watts, and frequency of 13 MHz, 95% of the electron heating is predicted to occur stochastically.

The sheath dynamics are being measured and related to the predicted stochastic heating for a plane parallel argon discharge. Depending on the details of the sheath motion, the enhancement factor of the stochastic heating can change, and consequently so can the ratio of electron to ion power at a given overall power level. The measured results, together with measurements of other plasma parameters, will be used to construct better predictive models of discharge behavior and parameter scaling.

Stochastic heating can be enhanced with a resonant helical discharge structure. This geometry is of importance for materials processing applications and is under investigation as part of the overall program to understand plasma heating and develop models of r.f. processing discharges.

University Of California/B

Dept of Mechanical Engineering **$120,603**
Berkeley, CA 94720 **01-B**
92-3

Thermal Radiation and Conduction In Microscale Structures
C.-L. Tien

Micro- and nanometer scale devices are becoming more and more prevalent in energy related applications. The rapid acceptance of microelectronics as commonplace control and data processing elements makes the systems using them vulnerable to heat instabilities. It is therefore of crucial importance to understand how heat is transported by radiation and by conduction on micro- and nanoscales. From the basic point of view problems arise because some of the characteristic lengths arising in heat transfer are not small as compared with the dimension of the heated or cooled objects, unlike the case usually encountered in heat transfer.

The proposed research is divided into three complementary parts:

1) Radiative properties of microstructures. Because of the small size of the objects of interest, it is expected that partial coherence theory of light will play a role in the emission of radiation by the small devices. To use that theory it has to be suitably generalized. At the same time microstructures themselves have significant effects on the optical constants. Experiments and analysis will be carried out to characterize those effects on the optical constants.

2) Radiative heat transfer in microstructures. Since the dimensions of microstructures are often comparable with the wavelengths typical of the radiated spectrum, geometrical optics may fail, and the intrinsic wave nature of the field must be taken into account. Theoretical studies will be carried out to determine how such phenomena as interference and diffraction affect radiative heat transfer.

3) Conductive heat transfer in microstructures. Unlike previous related work, here the size effects on heat conduction in multilayer films will be studied. Again both theoretical and experimental studies will be carried out. Of special note is the attempt to measure more reliably heat conduction in thin films, an area of experimental science which needs much more development.

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

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

A systematic development of models for turbulent transport in porous media with regular morphology is underway. Methods have been developed to close the integral terms in the turbulent transport equations that depend on the geometrical structure of the media. A tridiagonal non-monotonic algorithm has been designed to improve the numerical accuracy of the "one-temperature" model equation with irregular 3-nd kind boundary conditions for a highly porous medium.

Theoretical models for flow resistance and heat transfer have been developed for porous media with capillary and globular morphology (tubes, slits and beads free of interacting) that are valid over a wide range of parameters. Comparisons of the results obtained for these canonical models with coefficients of drag resistance and heat transfer for common non-structured porous media show good agreement for Re > 10.

Results have been obtained using one - and two-temperature turbulent transport models and comparison with effective coefficient one-temperature models will be made. Models have been developed for turbulent flow in a duct with roughness developed from regular two dimension shapes like ribs, rods, spheres and trapezoids. These models demonstrate the sensitivity of transport phenomena to the surface morphology of the solid surfaces whether a duct wall or interstitial space boundaries within the porous media. Methods of experimental confirmation are being developed for such regular morphology in porous media and other surfaces.

University Of California/LA

Physics Dept **$79,000**
Los Angeles, CA 90024 **06-C**
90-3

Wave Turbulence and Self-Localization in Continuous Media
S. Putterman

The fate of energy which is injected into fluids that are far from equilibrium is being investigated from the experimental, theoretical and computational point of view. These off-equilibrium systems can display a tendency to a) form structures b) develop a stochastic spectrum of energy and c) focus energy. Regarding a) the formation of solitons, domain walls and kinks in continuous media is being studied. Regarding b) the tendency of a spectrum of acoustic motion to become wave turbulent is being investigated and regarding c) the transduction of sound into light is being measured. This last phenomenon results from a self-focusing instability that concentrates energy by a factor of one trillion.

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

We are investigating methods for modeling fluid flows and plasma dynamics of relevance to energy problems when these physical phenomena exhibit motion on fractal objects called strange attractors. In these cases, which are quite common both in the settings indicated, and in electrical circuits and condensed matter systems, the time series have continuous broadband power spectra and quite irregular behavior. We are engaged in methods for identifying the space in which to work for these systems (phase space reconstruction), methods for computing the invariants of the motions, and methods for making physical models for prediction in these irregular systems. These systems are inherently less predictable than familiar linear systems, but their predictability is nonzero and may be extracted in a systematic fashion from the time traces themselves.

The work has concentrated on methods to extract chaotic, deterministic signals from noisy measurements. The noise may be due to environmental conditions or measurement errors or may have been imposed on purpose to mask the signal. With these "cleaning" tools, we will clean up laboratory and field data for use in the other parts of the signal processing effort.

University Of California/SD

Dept of App Mech & Eng Sci **$126,000**
La Jolla, CA 92093 **06-B**
90-3

Experimental and Theoretical Study of Fuel Droplets Subject to a Straining Flow
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 counterflowing streams which result in flat nonpremixed flames. A test rig which permits a wide variety of investigations including nonpremixed. premixed and partially premixed systems has been put into operation. Initial results involve a study of the extinction characteristics of these flames. A contribution including related theoretical work has been accepted for presentation at, and publication in the proceedings of, the International Combustion Symposium in Sydney. A phase doppler system permitting droplet size, two components of velocity and droplet population to be measured has now been set up and is undergoing initial testing so that a more complete set of data on droplet behavior in these streams will be obtained shortly. In addition the initial theory is being refined and improved. Attention is also being devoted to the applicability of the spray equation to counterflowing streams since there appear to be both theoretical and experimental difficulties arising when the droplet velocity goes to zero.

University Of California/SD

Department of Chemistry, 0340 **$183,512**
La Jolla, CA 92093 **06-C**
92-4

Noisy Nonlinear Systems
K. Lindenberg

Transport and reactions on fractals occur in many natural phenomena including geological processes and processes in the solid state or on surfaces. Our efforts have been directed toward gaining a theoretical understanding of these processes.

The time that it takes a walker to reach a given point on a fractal is relevant for events that are triggered when an excitation or molecule or charge reaches a designated point. Our analysis is based on a renormalization approach that yields exact results on some deterministic fractals. Whether these methods can be generally applied to random fractals is still an open question; we have applied them to certain classes of random fractals.

The rates of even the simplest diffusion-controlled reactions in low-dimensional (including fractal) systems behave very differently than the standard law-of-mass-action descriptions and have been called "anomalous" and indicative of "mathematical poisoning." Our calculation of reaction rates is based on scaling arguments that lead to parametrized results. Even this limited success has provided a great deal of insight.

We continue to make progress in the (unrelated) problem of the effect of colored noise on the evolution of a system. We have obtained analytic results for a dye laser driven by Gaussian fluctuations and also for bistable systems driven by dichotomous noise and by monochromatic noise.

University Of California/SD

Pure & Applied Physical Science **$98,000**
La Jolla, CA 92093 **06-C**
91-2

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 J and the Proceedings of the International Conference on Knot Theory and Related Topics, Osaka, Japan, 1990) 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 3 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. The same framework will also be applied to other one dimensional models such as the cellular automaton for Burger's equation. In addition one would like to begin investigating higher dimensional models, though this is expected to be much more difficult.

University Of California/SD

Inst for Nonlinear Science, R-002 **$94,458**
La Jolla, CA 92093 **06-C**
91-2

Formation of Three-Dimensional Singularities, Regularization Procedures and Markovian-Multifractal Description of Turbulent Flows
E. Novikov

A new approach to the problem of turbulent flows with high Reynolds number is developed. This approach is based on the conditional averaging of hydrodynamics equations for local characteristics with self-amplification (vorticity field in 3-D turbulence and vorticity gradient in 2-D turbulence). Some new exact results are obtained by this approach. The concept of conditional averaging is also applied to sub-grid modelling of turbulence for large-eddy simulations. Additional progress is made by a Markovian description of two-point characteristics of turbulence with the use of breakdown coefficients. Preliminary numerical experiments for the formation of singularities in viscous turbulent flows are performed. New results are also obtained for the chaotic vortex-body interactions.

University Of California/SD

Dept of Physics **$ 0**
La Jolla, CA 92093 **01-B**
90-3

Traveling-Wave Convection in Fluid Mixtures
C. Surko

While much progress has been achieved in understanding the dynamics of free convection in single-component fluids, much less is known about convection in fluid mixtures, yet in many realistic situations, the latter plays an important role. Examples of interest to engineering include the stability of doubly-diffusive systems such as solar ponds, the solidification of metal alloy casts, and convection in fuel droplets.

This research program addresses the role of traveling-waves in the dynamics of convective flows in fluid mixtures. Even in a relatively simple experiment, the behavior of the system is such that, by varying one or two control parameters, the whole gamut of states ranging from laminar traveling-waves to well developed turbulence can be explored. For example, in one experimental setup, a narrow annular channel is filled with a water-ethanol mixture and heated from below to produce free convection. For a range of parameters, this convective flow occurs in a pattern of traveling-waves, in the form of moving convective rolls, which propagate around the annulus. The resulting oscillatory convection exhibits a wide range of phenomena. One striking example is the occurrence of confined states, where regions of convection, confined to just a portion of the annular channel, co-exist stably with regions of quiescent fluid, even for uniform spatially values of the control parameter. In this case, we now understand that these convecting regions are stabilized by currents of concentration associated with the traveling-waves. The nature of convection in such mixtures is expected to be prototypical of effects arising in many contexts, ranging from oceanic flows to instabilities in liquid crystals.

Current research focuses on three related topics: measurement of the concentration field, study of the mechanisms of wavelength selection in one-dimensional traveling patterns, and study of traveling-wave patterns in large-aspect-ratio, two-dimensional geometries.

University Of California/SB

Dept of Physics **$130,000**
Santa Barbara, CA 93106 **06-C**
90-3

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

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

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

In pure fluids, we are investigating the mechanisms for the convective onset. In most physical systems the flow is initiated by properties of the experimental cell which lead to an imperfect bifurcation. Recently it has been possible, however, to perfect the apparatus to a point where stochastic effects control the evolution of the flow.

Beyond the convective threshold we are interested in the evolution and stability of various convective patterns in containers with simple sidewall geometries. We expect that our results will help in the development of theoretical models for pattern stability.

A particularly interesting pattern-stability problem occurs in binary-mixture convection. For certain values of the parameters of this system, there exist spatially localized patches of travelling waves of convective rolls. The existence of these states cannot be explained by the usual models with relaxational dynamics, but rather seem to require non-potential theories. We are studying quantitatively the wavenumber, frequency, amplitude, and spatial extent of these localized states. This information will permit a distinction between several competing theoretical models.

University Of California/SB

Dept of Chemical & Nuc Eng **$ 0**
Santa Barbara, CA 93106 **01-C**
91-3

Turbulence Structure and Transport Processes In Wavy Liquid Streams
S. Banerjee, G. Hetsroni

The first series of experiments in this program was to visualize wave-turbulence interactions near the shear-free gas-liquid interface. Waves were generated mechanically with different wavelength and amplitude without imposed shear at the interface to observe the effect of the waves on the underlying turbulence structure.

Oxygen bubble tracers lit by a laser sheet of light were imaged with high speed videography and single frame techniques. Turbulence quantities such as the mean velocity profiles, turbulence intensities, Reynolds stresses and turbulence production were evaluated near the interface. A paper has been submitted to Physics of Fluids summarizing these data.

Detailed measurements of these values within waves will be taken using the three-dimensional LDA with an ultrasonic gauge to define the instantaneous LDA distance from the interface. This work will clarify the identification of bursts within the surrounding fluid by using the flow visualization method to do conditional sampling of LDA data. When suitable criteria are isolated we will no longer have to rely on the visualization technique.

From a preliminary evaluation of the data already obtained it appears that the absolute value of the triple correlation between the three velocity fluctuation components, i.e. / u'v'w' / is a positive indicator of bursting motions.

Finally the contribution of surface waves versus bursting events to turbulence will be differentiated and compared for each run. To support the physical experiments, a program of direct solution of the Navier-Stokes equations will be continued using the pseudo-spectral method. With the new program we will incorporate free surface boundary conditions that allow the 2D wave trains of constant shape to be considered, and we have incorporated a scalar field (temperature or concentration) that will allow a computational assessment of relationships, if any, between large-scale flow structures and rates of heat and mass transfer.

California Institute Of Technology

Chemical Engineering 210-41 **$126,144**
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 can now be used to generate uncertainty descriptions relevant for robust control, PLS's performance advantages are clearer, and PLS can be applied to more general models.

Carnegie Mellon University

Chemical Eng Dept & Graduate **$160,000**
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 distillation, 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, travelling 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 a many examples, including a mixture of methanol, water, n-pentane and acetone. We shall next study 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 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 toplogy. The basic idea relies on a rigorous nonlinear convex NLP understimator 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 toplogies 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 Lyapunov-based stability theory has been developed and demonstrated. 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.

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 address the basic theories of reconfigurable modular manipulator systems that will culminate in the demonstration of these theories on experimental hardware. A modular manipulator system consists 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 RMMS design emphasizes modular manipulator components having consistent mechanical and electrical interfaces. The uniform interfaces will allow either semi-skilled field personnel or another manipulator to rapidly configure a RMMS manipulator to meet specific task requirements. 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 will develop methodologies that map the task requirements into a specific manipulator. The kinematic task requirements will be used to determine the link lengths and the orientation of the modules. And the dynamic task requirements will be translated to obtain the sizes and ratings of the actuators or joints. The use of both rule-based expert systems and optimization techniques will be investigated in obtaining a solution to this problem. For effectively controlling modular manipulators (RMMS), a methodology for automatically configuring a controller will be developed using model-based and/or adaptive control techniques.

University Of Chicago

Dept of Chemistry **$92,747**
Chicago, IL 60637 **06-C**
92-1

Finite-Time Thermodynamics and Effective Energy Use
R. Berry

The broad goal of this project is the development and application of methods to find the optimum performance of systems and processes amenable to thermodynamic analysis, and to find pathways that yield optimal performance. The current project has the goals of: a) extending to distributed systems the methods for treating lumped systems; b) finding how to select and use variables that describe nonequilibrium conditions, to study systems far from equilibrium; c) to find optimal performance, using these methods, for systems notable for high dissipation, such as separation processes. The results from the past year have been: development of a method for treating distributed systems with heat transfer by a generalization of distributed potential fields; analysis of the optimal performance achievable with heat-driven separation processes subject to realistic rate constraints; analysis of the efficiency of heat engines with distributed working fluid and subject to constraints of nonzero rate; determination of power and efficiency limits for internal combustion engines with distributed working fluids. In addition, papers on minimization of entropy production under conditions of finite rates of propagation of heat, and on a fully canonical formalism for thermodynamic evolution of systems at nonzero rates were submitted after the Grant period.

University Of Chicago

The Enrico Fermi Institute **$153,320**
Chicago, IL 60637 **06-C**
90-3

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. Recent developments cause the designs to be functionals of the acceptance angle. This permits new solutions which solve classical problems in illumination for the first time.

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, to understand the deposition of droplets or particles on the wall or their tendency to accumulate near the wall, a knowledge of such forces is important.

The approach used in the research involves a combination of analytical, numerical, and laboratory work. The analytical approach can provide useful asymptotic expressions 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. As a result, direct numerical simulations of the three-dimensional flow field around a sphere in a shear flow will provide the forces. In addition, experimental measurements of particle velocities in a vertical homogeneous shear flow apparatus will provide additional information and permit checks of the numerical study.

The asymptotic analysis portion of the project is done. A computer code has been developed for the direct numerical simulations. The code employs a hybrid spectral-finite volume technique to solve the incompressible Navier-Stokes equation. The program has been used to compute the lift force over the ranges of particle Reynolds numbers of interest. Further work is needed to determine the influence of the computational domain size. However, the results obtained to date are in reasonable agreement with the predictions of the asymptotic theory. A homogeneous flow apparatus has been constructed at Los Alamos National Laboratory and is being tested at Clarkson.

University Of Connecticut

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

Engineering Science Software

Smithfield, RI 02917 **$48,500**
01-A
88-3

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

The first part of this project has focussed on developing and experimentally verifying methods of predicting the deformation response of polycrystalline metals from models of single crystal deformation, based on crystallographic slip. A crystallographic slip based single crystal viscoplastic model was developed and then used in a mircomechanical model to predict the overall viscoplastic response of the polycrystal. Single crystal experiments were used to get all model constants from which polycrystalline response was predicted. Polycrystal experiments data was used to critically test the predictions and the predictions and experiments were found to be in good agreement.

In the ongoing research, the goal is to try to predict the degree of heterogeneity of deformation and verify these predictions experimentally. The existing self-consistent model is to be completed by a second model based on periodicity which is expected to be both more realistic and more computationally burdensome. The degree of heterogeneity of deformation will be studied by the different experimental techniques. Neutron defraction experiments are planned in which defraction from a few grains at a time is studied to determine lattice strains in individual grains. Many grains will be surveyed to get statistical measure of heterogeneity of grains including no surface grains. The Moire' strain analysis will also be done on large grained samples. The material studied is the same one's used in the first phase, so that all the single crystal mechanical properties are accurately known. The data collected will prove a unique complete set of data to test the ability of the models in this program and other models with respect to their ability to predict the degree of heterogeneity of deformation. Comparison of more data and the neutron defraction data will also provide insight into the difference between surface grain behavior and interior grain behavior. Developing models that realistically predict grain to grain heterogeneity and verifying those models is a basic element in modeling mechanical behavior. Heterogeneity is particularly important to fatigue in which the most unfavorably oriented grain is the site of failure.

Cornell University

Mechanical & Aerospace Engineering $62,989
Ithaca, NY 14853 01-A
91-3

Chaos in Fluid-Structure Systems
F. Moon

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 joint project with Argonne National Lab.

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 rows in crossflow is being studied in detail. Tube row with a motion-limiting stop configuration will be tested to investigate various response characteristics and a mathematical model based on the unsteady flow theory will be developed to predict the response characteristics of this classical fluid-structure system.

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. The understanding of dynamic characteristics, including periodic oscillations, random vibration, and chaotic motion, will impact the design and reliability of these systems in both the near and long term. In addition, fluid-structure systems are classical examples of autonomous systems that can exhibit chaotic behavior. Knowledge of the fluid-structure systems may provide some insights into the chaotic behavior of other energy system components.

Cornell University

Sibley School of Mech & Aero Eng $105,818
Ithaca, NY 14853 01-C
91-3

Experiments in Turbulent Mixing
Z. Warhaft

This project is concerned with experimental studies of scalar mixing in fully developed turbulent flows, a subject relevant to our understanding of chemical reactions, combustion and environmental pollution. Mixing in both homogeneous and inhomogeneous turbulence, with and without the effects of buoyancy is being examined.

The first experiment concerns scalar dispersion and mixing in a jet. This is studied using a novel method of introducing a scalar (temperature) into an air jet by means of placing thin heated wire rings, axisymmetrically, downstream from the jet origin. The diameter of the rings and their location from the jet is varied so that the effect of initial conditions on the subsequent evolution of the scalar mixing can be studied. The placing of a thin wire ring in a jet is analogous to placing a line source in homogeneous turbulence, a subject that has received much attention. We can anticipate that the thermal field will be more complex than that of a line source since as the flow evolves the thermal field from one side of the flow will begin to mix with that from the other side. This does not occur with a line source in grid turbulence. So far as we can determine there has been no previous study of a heated ring source in a jet. The effects of two scalar mixing is also being studied by adding a second ring. Preliminary findings show unexpected results concerning the evolution of the segregation and cross-correlation coefficients.

The second main experiment is concerned with scalar mixing in stably stratified decaying grid generated turbulence. A temperature (density) gradient is formed at the entrance to the plenum chamber of the wind tunnel and then the flow is passed through a turbulence generating grid.

Single and multiple line source dispersion experiments on mixing across sharp temperature steps, with and without buoyancy, are being attempted.

Dartmouth College

Thayer School of Engineering **$135,000**
Hanover, NH 03755 **06-C**
91-2

Mixing and Settling in Continuous Metal Production
H. Richter

For reasons of both energy conservation and environmental protection, tonnage oxygen has become an essential component in many ferrous and nonferrous smelting and refining operations. Innovative reactors such as the QSL converter for direct lead bullion production are also suitable for direct coppermaking and a modification of the reactor is also very attractive for steelmaking.

Oxygen and fuel are bottom-injected into the molten bath of these essentially horizontal reactors in controlled rates required for heating, physical mixing and chemical reaction purposes. Sufficient turbulence is generated to maximize heat and mass transfer rates. However, such bath turbulence is opposite to the process requirement for continuous countercurrent flow of liquids at specific temperature, compositional and oxygen potential gradients. The powerful stirring effected by submerged gas injection is therefore judiciously localized so as to provide adequately calm settling zones between the active turbulence zones in a staged mixer-settler.

The research objectives of the work are to learn about the behavior of gas and particulate matter in turbulent liquids, the nature and paths of liquids and particulate entrainment into the plumes, and separation phenomena including travel to and behavior in the settling zones. Such knowledge is of fundamental value in designing reactors for continuous, direct metalmaking.

The new information will predict bath mixing, heat and mass transfer and settling parameters under the variety of operating conditions which will prevail in continuous, direct metalmaking oxygen reactors of the future. Therefore, it is proposed to study gas injection through submerged injectors, and also particulate addition from above, into a liquid bath consisting of two immiscible layers of liquids having roughly the same viscosities as slag and matte or metal and with roughly comparable density ratios.

Dartmouth College

Thayer School of Engineering **$120,599**
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

Mech Eng & Mat'ls Sci Dept **$50,000**
Durham, NC 27706 **01-C**
90-3

Analytical and Experimental Study of Instabilities in Buoyancy-Driven Convection in Porous Media
J. Georgiadis

The mission of this research project is the study of thermal instability phenomena associated with natural convection in two classes of fully-saturated porous media systems: (1) porous media saturated with pure fluids, and (2) porous media saturated with binary fluids. Our primary objectives are: (1) the delineation of the various stability domains for the convective flows and an exploration of the convective states after the onset of secondary instabilities, (2) the development of novel experimental techniques for high precision measurements and determining the flow patterns in porous media, and (3) the validation of macroscopic governing equations for natural convection in porous media.

Emphasis is put on the first two objectives. An experimental investigation of the onset of natural convection in a porous medium with internal heat generation is initiated. The potential of Magnetic Resonance Imaging (MRI) techniques in visualizing low-speed flows in porous media is also investigated. We will explore ways of obtaining quantitative information on interstitial velocity profiles by using a combination of spin tagging and spatial encoding MRI processes. Direct numerical simulation and stability analysis of the pertinent convective states will be performed in conjunction with the experimental component of this investigation.

Idaho National Engineering Lab

Biotechnology and Geosciences **$109,000**
Idaho Falls, ID 83415-2210 **06-A**
89-3

Three Phase System Modelling
G. Andrews

Many unit operations in environmental engineering, including biological wastewater treatment and flotation (used to remove colloids from wastewater and sulfur from coal), involve bubbles rising through water containing both surface-active materials and suspended particles. There is no general theory to predict the hydrodynamics near millimeter-sized bubbles in this situation, which makes it difficult to predict the gas/liquid mass transfer rate (in biological wastewater treatment) or the number of particles that strike the bubble (in flotation). This task will develop a mathematical model of the situation on the upper surface of the bubble where most mass transfer and particle capture occurs. The model will be based on integral boundary layer theory for the hydrodynamics and the transport of surfactant to and from the interface, and will include the effect of adsorbed surfactant on the force balance at the bubble interface.

The results will be compared with experiments designed to measure the particle capture rate as a function of surfactant concentration (i.e., interfacial tension) and particle concentration. Particle capture rate is measured because it is a very sensitive indicator of bubble interface motion.

Idaho National Engineering Lab

Applied 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 measurement of temperature, velocity, enthalpy, and species concentration in high temperature gases such as weakly ionized thermal plasmas has considerable importance in the areas of plasma thermal spray and the thermal plasma synthesis of materials. In particular, the dynamics of the plasma, the interaction of the plasma with its surroundings and the behavior of particles immersed in the plasma surrounding it are important in the understanding, development and optimization of plasma process that involve fine powders.

Traditional measurement techniques, such as emission spectroscopy, have severe limitations and often yield excitation temperatures which reflect neither the true gas kinetic temperature nor the temperature of the electrons. Laser based measurement techniques which have been developed and applied to the study of thermal plasmas at this laboratory include Coherent Anti-Stokes Raman Spectroscopy for species measurement, Rayleigh and coherent Thompson scattering for heavy particle, electron temperature and number density measurement, laser scattering Doppler shift plasma velocity measurements, and the simultaneous measurement of particle size, velocity, temperature, and number density. In addition to the laser techniques enthalpy probes coupled to a mass spectrometer also provide temperature, velocity and concentration information. The experimental data produced is used to benchmark the modeling work done under a related program in "Modeling of Thermal Plasma Prccesses" (see J. Ramshaw, Idaho National Engineering Lab).

Idaho National Engineering Lab

Energy & Systems Tech Grp **$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 transient compressible Navier-Stokes equations. Multicomponent diffusion is calculated by a self-consistent effective binary diffusion approximation, including 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 kinetic and equilibrium chemistry routines. 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 (LTE) are accounted for by a two-temperature model which permits the electon and heavy-particle temperatures to differ. Nonequilibrium populations of excited levels will be 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 simulations of plasma jets and plasma spraying.

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, W. Lloyd, J. Epstein

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluation guiding the direction of experimental testing. Tests are being conducted on a material (a modified ASTM A-710) exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength. As test temperature increases, the specimen configuration-fracture toughness relationship complies initially with requirements for linear elastic-fracture mechanics and extends beyond the range of a J-controlled field. Presently, compact tension and bend specimens are being used to develop state-of-the-art fracture mechanics data for comparisons with data developed from specimens containing surface cracks.

These comparisons are presently underway for 6.4 and 12.7 mm thick surface- flawed specimens. Metallographic techniques are being used to measure crack tip opening displacement and remaining ligament configurations for comparison with analytical models. Other techniques including microphotography and replicating of the crack tip region to complement the above measurements are being used to identify limits and capabilities of each technique. Moire interferometry techniques are being used to evaluate and quantify the deformation in the crack region. These data are being used to experimentally measure J and CTOD for standard (CT and SENB) specimens as well as for specimens containing surface cracks. The above tests have been supplemented by using specimens fabricated from aluminum (dimple rupture only) and titanium. The titanium specimens are being used to study the fracture behavior and the ability of existing models to predict failure for weldments. Moire interferometry techniques are being used to study the local constitutive behavior and the fracture process at the crack tip region of the weldment. Automated techniques are being developed to obtain, store and analyze the moire data.

This project is carried out in collaboration with Professors Parks and McClintock at MIT.

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 six years. Research is being conducted on an extension of the fundamental process physics, application of neural network-like dynamic controllers and signal/image processors, and development of noncontact sensing techniques. Tasks include physics of nonlinear aspects of molten metal droplet formation, transfer, and substrate thermal interaction; understanding the relationship of neural network structure and associated learning algorithm to model development and learning dynamics in neural networks with the objective of obtaining a fundamental understanding of network transfer functions; and advanced 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 MIT.

Idaho National Engineering Lab

Nondestructive Mat'ls Charac Group $200,000
Idaho Falls, ID 83415-2209 03-B
90-3

Nondestructive Evaulation of Superconductors
K. Telschow

The purpose of this task is to perform fundamental research which will lead to the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of high-temperature superconducting materials. In the near future, application of these new superconductors will require NDE methods for evaluating the properties of wires, tapes, and coatings. Microstructural and, particularly, superconducting properties, must be measured noninvasively in a manner capable of providing spatial information so that fabrication processes can be optimized. Although the fabrication of these ceramic materials is being pursued by many different techniques at present, there is enough similarity in the different superconducting materials and the fabricated forms to begin research into NDE measurement techniques. A noncontacting AC induced current measurement technique has been developed which can determine critical currents on a local scale with resolution down to 1 mm. This technique can be used in conjunction with DC transport currents to determine spatial variations in critical current dissipation. It also can be used alone to induce 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 can be determined without any connections to the sample. These measurements are being applied to coating and wire geometries and the results are being correlated with material microstructure information. Nonlinear flux trapping signals are being recorded with a new pulsed probe extension of this technique.

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 modeling, optimization, stabilization and coordination, as well as in the development of computational schemes for generating 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.

Current research is concentrated on the design of robust controllers for linear and nonlinear systems under various types of uncertainty which appear as unknown parameters, external (time-varying) disturbances, or nonlinearities whose functional forms are not exactly known. We study linear systems which exhibit time-scale separation in open-loop dynamics (such as singularly perturbed models), which are subjected to unknown external disturbances of finite energy. Here the robustness is with respect to these external disturbances and the unknown singular perturbation parameter, and the criterion is minimization of a worst-case performance. We also study nonlinear systems where the uncertainties are either parametric or structural, with the criterion being one of stability.

University Of Illinois

Dept of Chemical Engineering **$108,337**
Urbana, IL 61801 **01-C**
89-3

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 predict when slugging will exist in horizontal flows, based on an understanding of interfacial waves, (2) to develop a model for slug flow in horizontal pipes, (3) to develop an understanding of vertical and horizontal annular flow by studying droplet entrainment and deposition and (4) to develop a basic understanding for the dispersion and deposition of particles in a turbulent flow. Vertical experiments are conducted in pipelines with diameters of 3/4 in., 1 1/2 in., and 2 1/4 in. The horizontal flow facility has 1,2,3,4 in. pipelines mounted on a specially designed platform whose angle can be controlled to within 0.01 degree.

Slugs have been observed to develop by a nonlinear Kelvin-Helmholtz mechanism at superficial gas velocities less than 3 m/s. Gravity waves formed at the entry grow and double their wavelength. These waves can tumble or grow to a height such that they are unstable, depending on the liquid height. At gas velocities greater than 3 m/s, the process is enhanced by coalescence of waves.

Detailed temporal variations of pressure profiles have been made during the passage of slugs. These have been used to develop a hydrodynamic model.

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. Photographic studies of drop size and drop configurations are being used to obtain an understanding of this phenomenon.

Particle dispersion and deposition in turbulent flows are not easily described by classical Eulerian methods. Therefore, Lagrangian methods are being explored whereby the concentration profiles and deposition rates are described as resulting from a distribution of point or line sources. These techniques have been used to study vertical annular flow, horizontal annular flow and sediment transport.

University Of Illinois At Chicago

Energy Resources Center **$73,391**
Chicago, IL 60680 **01-B**
91-2

Momentum and Heat Transfer Processes in Viscoelastic Fluids
J. Hartnett

Recent studies of the heat transfer performance of viscoelastic aqueous polymer solutions have been directed to the pool boiling behavior of such solutions. The heat transfer coefficients of aqueous hydroxyethy cellulos (Natrosol) solution boiling on horizontal wires were found to be considerably higher than the values found for water alone, whereas the pool boiling performance of other polymer solutions (including polyacrylamide solutions) was inferior to that of water. A distinguishing characteristic of the Natrosol solutions is their lower surface tension values. Accordingly an investigation of the influence of two different surfactants (i.e. agents which reduce surface tension) on the pool boiling behavior of aqueous polyacrylide solutions was carried out. When the surfactant polyoxyethylene sorbitan monooleate (Tween 80) was added to the aqueous polyacrylamide solution the surface tension decreased by 10 to 20% but the boiling performance was not affected. In contrast, the presence of sodium lauryl sulfate (SLS) resulted in a similar decrease in surface tension but a significant increase in the boiling heat transfer coefficient was recorded relative to the pool boiling performance of deionized water. On the basis of these experimental results it can be concluded that lowering the surface tension of an aqueous polymer solution does not guarantee enhancement of the boiling heat transfer performance.

Jet Propulsion Laboratory

Pasadena, CA 91109 **$109,200**
03-C

Neural Learning Formalisms for Global Manipulator Redundancy Resolution Problems in Unstructured Environments **89-3**
J. Barhen

In many applications the robotic arm needs to have sufficient maneuverability so as to carry out its tasks in the presence of obstacles and in constricted locations. One way to achieve that is to endow the arm with an extra degree of freedom.

While mechanically that is easy to implement, say by the addition of an extra joint, the mathematical problem associated with the guidance of the arm becomes very difficult. The reason for that is that with the conventional six-degree-of-freedom system the relationship between the location and orientation of the arm's joints and the location of the arm's tip is uniquely determined, while the redundancy accompanying additional degrees of freedom yields an infinity of such relationships. The proposed research will address the resolution of the mathematical problems arising in the latter case.

Specifically, neural networks will be used to permit the robot arm to learn which of the possible motions of the arm are the most appropriate under given conditions. These networks are really models of the way we think, learn, and remember. Those functions are represented by a set of differential equations with many possible solutions, each of which is accessible from well defined initial conditions. In effect the individual solutions serve to encode a learned response to a given stimulus.

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 put the widely used engineering averaged-equations models of multi-phase flows on a firmer basis by comparing their results with those of direct numerical simulations.

Viscous effects on slip-free spheres (a useful approximation for gas bubbles) have been studied computationally to determine the validity of the Lagrangian method often used in the derivation of the equations for such systems.

A new approach to phase averaging has resulted in a rather unexpected form of disperse-flow equations in the dilute limit. The properties of the equations and the advantages and limitations of this new approach are being investigated.

A study has 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 flows in which the compressibility of the particles (bubbles) plays an important role.

Robert H. Kraichnan, Inc.

303 Potrillo Drive **$64,303**
Los Alamos, NM 87544 **01-C**
90-3

Turbulence Theory and Reduced Hydrodynamic Description
R. Kraichnan

Turbulent flow is omnipresent in geophysics and in energy-producing devices. Atmospheric turbulent transport plays an essential role in the movement of heat, moisture. and pollutants. Turbulent flows typically contain an enormous amount of information. Both for practicable computation and for physical understanding, it is necessary to extract essential information in compact form. This project explores novel approaches to economical and meaningful description of turbulence. Concentration in the past year has been on a method of modeling turbulence by nonlinear distortion (mapping) of fields with simple, known statistics. This method has been very successful for Burgers model of turbulence and is being applied to chemical reaction problems by an increasing number of researchers in the chemical engineering community. New developments in the method now enable easily computable applications to Navier Stokes turbulence and these are being actively pursued. In collaboration with workers at Los Alamos National Laboratory, we are also carrying out related turbulence computer simulations with a resolution not previously attainable.

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

This project involves studies of fundamental properties of nonlinear dynamical systems which arise in physical situations of importance to energy research. A major area of theoretical investigation concerns several different aspects of wave systems. Special focus is given to wave packets; the role played by the Maslov index in multidimensional wave problems; the occurrence of Berry's phase in wave and other dynamical systems; the role of periodic orbits in the spectrum of chaotic wave systems; and linear mode conversion. Recent progress includes the exploration of the relation between the Maslov index and the phase space structures of nonlinear Hamiltonian dynamical systems; new methods of computing the Maslov index, both for finding wave functions and eigenvalues; elucidation of the relationship between the Bohr-Sommerfeld and Maslov phases and the recently discovered "Berry's phase"; a discovery of Berry's phase in the adiabatic motion of charged particles in magnetic fields; a study of complex rays in eikonal theory, and their relation to complex Lagrangian manifolds, Stokes' lines and turning points; a numerical exploration of the role of periodic orbits in the spectrum of a chaotic wave system; and the first treatment of mode conversion phenomena for multidimensional systems, involving novel "reduction" techniques. Emphasis is given to the use of a phase space approach to wave phenomena in all these applications. A second area of investigation concerns action principles, which are being used to imbed single-particle Lie transform perturbation methods in collective models, such as Vlasov-Maxwell systems. Nonlinear phenomena (e.g., ponderomotive forces) are thus dealt with systematically.

Lovelace Medical Foundation

Bioengineering Research **$52,686**
Albuquerque, NM 87108 **01-C**
91-2

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

This project will develop nuclear magnetic resonance (NMR) methods to measure velocity and concentration distributions of both phases in two-phase flows. Systems to be studied include concentrated suspension flows in circular tubes, solid-liquid flows in Couette geometries, gas-liquid, and liquid-liquid flows.

One approach to velocity measurements is to measure an incremental spatial displacement of nuclear spins that are non-invasively tagged whereas another is to measure the phase evolution of the spin precession which depends on the translational velocity. The first method is best suited for flows in uniform geometries such as pipe flows whereas the second, more complex method, is better suited for non-uniform cases such as for non-neutrally buoyant flows in a Couette geometry.

Several steady flow studies such as concentrated suspensions in pipes and Couette have been performed, to date. In order to move on to nonsteady flows, faster velocity imaging techniques need to be developed and a new commercial shielded gradient coil is in its extended installation stage right now (in June, 1992). Preliminary images of bubbles rising in a fluid look promising and further attempts to image gas-liquid flow systems will be made.

University Of Maryland

Dept of Mechanical Engineering **$55,473**
College Park, MD 20742 **03-C**
90-3

The Use of Stereo Optical Flow Fields in the Determination of 3-D Motion and Stereo Correspondence
J. Duncan

In this study, the optical flow fields in the left and right image sequences of a stereo camera pair are being used to determine the three-dimensional motion and position of the camera platform relative to objects in the field of view. A method has been found that uses a robust statistically based calculation to determine the camera motion and feature points in one image that correspond to given features in the other image (stereo correspondence). This method is presently being evaluated experimentally. Preliminary results from tests with synthetic images show that the method produces accurate results when there are not too many points without stereo matches in the two images, when all the points in the left and right images belong to objects with the same three-dimensional motion relative to the cameras, when the noise levels are less than about 10%, and when the cameras are accurately mounted in a parallel configuration. Techniques are currently being developed to extend the method to situations where the four conditions mentioned above are not met.

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

Our research, which was originally focused on light propagation in inhomogeneous optical fibers, has broadened in scope to include studies of solid state rib waveguides and Y-junctions which are used to guide and switch light. The work on optical fibers is divided into two research projects.

The first project concerns long-distance communication using solitons. We have been particularly concerned with the effects of randomly varying birefringence, and we have shown that its effect is benign. From the basic equations, we were able to show from an appropriate ordering expansion that the nonlinear Schrodinger equation is the lowest order equation, and, hence, we expect its behavior to dominate the soliton evolution even in a highly birefringent fiber, as long as the birefringence is rapidly varying. We have also studied optical fiber soliton switches based on trapping and dragging. To do the work on optical fibers, we have collaborated with scientists at AT&T Bell Laboratories. The first solid state project was to find the effect of a quantum well on the propagation characteristics of a rib waveguide. Using a planar guide as reference, we were able to show that the effect of the real geometry is qualitatively small but can have a significant quantitative effect. The second solid-state project is to determine the effect of dry-etching on the mode-holding characteristics of the device. As a consequence of the etching, the height at which the junction splits can vary. We showed that the rounding has a very small effect, in contrast to blunting which occurs when the materials are chemically wet etched.

University Of Maryland

Dept of Mechanical Engineering **$75,000**
& Systems Research Center **03-C**
College Park, MD 20742 **92-3**

The Mechanics of Redundantly Driven Robotic Systems
L. Tsai

The objective of this research is to gain better understanding of the kinematics, dynamics and control laws associated with manipulators having redundant actuators but no redundant degrees of freedom. The major advantages of a redundantly driven manipulator are zero backlash, better repeatability, and fail-safe.

Force transmission characteristics associated with tendondriven manipulators have been investigated. It is shown that the effect of tendon routing can be characterized by a condition number and by the direction of its homogeneous solution. It is also shown that isotropic transmission can be achieved for certain types of tendon routing. To resolve the redundancy in tendon forces, an efficient algorithm is being developed. It is hoped that this algorithm will make realtime, computed-torque control feasible.

Gear backlash introduces discontinuity, positioning uncertainty, and impact in mechanical systems. To overcome these difficulties, an innovative concept utilizing unidirectional redundant drives to ensure positive coupling of gear meshes has been conceived. A two-DOF prototype manipulator has been designed and tested. The experimental results indicate that use of unidirectional redundant drives improves the repeatability by an order of magnitude.

A two-DOF wrist mechanism is also being investigated. Two types of mechanical transmission arrangements are considered. The first uses gear trains in all three transmission lines while the second uses gear trains as well as tendons. The purpose is to demonstrate that precise control can be achieved via mixed rigid and flexible transmission elements. A computer simulation model including compliance and backlash as fundamental concern will be developed.

University Of Maryland

Dept of Mechanical Engineering **$132,000**
College Park, MD 20742 **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 containment 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.

300 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. 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 **$121,000**
Goessmann Laboratory **03-A**
Amherst, MA 01003-0011 **90-3**

A General Procedure for the Synthesis of Process Flowsheets

J. Douglas, M. Malone

This research is focused on developing a more general procedure for the systematic synthesis of flowsheets for chemical processes. These procedures are intended to identify the most important process alternatives, the dominant design variables, and the minimum energy consumption for each alternative in processes containing vapor, liquid-liquid and/or solid phases. This work will substantially expand process synthesis capabilities, building on earlier results which were the basis of a hierarchical synthesis procedure for continuous processes containing mixed vapor/liquid phases.

A hierarchy of decisions and rules for the synthesis of liquid-liquid separation systems and for crystallizer, filter dryer steps have been developed. The generalized flowsheet structure has also been identified and an evaluation of the interactions with other separation steps is being studied. One important difference between vapor/liquid processes and solids processes arises on account of the optimum operating temperature for decanters, dissolvers, and crystallizers. The popular energy integration procedures, which have led to major energy savings in continuous processes over the last decade, must be modified to include this unknown temperature.

Noncontinuous processes which include one or more important batch processing steps are also being studied. An algorithmic approach based on simulated annealing for the scheduling of batch processes including due date and inventory considerations has been developed and the interactions of the design with the production schedule are under study.

University Of Massachusetts-Lowell

Department of Electrical Engineering **$79,995**
Lowell, MA 01854 **01-C**
91-3

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

This project represents an analytical/experimental effort directed toward understanding the processes responsible for the generation of boundary layer instabilities in time-modulated flows. In particular the temporal modulations of the basic state by harmonic and free-stream vorticity is considered. The objectives of this work are to: 1) Develop analytical models describing instability in temporally modulated flows. The dynamics of the system is examined using stability analysis and validated against experimental observations.
2) Determine the growth and propagation of unstable disturbances occurring in the viscous region. The influence of the modulation amplitude and wall features such as wall curvature are considered. 3) Examine the stabilizing influence of steady-flow. 4) Examine global and local instability resulting from modulation of the free-stream near points of mean-flow stagnation.
5) Categorize results suggestive of possible mechanisms for heat transfer.

Models for the transition to chaotic fluid motion in time modulation flow have been developed. It has been shown that oscillatory modulation of the basic flow results in successive period-doubling bifurcations of three-dimensional vortical disturbances. Above an amplitude threshold these disturbances exhibit temporally chaotic behavior.

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 present research is part of a cooperative program among faculty at MIT and staff at the Idaho National Engineering Laboratory (INEL) to develop a sound understanding of the arc welding process and to develop sensing and control methods that can be used to automate the gas-metal arc process.

Previous research on this project mapped the light emissions from a welding arc spatially, temporally, and spectrally. This work identified windows where it is best to photograph or otherwise view the weld pool. Later work developed an understanding of the forces controlling metal transfer in gas-metal arc welding. Welds were made with steel, titanium, and aluminum using a variety of shielding gases and varying the welding current to achieve different metal transfer modes. This work was done using a laser back-lighting technique developed at MIT which allows one to estimate the anode spot attachment on the melding electrode. These experiments have led to a new hypothesis to explain the transition from globular to spray metal transfer. A mathematical model was based on this model which accounts for the forces due to gravity, surface tension, electromagnetic, and plasma jet drag. By studying the relative importance of each of these forces, it was shown that 10 to 20 percent higher weld deposition rates could be achieved with pulsed current welding using different shielding gases.

The research during the current year has reviewed methods of filtering the voltage and current waveforms during pulsed current welding in order to extract signals which can be used to control the process. A new process control system has been developed and integrated with the welding equipment. Work has begun to study methods of mechanically controlling droplet detachment from the welding electrode.

Massachusetts Institute Of Technology

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

Synthesis and Optimization of Integrated Chemical Processes
L. Evans

The objective of this research is to investigate and develop improved systematic methods for the synthesis and optimization of chemical processes. The work to date has focused primarily on synthesis of heat and work integration systems for large-scale continuous chemical plants. In the past year we have redirected the project to address methods for synthesis and optimization of batch and semi-continuous processes.

The synthesis of heat and work integration systems in process plant is important in the design of new plants and in the retrofitting of existing plants for energy conversion. A typical process plant, such as a petroleum refinery, a petrochemical plant, or a paper mill, requires energy in the form of heat to raise the temperature of process streams and in the form of work to drive pumps and compressors and meet other mechanical energy needs. The goal of heat and work integration is to reduce this external energy requirement through better process integration. For example, the heating requirement can be reduced by allowing hot streams that must be cooled to exchange heat with cold streams that must be heated. Also, the process itself can be used to generate mechanical energy by introducing heat engines.

This research has focused on developing computer-based methods to help engineers synthesize a process with improved energy integration. The strategy has been to combine modern mathematical programming techniques, sophisticated rigorous models of the process utilities system and heat recovery network, and heuristic methods to develop an overall methodology that is more powerful than traditional approaches. Methods and computer programming techniques of artificial intelligence have been used where appropriate. An effort was made to overcome the idealizations characteristic of much previous process synthesis research to develop methods that will help engineers solve realistic industrial problems. The net result of the research has been an improved understanding of the nature of the problem of energy integration in process plants.

With the completion of three doctoral theses on the project in the area of heat and work integration, the research is now being redirected to address the synthesis and optimization needs of batch and semi-continuous manufacturing processes. These processes are of increasing importance for the manufacture of high-value performance products such as those produced by biotechnology. Yet, the development of systematic computer-based methodologies for batch process is only in its infancy.

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

The Gas-Metal Arc Welding Process (GMAW) is a highly productive means for joining metals and is being used increasingly for structures and pressure vessels. It presents a challenging multivariable control problem entailing both geometric and thermal outputs. These outputs all combine to determine the strength and toughness of the resulting joint. The overall objective of this work is to examine the problem of simultaneous regulation of all real-time attributes of a weld. Past work has established the viability of independent control of thermal characteristics and the present work is examining the geometric aspects of weld pool control.

One objective of this work is to develop basic process modeling and control schemes to allow independent regulation of the weld bead width and height. A control model relating wirefeed and travel speed to width and height was developed using transfer function identification techniques applied to a series of step welding tests. The resulting discrete transfer function was found to be nonlinear in both the static and dynamic parts owing to a strong dependence upon the input magnitudes. This model was then used to develop a decoupling controller design that cancels the nonlinear behavior using gain scheduling. Proper regulation of the process was demonstrated, but the limited range of control afforded by this process and the significant process delays that were in evidence led to very poor disturbance rejection. It is apparent that the GMAW process will need significant modifications to overcome these problems.

In an attempt to merge previous results on the regulation of thermal characteristics in real-time with the geometry control work, we are developing a control system to independently regulate the weld bead width and the width of the heat affected zone. Initial work is concentrating on simulation of wide seam welding using an analytical heat transfer model as well as a finite difference process model. A key issue in the problem is the strong coupling between the inputs (current and travel speed) and the outputs. The use of high frequency transverse motion of the torch is being investigated as a means of overcoming this coupling. Once the control latitude is increased, a two variable control scheme based on both video and infra-red sensing will be implemented.

Finally the depth of penetration of a weld is the most important indicator of weld strength, yet it is the one variable that is essentially impossible to measure directly. A real-time depth estimator has been developed based on solution of an inverse heat transfer problem. Surface temperature measurements are used as inputs to the analytical model, which then tunes the unknown parameters until predicted temperatures match the measured. Initial experiments with this model, using surface temperature measurements from the top and bottom of the weld, have shown accurate and rapid convergence and development of a depth control system based on this estimator is now being processed.

This project is a collaborative program with INEL.

Massachusetts Institute Of Technology

Dept of Mechanical Engineering **$88,020**
Cambridge, MA 02139 **01-D**
91-2

Cryotribology: Development of Cryotribological Theories and Application to Cryogenic Devices
Y. Iwasa

The principal objective of this cryotribology (low-temperature friction and wear) project is to contribute towards the advancement of cryogenic systems by examining the basic mechanisms of cryotribology. Because relative motion is essential to the operation of many cryogenic devices, an improved understanding of cryotribology will place us in a much better position to meet the future demands that will be required of these low-temperature system. While continuing to generate more cryotribological data, we have also been expanding our efforts to emphasize the development of cryotribological theories which will enable a more systematic approach towards the design of cryogenic devices, including helium-temperature (4.2 K) as well as high-Tc superconducting magnets.

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

This research focuses on the analysis of ductile crack initiation, growth and instability in part-through surface-cracked plates and shells. The overall approach consists of careful calculations of crack front stress and deformation fields, and correlation of cracking with experimental observations being conducted at the Idaho National Engineering Laboratory.

Recently, significant progress has been achieved in developing and applying a two-parameter description of crack front fields. The amplitude of crack tip deformation is characterized by J or CTOD, while the hydrostatic constraint in the near-tip region correlates well with a parameter related to the so-called T-stress, or second elastic Williams' eigenfunction.

Simplified engineering applications of surface crack analysis are being developed in the context of the line-spring model. Specific enhancements include improved elastic-plastic procedures for the practically important case of shallow surface cracks, as well as simple methods for calculating the T-stress along surface cracks fronts.

Detailed elastic-plastic stress analyses of cracked structural geometries provide a basis for interpreting experimental observations, for quantitatively assessing inherent limitations of nonlinear fracture mechanics methodology, and for extending these boundaries through development of two-parameter characterization of crack tip fields. Simplified but accurate analytical methods are also under development for analysis of surface-cracked plates and shells. Emphasis is placed on better understanding complex three-dimensional features of elastic-plastic crack tip fields.

Massachusetts Institute Of Technology

The Energy Laboratory **$133,000**
Cambridge, MA 02139 **01-A**
91-3

Basic Engineering Sciences of Solids Comminution
C. Peterson

This work is a study of the energy and force requirements for fine grinding of minerals and coal. Fine grinding is a low-efficiency process at best, and it can become excessively energy intensive as finer grinding is required for better cleaning of coal or for beneficiation of lower grade ores.

Research is directed to the crushing behavior of individual particles, of particles within particle beds subjected to compressive loading, and to the transport of materials into and through the comminution device, with particular attention to the separation and transport of fine particles from the active crushing zone.

Although the program conducts basic research, a machine has been conceived to provide focus for the various aspects of the research. It was known from the outset that both crushing behavior within the bed and material transport through the device were critical to the achievement of high efficiency. It is essential to remove fine material from the bed as it is formed if the remaining coarse material is to be efficiently fractured. The machine concept, therefore, combines the crushing action of a jaw crusher with upward transport of granular material, driven by an upward fluid flow, the mixture being in a fluidized or near fluidized state. Since fine particles are more easily fluidized than coarse, it was argued that fluidized transport would preferentially transport fine material, leaving coarse material behind for further crushing action. Preliminary experiments have shown that such size-dependent segregation and transport is indeed achieved, but research continues to establish an understanding sufficient for design.

Early work concentrated on crushing behavior, both of individual spheres (between flat plates and subjected to multiple side loads in addition to loading from the plates), and of particle failure within particle beds. Computer simulation of 2-dimensional beds composed of 3-dimensional spheres provided a good picture of load distribution within beds and of failure of individual particles within such beds. Simulations correlated well (qualitatively) with experimental crushing within beds of spherical glass particles. It was determined that, for brittle materials, particle failure was adequately predicted by a size-dependent critical value of the maximum single load on the sphere, regardless of the magnitude and number of lesser loads. Failure of plastic materials, however, is inhibited by the presence of significant secondary loads.

A "bed efficiency" was defined as the energy necessary to fracture an individual sphere between flat plates to that necessary to fracture a similar sphere subjected to multiple loading within a particle bed. As expected, the value of this efficiency falls rapidly from a value of one (by definition) for a bed of one particle depth to lower values as bed depth increases, and energy is wasted on frictional motion within the bed. However, for bed depths above about 5 particle diameters, the bed efficiency seems to level off at about 40%. This is of significance since all particle beds (i.e., beds treating through flow rates of interest) will be of depths much greater than five particle diameters. Bed efficiency is also a function of the extent to which the bed is compressed. Since initial bed loading results in bed movement and compaction, with energy consumed in friction but with little or no fracturing, initial bed efficiency is zero. As compaction continues and fracturing begins, bed efficiency rises and peaks at about 40% for a compaction to about 80% of initial bed height. Thereafter, while further compaction continues to break particles, the necessary force rises rapidly and, hence, the work input increases disproportionately. This sudden rise of required force correlates with filling the voids between coarse particles with the fine fragments of the crushed particles. Peak bed efficiency is about 40%--that is, it takes at least two and one-half times as much energy to crush a particle within a bed as it would take if the particle could be crushed individually between flat plates. At the peak efficiency compaction, about 40% of the initial coarse material has been fractured within the bed.

With this understanding of crushing action within beds, the focus has shifted to studies of fluidized bed behavior and the relative motion of particles of different sizes within the bed. Preliminary work with mixtures of 2 and .8 mm glass spheres demonstrated segregation will be rapid enough for practical devices. More sophisticated research is now underway to provide quantitative data on particle velocities and to explore a wide range of flow conditions and geometries. Much finer particles, typical of those observed upon crushing of brittle coarse particles, are being used, which should enhance the segregation behavior.

Massachusetts Institute Of Technology

Dept of Mechanical Engineering **$116,76**
Cambridge, MA 02139 **01-C**
92-3

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

The efficient utilization, transport, and handling of dense multiphase slurries containing high volume fractions of solid particles, distributed in size from submicron to several hundred microns, requires the ability to predict the rheological and flow properties as a function of the various physical parameters including solids loading, particle shape and size distribution, stability characteristics, and solid and fluid properties. Under the grant a rational theoretical and experimental methodology will be developed for the rheological and flow property prediction of dense-phase slurries. 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.

The bimodal model has been shown to be very successful in application to a truly bimodal suspension, where the shear dependent viscosity behavior of the colloidal fraction is determined experimentally. For polymodal multiphase flows the bimodal model is being extended, through analysis and experiment, to find a rational method to divide a continuous size distribution into a colloidal and a coarse fraction, and to define the effect of a non-uniform size distribution of each fraction. Additional rheological information on the colloidal fraction, including the effects of the electrochemistry, and the particle shape and size distribution is also being obtained.

Massachusetts Inst Of Tech[1]

Dept of Chemical Engineering **$63,000**
Cambridge, MA 02139 **06-C**
91-3

Los Alamos National Lab[2]

Design Engineering Division **$108,000**
Los Alamos, NM 87545 **06-C**
91-3

Sandia National Laboratories[3]

Fluid & Thermal Sciences Dept **$198,000**
Albuquerque, NM 87185 **06-C**
91-3

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

This research aims to correlate the macroscopic rheological behavior of suspensions with their statistical microstructure. This fundamental knowledge will benefit a host of technologies, including geothermal energy production, petroleum production and refining, and synfuels processing. The approach involves a novel combination of experiments, numerics, and theory. Experiments primarily involve tracking small balls as they fall slowly through otherwise quiescent suspensions of neutrally buoyant particles. Detailed trajectories of the balls, obtained either with new experimental techniques or by numerical simulation, are statistically interpreted in terms of the mean settling velocity and the dispersion about the mean. Determining the mean settling velocity of balls that are small relative to the suspended particles is a means of measuring the macroscopic zero-shear-rate viscosity without significantly disturbing the original microstructure; therefore, falling-ball rheometry is a powerful tool for use in studying the effects of microstructure on the macroscopic properties of suspensions. The dispersion about the mean yields information about the particle interactions. To date, the mean and dispersivity of a falling sphere's velocity has been determined as a function of the tracer sphere size and the suspended particle size, shape, and concentration. Currently, the pressure drop caused by the falling ball is being measured also. This will provide a much needed benchmark problem for numerical studies, as well as provide another measure of the macroscopic response of a suspension as a function of its microstructure. Also begun recently are two studies of boundary effects in two-phase fluids: the determination of the torque on a small ball spinning in a suspension (a sensitive measure of apparent slip at the boundary) and the determination of the velocity of a small ball rolling down the wall of a container holding a suspension. Numerical studies are also continuing, in which the three-dimensional dynamics of many interacting suspended particles are calculated using the boundary element method.

University Of Minnesota

Dept of Aero Eng & Mechanics **$ 0**
Minneapolis, MN 55455 **01-C**
90-3

Stability Studies of Core-Annular Flows
D. Joseph

The objectives are to understand and control drag reduction in water lubricated pipelines and to determine conditions of stability in water film cooling of water vapor (with phase change) for possible application to nuclear safety. We have developed a successful linear theory for predicting regimes of lubricated flow of oil and water and we have new experimental results in lubricated flow in vertical pipes. We are now doing nonlinear theory and preparing experiments on water lubricated pipelining of coal-oil dispersions. We are generally supported and encouraged by Shell Development in Houston. We are world leaders in this subject. We are going to apply the methods we use for water lubricated pipelining to nuclear safety, but we don't know how it will turn out.

University Of Minnesota

Dept of Mechanical Engineering **$141,928**
Minneapolis, MN 55455 **06-C**
92-4

Thermal Plasma Processing of Materials
E. Pfender

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 films.

During the past year our efforts have concentrated on characterizing the thermal plasma chemical vapor deposition (TPCVD) process of diamond films onto various substrates. In our studies we have used the triple torch reactor developed previously under this program to obtain good mixing of the reactants CH_4 and hydrogen with the argon-hydrogen plasma jets.

Based on systematic studies, the effects of pressure, plasma composition, substrate material and temperature on deposition rate and quality of the films have been determined with deposition rates up to 60 m/hr. Homoepitaxial films have been grown on diamond seed crystals with growth rates up to 200 m/hr.

Modeling of the situation close to the substrate indicates extremely steep temperature and concentration gradients pointing to the importance of thermal diffusion.

Another plasma reactor with counter flow liquid injection has been previously used for the synthesis of fine powders but recently also for diamond deposition. The configuration of this reactor gives rise to recirculation eddies enhancing the residence times of the reactants and products in a relatively uniform temperature zone. Very high diamond deposition rates up to 1 mm/hr have been observed with this reactor. A series of diagnostic studies have been initiated to facilitate an understanding of the main reasons for the observed high deposition rates.

National Academay of Sciences/ National Research Council

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

Recent concern for the loss of competitiveness of the United States in manufacturing has motivated a number of studies for the underlying causes and possible cures for this state of affairs. An important conclusion of those studies with important consequences for the future is the recognition of the need for a more integrated approach to manufacturing than that prevailing in our industry. There are two related aspects of this situation: first is the traditional separation of the product design function from the manufacturing function, and second is the lack of an appreciation for the process of manufacturing as an integrated system, similar to that prevailing in the chemical process industry. The proposed fellowships are a step towards ameliorating that situation.

The proposed program calls for twelve doctoral fellowships under the aegis of the National Academy of Engineering. The fellowships will be awarded following a nationally advertised competition. The selection of the fellows will be carried out by a panel of 25 distinguished scholars in engineering and knowledgeable industrial experts. Each fellowship will be for a three year nonrenewable period.

The objective is to create a pool of Ph.D.'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.

Based on recent experience in chemical process industry, it is natural to expect that improved manufacturing methods will contribute to improved energy efficiency, to better utilization of scarce resources, and to less degradation of the environment.

National Institute Of Standards & Technology

Chemical Eng Science Division — **$104,000**
Boulder, CO 80303-3328 — **01-C**
90-3

Convection and Dispersion in Coarse-Packed Beds
M. Jones, J. Wolfe, R. Nassimbene

One of the most widely used items of industrial equipment is the packed bed in which, commonly, a vertical throughflow exists through a packing which is relatively coarse. The presence of temperature or compositional gradients in conjunction with the stochasticity of the packing on the scale of observation leads to flow structures which may be hard to predict but which are, in any case, not uniform. The flow structures observed under these conditions are being studied with the aid of an array of fiberoptic probes which detect the concentration of a fluorescent dye injected with the throughflow. This technique allows time-resolved imaging of the flow structure in the plane of the array. Considerable insight into the state of convection may be obtained from some of the statistics available from individual probe responses. These include the residence time distribution, the spatial distribution of transit times, and their means and standard deviations.

Experiments have been performed with downward flow of water in a packing of uniform diameter, poured, glass spheres with a vertical temperature gradient. The transition of the flow structure has been observed for a range of temperature gradients characterized by a Rayleigh number, and different flow rates characterized by a thermal Peclet number. The transition to mixed forced-free convection is not abrupt as would be predicted from the volume-averaged equations of motion and energy. Instead, the flow structure undergoes distributions which indicate a random structure which gradually changes to approximate modes determined from the confining geometry. Dispersion obtained from the standard deviation of dye transit times at the plane of observation shows a generally increasing trend, with a small maximum preceding the occurrence of circulating (free convection) flows. The interpretation of these observations is aided by numerical solution of the governing equations for grids with randomly distributed porosity. These show similar precursors to circulating flow associated with neutrally buoyant stagnant regions of the bed.

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 research is being done jointly by two groups within the Thermophysics Division of the NIST Chemical Science and Technology Laboratory; one group is located in the Gaithersburg, MD laboratories and the other at the Boulder laboratories. The specific measurement capabilities to be developed in this project include new apparatus for transport properties (thermal conductivity and viscosity), for thermodynamic properties (pressure-volume-temperature data and enthalpy), for phase equilibria properties (vapor-liquid equilibria, coexisting densities, and dilute solutions), and for dielectric properties (dielectric constant). 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 systems containing alternative refrigerants, on aqueous solutions, and on carefully selected systems with species of diverse size and polarity that are important to the development of predictive models for energy-related fluids.

National Institute Of Standards & Technology

Electromagnetic Technology Div $98,488
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 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 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 $129,703
The Benjamin Levich Institute 01-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 high 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 a shear flow, a settled bed of heavy particles can resuspend even under conditions of vanishingly small Reynolds numbers.

Viscous resuspension is being studied both theoretically and experimentally in various unidirectional flows, e.g. a 2-D Hagen-Poiseuille flow, as well as a Taylor-Couette system. 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.

The City University Of New York

The City College $126,000
The Benjamin Levich Institute 03-A
of Physico-Chemical Hydrodynamics 91-3
New York, NY 10031

Partial Control of Complex Processing Systems
R. Shinnar, I. Rinard

Most control theory applies only to systems in which the number of manipulated variables equals or exceeds the number of controlled variables. However, in complex systems such as chemical reactors, refineries, or entire chemical plants, the number of variables that need to be controlled is larger than the number of manipulated variables available.

In many systems one can find a small square control matrix in which exact control of a few dominant variables allows one to keep a larger number of output variables within an acceptable domain. The choice of the manipulated variables as well as the controlled variables is very critical to ensure stability as well as controllability.

The goal of the research is to develop a better understanding of how to approach the control of such complex systems characterized by both a large number of state variables and large uncertainties in the model describing them and to provide a systematic theoretical framework for such design.

This will be done by studying a few well-defined complex systems such as a fluid catalytic cracker and some polymerization reactors. In the first phase a model of a fluid catalytic cracker suitable for this purpose was developed. It will be suitable for both steady state control which is nonlinear and dynamic control and will allow comparisons of different current decisions and critical review of the field.

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 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 propagating 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

Dept of Civil Engineering **$ 0**
Evanston, IL 60208 **03-B**
89-3

Quantitative Non-Destructive Evaluation of High Temperature Superconducting Materials
J. Achenbach

A crack in a solid body can, in principle, be detected and characterized by its effect on an incident pulse of ultrasonic wave motion.

The work on this project is concerned with applications of the scattered field approach to the detection and characterization of cracklike flaws. The work is both analytical and numerical in nature. Several forward solutions to model problems have proven to be very helpful in the design of experimental configurations. They are also valuable in interpreting scattering data for the inverse problem.

The efficacy of ultrasonic methods to detect and characterize a crack depends on topographical features of the crack faces, the presence of inhomogeneities in the crack's environment, and on the mechanical properties in the near-crack region. In this work the effects on the scattered ultrasonic field of various features of fatigue and stress corrosion cracks, such as partial crack closure, the presence of microcracks and microvoids, and near-tip zones of different mechanical properties have been investigated. Most of the results have been obtained by formulating a set of singular integral equations for the fields on the boundaries of the scattering obstacles. These equations have been solved numerically by the boundary element method, and the scattered fields have subsequently been obtained by using representation integrals.

For the configurations examined in this work, crack closure has the most significant effect on far-field scattering.

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 (including contact-line motions) of thin liquid films, especially with heat and/or mass transfer. The two- and three-dimensional structure of surface waves on a heated inclined plane, has been examined and the experimental technique has been developed to measure accurately the surface-wave shapes, frequencies and amplitudes on thin liquid films draining down an inclined plate under adiabatic or heating conditions, for comparison with theoretical predictions.

The evolution equation for two-dimensional disturbances incorporates viscosity, gravity, surface tension, thermocapillarity, and evaporation effects. The linear theory derived from this describes the competition among the instabilities. Numerical solutions of the evolution equation describe the finite-amplitude behavior that determines the propensity for dryout of the film. Among the phenomena that appear are the tendency to wave breaking, the creation of secondary structures, and the pre-emption of dryout by the mean flow. A three-dimensional evolution equation was also derived that contains surface-wave instability and nonlinear saturation. A new secondary three-dimensional instability was identified. Unlike other secondary instabilities found in many shear flows, the instability does not require a threshold amplitude, so that all two-dimensional permanent waves on vertical plates become unstable to three-dimensional disturbances. The nonlinear evolution of three-dimensional layers, including the finite-time behavior of the secondary instability, is studied by posing various initial-value problems and numerically integrating the long-wave evolution equation.

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.

One of the central concerns of this work will be to understand how the motion of the contact line, i.e., the line of intersection of a liquid/liquid or liquid/gas interface and a solid, influences the motion of the fluids. Recent work has been directed to solving for the evolution of a contact line using analytical and numerical methods. Also recently the dissipation associated with the motion of a contact line and how this dissipation manifests itself in a macroscopic model of wave propagation in a partially saturated porous material has been investigated. The microscopic flow problems in a porous material can now be studied using these results. Also attention will be directed to problems concerned with the fundamental modeling of the motion of a contact line. This is an important aspect of the work since the dynamics and dissipation associated with the motion is very dependent upon the model used for the contact line motion.

Northwestern University

School of Eng & Applied Science **$ 0**
Evanston, IL 60208-3120 **06-C**
91-3

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

This project seeks basic experimental and theoretical understanding of mixing and dispersion of viscous fluids, and it is relevant to applications such as processing of polymers. The work consists of several inter-related sub-parts: (i) stretching and breakup of filaments under supercritical conditions in chaotic flows, (ii) analysis of details of breakup and sub-satellite formation at small scales, (iii) understanding of the statistics of drop size distributions produced for different viscosity ratios. Issues (i-ii) form the basis for the understanding of (iii). The drop size distribution is consistent with scaling assuming that moderately extended filaments behave passively and that stretching in chaotic flows behaves as a multiplicative process with weekly correlated steps.

More recently we have extended our investigation in two new directions: (iv) Mixing of equal volumes of fluids using the marker and cell technique; and (v) Investigation of the role of rheology in chaotic mixing processes. Item (iv) focuses on the early stages of the mixing process, before scenario (i) takes place. Studies under item (v) comprise both experimental and computational investigations of steady and time-periodic flow of a constant viscosity, elastic fluid in a two-dimensional eccentric cylindrical geometry. Several results have already been obtained for this case.

Northwestern University

Dept of Eng Sci & App Math **$74,814**
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. Examples of such non-equilibrium structures are found in fluid dynamics - Rayleigh-Benard convection and Taylor vortex flow - and in solidification - Mullins-Sekerka instability. Such structures also serve as paradigms for non-equilibrium structures in general which arise in other fields such as chemistry and mechanics. Structures in spatially extended systems provide a link between low-dimensional systems and high-dimensional ones which are fundamental in developed turbulence.

Solitons in integrable conservative systems are well understood. Since Hopf bifurcation in binary mixtures gives rise to coupled complex Ginzburg-Landau equations, the localized wave trains have been described as dissipative perturbed solitons. However, it has been found that the predictions of the complex Ginzburg-Landau equations disagree with certain aspects of experimental observations. The PI proposes to investigate binary-mixture convection building on the extended Ginzburg-Landau equations which he has derived recently. His extended Ginzburg-Landau equations incorporate an additional slow time-scale due to the presence of slow mass diffusion.

The proposed research will be conducted in the following areas: (1) Ginzburg-Landau (GL) equations coupled to a mean field for binary-mixture convection with emphasis on the microscopic equations, derivation of the extended GL equations, and investigation of the extended GL equations, (2) evolution of domain structures with emphasis on steady structures and oscillatory structures.

University Of Notre Dame

Department of Chemical Engineering **$62,916**
Notre Dame, IN 46556 **01-C**
92-3

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

Liquid films falling under the force of gravity is extremely unstable with several unique dynamic characteristics. The interfacial waves which result from these instabilities are able to transfer large amounts of heat or mass into and across the liquid phase. However, both the nonlinear wave evolution and the fundamental transfer enhancement mechanism remain largely unexplored. The project aims to carry out a fundamental study of the nonlinear and spatial evolution of the interfacial waves from first principles. A weakly nonlinear analysis will scrutinize the evolution of wave spectra downstream especially the unique cascading of energy to lower wave frequencies. A mixed spectral finite-element scheme for free surface problems will then be used to extend the analytical results. The feasibility of preventing or delaying this transition to turbulence using a recent theory for chaos control will be analyzed. A strongly nonlinear theory will be developed to consruct the large solitary waves that are created downstream by secondary transition due to nonlinear excitation. Interaction of these solitary waves that cause non-stationary three-dimensional waves will be examined and the results wiii be used to achieve quantitative understanding of the heat/mass transfer enhancement mechanism. Of particular interest is the role of chaotic mixing which allows transport across the separating streamline of the circulation regions in large solitary waves.

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 an understanding of various types of small-scale (e.g. waves) and large scale (e.g. slugs) disturbances which are observed in cocurrent gas-liquid flows.

Typical gas-liquid systems are "open" flows where there is no feedback of information between the inlet and exit. It is important to determine to what extent the ubiquitous time-varying fluctuations at the inlet, which may be of small or large amplitude, can be expected to affect the qualitative or quantitative behavior of the downstream flow. For example, it appears that close to neutral stability in a stratified flow, conditions exist where the irregularity in the interfacial waves can be traced to inlet noise. However for other nearby conditions the waves show no evidence of the effects of inlet noise.

The present approach is to characterize these flows by using experimental measurements of wavelength and amplitude for periodic waves, and amplitude and time-spacing between irregular disturbances. These measurements are interpreted using linear and nonlinear analysis, based on spatially-varying disturbances, of the Navier-Stokes equations. Additional insight comes from some of the recent developments in understanding the generic behavior of nonlinear dynamical systems (e.g. intermittency and chaos) but with careful recognition of the differences between open systems and the typically-studied closed systems (e.g. Taylor-Couette flow).

Oak Ridge National Laboratory

Engineering Physics $1,096,000
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.

Oak Ridge National Laboratory

Chemical Technology Division **$108,000**
Oak Ridge, TN 37831 **06-A**
89-3

Bioprocess Engineering Research for Energy Applications
C. Scott

This program will support engineering research in three primary areas that are critical to an expanding use of advanced bioprocessing systems for energy production and conservation: (1) efficient biocatalytic systems, (2) innovative bioseparations approaches, (3) advanced bioreactor concepts.

Efficient biocatalytic systems - Several advanced bioreactor concepts require that the biological catalyst (microorganisms or active fractions) be retained in the bioreactor at high concentrations in a microenvironment that enhances biological activity. A fundamental understanding of the basic kinetics and dynamics of such biocatalyst systems and a predictive mathematical model will be developed.

Innovative bioseparations approaches - Advanced separations concepts will be needed to isolate or concentrate the dilute aqueous components of bioconversion systems or waste streams from energy processes. The research emphasis will be on separation concepts that utilize solid-fluid interactions with an initial study of the use of biological materials (certain microorganisms and plant and animal tissue) as bioadsorbents for the isolation and concentration of dissolved metals.

Advanced bioreactor/biosorber concepts - Fixed- and fluidized-bed bioreactors and/or biosorbers using immobilized bioreagents are advanced concepts that have the potential for significantly increasing productivity. However, such systems are not well defined, since they may contain three or four interacting phases, including a changing gas phase. The coupling of hydrodynamics, gas generation or depletion, gradients of phase fractions, and biokinetics in continuous columnar systems will be investigated and predictive mathematical models will be developed.

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 non-linear systems with many degrees of freedom.

An important issue in this area concerns the extent to which deterministic chaos can simulate the effect of external noise. Effective stochastic equations that describe the long wavelength properties of partial differential equations (such as the Kuramoto-Sivashinsky equation) are being studied. This is done numerically by explicit elimination of short wavelength modes with an emphasis on interpreting the physical basis of the parameters in the effective equations.

A focus of current research in the field is generic scale invariance (algebraic decay of spatial correlations without tuning external parameters). The aim 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.

Interface models with a finite density of positive Liapunov exponents and structure functions that grow as power laws are being investigated to understand features of fully developed turbulence.

Extensive numerical simulations of resistively shunted junction models of Josephson junction arrays and complex Ginzburg-Landau equations are being carried out to understand spatio-temporal chaos and pattern formation.

Ohio State University

Mathematics Department **$66,116**
Columbus, OH 43210 **06-C**
92-3

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

A cell consisting of two parallel plates separated by a thin layer of liquid, the so-called Hele-Shaw cell, serves as a model of a porous medium. Using it one can perform laboratory experiments which may be difficult to carry out in an actual porous medium. For example one can readily observe the displacement of a more viscous fluid by a less viscous one, such as is taken advantage of in secondary oil recovery methods. Most mathematical models of the displacement process studied to date have dealt with steady states and their stability. Under those conditions solutions can be obtained even if the surface tension at the interface between the two fluids is ignored. As to the initial value problem, it has been found that ignoring surface tension leads to an ill-posed problem in the sense that nonphysical cusps form at the interface in a finite time.

Experimentally it is found that when the surface tension is small no steady state is reached and the interface continues to deform into a finer and finer fractal-like structure.

Recent work by the proposer has revealed that it is possible to imbed the ill-posed problem into a well-posed one so as to clarify what happens when the surface tension tends to zero. The proposed research is a logical extension of the preliminary results obtained heretofore.

Specifically, detailed calculations will be carried out to examine how the singularities in the model equations are related to the evolution of the shape of the interface; second, the results obtained for the Hele-Shaw cell will be extended to study the time evolution of the surface of a growing crystal with dendrites; third, statistics of the observed patterns will be related to the statistical distribution of singularities in the model equations; next, more general boundary conditions will be considered to conform to a broader class of physically realistic situations; finally some intrinsically nonlinear aspects of dendritic growth will be examined.

Oregon State University

Dept of Mechanical Engineering **$105,479**
Corvallis, OR 97331-6001 **01-B**
91-3

Radiative Transfer Through an Array of Discrete Surfaces
J. Welty

Determination of the radiative heat transfer through a given volume is straightforward when the number of objects in the volume is small or when the volume is occupied by a continuous medium, such as an aerosol or gas. However, when the volume is occupied by a large number of discrete objects, either a Monte Carlo numerical model must be used, or some assumptions must be made to treat the collection of objects as though it is a continuous medium. This research is directed at characterizing the radiative transfer through arrays of objects as a function of array geometry.

The primary goal of this research has been the experimental measurement of radiative transfer through arrays of fixed, discrete surfaces. The independent variables are array packing arrangement and density, array element shape, and angle of the incident beam. The results are in the form of a forward scattering phase function for each discrete position across the exit plane of each array. In addition, a bi-directional reflectometer covering a full hemisphere has been designed and built for use in accurately determining array surface properties, a necessity for accurate numerical modeling of the radiative transfer process.

This research is being conducted in coordination with a project at Battelle, Pacific Northwest Laboratory, to numerically model radiative transfer through an array of fixed discrete surfaces.

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 the model the array as a participating medium.

FY 1992 accomplishments consist of: 1) the Monte Carlo code has been completed and validated against other Monte Carlo, 2) preliminary parametric studies have been conducted and show that typical arrays have strongly nonhomogeneous and anisotropic optical properties making it difficult to model the arrays as participating media, 3) parametric studies have shown that three dimensional surface properties variations can have a significant effect on Monte Carlo simulations and need to be considered by other researcher. 4) One technical paper was published in FY 92 and two journal articles have been prepared for publication in FY 1993.

University Of Pennsylvania

Mechanical Engineering Dept **$101,381**
Philadelphia, PA 19104 **06-C**
92-3

Active Control of Convection
H. Bau

It is proposed to study theoretically and experimentally the use of active, feedback control strategies to alter the structure of convection. The work focuses on controlling convective currents in a fluid layer contained in a vertical upright cylinder heated from below and cooled from above (the Rayleigh-Benard problem). By introducing small perturbations in boundary conditions, it is planned to (i) stabilize the no-motion state of the 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. The proposed work is the 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 the proposed work may be of importance, among other things, to materials processing and crystal growth applications in which it is desired 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.

Pennsylvania State University

Mechanical Engineering Dept **$111,417**
University Park, PA 16802 **06-B**
92-3

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

Flame sprays are an alternative to thermal plasma sprays for coating materials. However, until now the quality of the coatings produced with flame sprays was lower than that produced with thermal plasmas. Recently high velocity oxy-fuel (HVOF) sprays have been shown to share some desirable characteristics with thermal plasma sprays, including the possibility of producing high density coatings. Since they operate at lower temperatures, HVOF sprays seem to offer an economical alternative to thermal plasma processing, as well as some technical advantages, such as lesser decomposition and oxidation rates.

While some commercial HVOF equipment has been developed, it appears that none of it has implemented the basic principles of gas dynamics in its design. The main objective of this research is to conduct an experimental study of the gas dynamics of HVOF thermal sprays. The results of the experiments will serve as the basis for a model of the process, which then can be used to control and optimize it.

An attractive aspect of the proposal is the possibility of utilizing in this context much of the knowledge gained in advancing high-speed aeronautics and rocketry.

Specific topics to be addressed are:

1) Nozzle design and operation - controlling the expansion of the spray jet.

2) Turbulent mixing with the surrounding air - minimizing the effects of compressible turbulence on the quality of the spray jet.

3) Analysis of coatings produced with an experimental apparatus embodying gas dynamics principles in its design.

The results of the experiments will be incorporated in a physical-mathematical model of the coating process.

Physical Sciences Inc.

20 New England Business Center **$129,861**
Andover, MA 01810 **06-A**
92-4

Experimental and Theoretical Studies of Multicomponent Vapor Condensation
M. Frish, G. Wilemski

This research program comprises experimental and theoretical studies of nucleation and condensation in multicomponent gas mixtures. The program goals are: (1) to improve basic understanding of 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.

Experimental and theoretical results on water vapor condensation have shown that the latent heat release disturbing the gas flow at onset is due mainly to the condensational growth of large numbers of large (5-9 nm radius) droplets. These results amend an older view that attributes onset solely to the rapid nucleation of very tiny microclusters. Currently, nozzle experiments on binary vapor condensation are being conducted, and a new experimental apparatus is being constructed to study binary nucleation in mixtures of sulfuric acid and water vapor.

Princeton University

Dept of Mech & Aero Eng **$96,000**
Princeton, NJ 08544 **06-B**
90-3

Mechanisms and Enhancements of Flame Stabilization
C. Law

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

A unified chain-thermal theory of flammability limits was formulated. This theory describes the steady propagation of the one-dimensional planar flame, with radiative heat loss, in the doubly-infinite domain; the incipient failure for such a propagation mode would indicate the limit of flammability. Detailed transport and reaction schemes are allowed through numerical simulation. Results reproduce the characteristic extinction turning-point behavior due to heat loss. It is further shown that at the state of the turning point, the relative sensitivity of the dominant termination reaction to the dominant branching reaction varies exponentially with system parameters, indicating the signilficant reductin in the net reaction rate and thereby the propensity to extinction in the presence of heat loss. The present study allows first-principle determination of the flammability limits of gaseous mixtures.

An investigation was conducted for the stabilization of an inverted flame. Contrary to prevailing concepts, present experimental results show that flame stabilization and consequently blowoff can be achieved without heat loss to the stabilizing rod. A theory was formulated, allowing for the active modification of the flame speed by flame curvature and flow nonuniformity characterizing the rear stagnation flow in the stabilizing region. Predicted results using this alternate stabilization mechanism agree well with the experimental observations.

Princeton University

Dept of Civil Engineering **$70,676**
Princeton, NJ 08544 **06-A**
92-1

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. 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 cales obtainable from Nuclear Magnetic Resonance experiments have been derived.

Purdue University

School of Mechanical Engineering **$93,290**
West Lafayette, IN 47907 **01-C**
90-3

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 two-dimensional, aqueous salt solutions 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.

The primary objective of current studies is to determine the manner in which externally imposed forces influence thermo/solutal convection in the mushy and liquid regions during solidification of a binary mixture. A special goal is to determine means by which the forces may be used to offset or dampen thermo/solutal convection, thereby reducing macrosegregation and attendant casting defects. Separate consideration is being given to the effects of magnetic and centrifugal forces on solidification in binary metallic alloys and aqueous salt solutions, respectively. Predictions based on the continuum model are being compared with measurements obtained for metallic (Pb-Sn) and aqueous (NH_4Cl-H_2O) systems.

Purdue University

School of Nuclear Engineering **$108,000**
West Lafayette, IN 47907 **01-C**
90-3

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

The objective of the research program is to develop instrumentation methods, experimental data base and analysis leading to predictive models for describing the interfacial structure and behaviors of two-phase flows. In terms of the flow structure, the local void fraction, interfacial area concentration, fluid particle size distribution and flow patterns in vertical two-phase flow systems are studied in detail. For the purpose of understanding the dynamic behaviors, the interfacial velocity, wave characteristics and coalescence and disintegration of fluid particles are investigated. Special emphasis is placed on developing the four-sensor and five-sensor resistivity probe method and improving the double-sensor resistivity probe method. A second emphasis is on the system size and entrance effects on the interfacial characteristics described above. The changes in the interfacial structures and flow regimes as a function of an axial location are measured experimentally. This information together with the local measurements from the probe method are used to study the mechanisms of flow regime transitions. This research is part of a joint program between the University of Wisconsin-Milwaukee (Kojasoy) and Purdue. The research program is expected to lead to a) local instrumentation methods for detailed interfacial characteristics, b) data for local interfacial area, void fraction, relative velocity and wave propagation velocity, and c) phenomenological models for interfacial area and interfacial structural changes.

Rensselaer Polytechnic Institute

Dept of Mechanical Eng, **$125,500**
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 sub-cooled 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, usually presented as a boiling curve, are unknown at such high heat fluxes.

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 geo-metrical variables using the present data base of over 200 points as well as data obtained by other investigators. The experiments are complemented by visual observations and mechanically-based models for CHF under normal and enhanced conditions.

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

Rensselaer Polytechnic Institute

Dept of Mechanical Engineering, Aeronautical Eng & Mechanics
Troy, NY 12180-3590
$134,000
01-A
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. Creep-fatigue interaction and ratchetting are of special concern. The long-term goal is the development of a finite element program that can directly calculate the life-to-crack initiation of a component under a given load history.

An MTS servohydraulic axial/torsion test system together with an MTS Data/Control Processor provides biaxial rate controlled loading of suitably designed tubular specimens. Induction heating (10 kHz frequency), MTS biaxial grips and an MTS biaxial extensometer are available together with a reversing direct current potential drop facility for testing from ambient temperature to 1000°C. The potential drop measurements are intended for early monitoring of damage during cyclic loading.

Biaxial experiments on AISI Type 304 under low-cycle fatigue conditions were performed at 538°C with several probes for potential drop measurements on the gage section. Voltage drop readings increase with cycles and are high in regions close to the final fatigue crack. Data analysis based on Fast Fourier Transform techniques are being used for the interpretation of the readings.

Uniaxial testing on modified 9Cr-1Mo steel at 538°C showed significant rate sensitivity, relaxation and evidence of influence of recovery of state on the deformation behavior. Accordingly the viscoplasticity theory based on overstress (VBO) was modified to include the representation of recovery of state. The new formulation was able to reproduce the observed behavior. The uniaxial VBO theory is now being generalized for finite deformation and three dimensions.

Rensselaer Polytechnic Institute

Dept of Nuc Eng & Eng Physics
Troy, NY 12180-3590
$128,000
06-C
89-4

The Continuum Modeling of Two-Phase Systems

R. Lahey, Jr., D. Drew

The primary objective of the research being conducted is to develop a mathematically consistent multidimensional two-fluid model which agrees with data and satisfies all the constraints implied by physical laws and the postulates of continuum mechanics.

To this end, interfacial closure laws are being developed such that two-fluid models can be used to predict many important phenomena, such as the evolution of interfacial area density and flow regime transition. Void wave phenomena are also being investigated, both analytically and experimentally, in order to assess and thoroughly understand the effect of the proposed closure laws on the void wave eigenvalues of the two-fluid model (i.e., to study well-posedness).

It is intended that the results of this research will significantly advance the state-of-the-art in the two-fluid modeling of two-phase flows such that, in the future, multidimensional two-fluid models can be used with confidence for many problems of practical interest.

Rensselaer Polytechnic Institute

Dept of Chemical Engineering
Troy, NY 12180-3590
$87,500
01-C
89-4

Microcomputer Enhanced Optical Investigation of Spreading and Evaporative Processes in Ultra-Thin 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 equipment 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 polar and non-polar fluids, with and without heat transfer, are being experimentally studied and analyzed.

Using the results of these studies, an ellipsometer with a complementary interferometer has been designed and is being constructed. The long term objective is to determine the heat transfer characteristics of evaporating ultra-thin films. The near term objective is to develop microscopic image-processing equipment and a complementary heat transfer 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

A new technique is developed to evaluate the response statistics of a Tension Leg Platform subject to viscous and potential first and second order forces. Since the drag force nonlinearity is not of a polynomial type, it is treated by the equivalent quadratization method. Accordingly, the function representing the drag forces is replaced by a multidimensional polynomial the coefficients of which are evaluated so as to minimize the norm of the approximation error. A third order Gram-Charlier expansion of the probability distribution of the response is then implemented to estimate the probability distribution of the nonGaussian response quantities. The quadratization results agree very well with simulation results for a wide range of sea states. For moderate to severe wave states, the surge response of a Tension Leg Platform is significantly affected by higher order wave forces. Of the quadratic forces considered, all have a significant influence on this response. The Neumann approximation is found to be non-conservative for predicting the magnitude of the low frequency surge response. For operational wave states, both linear and quadratic forces induce significant responses in the pitch mode, and consequently in the axial tendon force. In particular, the high frequency response at the pitch natural frequency will have a significant impact on the fatigue design of the tendons.

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 motion of vortex structures, in response to applied currents, is a major source of resistance in superconducting networks in magnetic fields. Systems of interest include regular Josephson junction arrays and type II superconductors, such as the new granular high Tc ceramics. Numerical simulations of finite temperature, current carrying, networks will be carried out to provide a characterization of vortex response in non-equilibrium situations. For periodic networks, current-voltage (I-V) characteristics will be computed and compared with experimental results. The effects on resistivity of transitions from pinned to unpinned or to melted vortex structures, will be investigated. For disordered networks, the effects of pinning in producing metastable vortex structures leading to glassy behavior will be explored.

To date, simulations have been carried out for two dimensional regular Josephson junction arrays, as well as arrays with random vortex pinning sites. Various values of applied magnetic field have been studied and I-V characteristics and resistivity were computed and related to vortex structure. We have also simulated the equilibrium behavior of fluctuating vortex lines in a three dimensional network, as a model for high Tc superconductors. Melting of the vortex line lattice into a line liquid, and properties of the line liquid, have been investigated and compared with recent theoretical results.

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

University Of Rochester

Dept of Physics and Astronomy **$93,186**
Rochester, NY 14627 **06-C**
90-3

Coherence Effects in Radiative Energy Transfer
E. Wolf

The main objective of this research is the elucidation of how coherence properties of sources affect the spatial and the spectral distribution of energy in optical fields. The clarification of such questions is of importance for the theory of radiative energy transfer and for radiometry with sources of different statistical properties. The influence of source correlations in the physical parameters of random media with which a field may interact on the spectral properties of the scattered radiation is also being examined.

The progress made so far includes the clarification of the relationship between the radiance of a field produced by a class of partially coherent optical sources and the radiance (specific intensity) of the phemomenological theory; elucidation of effects of diffracting apertures on spectra of partially coherent fields; and formulation of laws for propagation of the radiance through paraxial optical systems.

Current research includes the formulation of new conservation laws in which spectral changes take place and investigations of spectral modifications produced in multiple scattering. The possibility of determining correlation functions of media from observed spectral changes of scattered radiation is also being examined.

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. An investigation of the new types of diffusion, discovered in Lorentz lattice gas cellular automata, is continued. In this gas point particles move on a lattice, which is randomly occupied by deterministic scatterers. This gas can be considered as a dynamical system in a random environment and a beginning has been made to prove theorems on its abnormal diffusive behavior. In addition, the connection with polymer statistics on a lattice, noticed before, will be further pursued. 2. A general relation between the transport coefficients of a fluid in a stationary nonequilibrium state, near or far from equilibrium, and its two maximal Lyapunov exponents found before, is further investigated. This relation is based on a pairing rule of conjugate Lyapunov exponents. The class of systems for which this pairing rule holds is being determined. In addition, computer studies are done to cheek its use under extreme nonequilibrium conditions. 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 rheological behavior of concentrated colloidal suspensions are made, providing a microscopic approach to fluid rheology.

Sandia National Laboratories

Fluid, Thermal, and **$14,000**
Structural Sciences Division **03-B**
Albuquerque, NM 87185 **92-1**

Two-Phase Flow Measurements by NMR
R. Givler

This project will develop nuclear magnetic resonance (NMR) methods to measure velocity and concentration distributions of both phases in two-phase flows. Systems to be studied include concentrated suspension flows in circular tubes, solid-liquid flows in Couette geometries as well as to gas-liquid and liquid-liquid flows.

One approach to velocity measurements is to measure an incremental spatial displacement of nuclear spins that are noninvasively tagged whereas another is to measure the phase evolution of the nuclear spin precession which depends on the translational velocity. The first method is best suited for flows in uniform geometries such as pipe flows whereas the second, more complex method, is better suited for non-uniform cases such as for nonneutrally buoyant flows in a Couette geometry.

In order to improve the capabilities of the apparatus to make rapid measurements, a major instrumentation upgrade is being performed during summer and fall of 1991. This consists in a new operating system and computer, hardware improvements to the rf electronics, and a shielded magnetic field gradient coil system. The studies of concentrated suspensions in pipe flow for velocity and concentration distributions is complete except for measurements of particle velocities. The next major experimental emphasis will be on liquid-solid flows in an asymmetric Couette device.

This work is carried out in collaboration with the Lovelace Medical Foundation.

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

The principal focus of this research program is the development of a turbulent mixing model applicable to combustion flows. In work to date, a novel computational approach has been formulated in which turbulent stirring is represented by non-linear mappings on a line, iterated according to a stochastic rule that incorporates key aspects of the Kolmogorov cascade picture of turbulence. Computations and analysis demonstrate substantially better predictive capability than achieved by previous models of molecular mixing in turbulent flow. Future work will involve further analysis of the mathematical origins of the computed results, refinement of the model to capture subtle effects such as the influence of molecular diffusion on turbulent transport, and application to unsolved problems of turbulent mixing in non-reacting turbulent shear flows and turbulent combusting flows.

Aspects of heterogeneous combustion are also addressed in this program. Stochastic network-breakup models are applied, on a macroscopic scale, to the morphological evolution of a reacting porous solid, and on a microscopic scale, to the thermochemical dissociation of a macromolecular fuel such as coal.

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 research project investigates the structure of inverse diffusion flames in supercritical fuel/water mixtures. Inverse diffusion flames have received very little attention in the literature although they possess unique characteristics that are applicable to chemical processing and materials synthesis. The focus of this project is the specific class of inverse diffusion flames in which a laminar jet of oxidizer is introduced into a background of hydrocarbon fuel and water at a temperature and pressure above the thermodynamic critical point of the fuel/water mixture. These flames have direct application to the destruction of aqueous and mixed hazardous wastes, but little is currently known about the ignition, extinction, or stability of flames at high pressures, particularly flames at supercritical water conditions. Sandia has built a laboratory-scale supercritical reactor and demonstrated the capability to obtain quasi-steady inverse diffusion flames in supercritical mixtures of water and methane. The reactor provides optical access to the reaction zone, and a mapping of temperature, species, and velocity fields is planned. Both analytical and numerical models of laminar diffusion flames are available to support the experimental efforts, however these models must be modified to include a supercritical fluid equation of state and supercritical 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. Such forces are responsible for the attrition of fluidized particles and postulated behaviors of the particle pressure have been used as a mechanism to explain the stability of homogeneously fluidized beds. But, until recently there have been no measurements of the particle pressure. 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. The purpose of the present investigation is to continue this work to better understand the mechanisms that lead to particle pressure generation in both gas and liquid fluidized beds. In two-dimensional gas bed, the goal is to determine the distribution of particle pressure around an injected two-dimensional bubble as a way of understanding the distribution of particle pressure across the bed. The studies in the liquid bed will be used to try and understand the behavior of the particle pressure near the point of initial instability of the bed and the pressure that are generated in the early stages of unstable behavior. In the first year of the project we have developed and improved version of the particle pressure transducer. The results show that particle pressures are largely generated in the wakes of bubbles. The same may not be true for a slug, in which case, the bubble spans the bed. We have some qualitative evidence that, in that case, the largest particle pressures are generated between the nose of the slug and a boundary wall. So far, it appears that the particle pressures generated in a liquid bed are so small (a few Pascals) that they are at the lower boundary of the region that can be resolved with the current transducer; we are planning another radical change in the transducer design that will hopefully resolve these pressures.

Southwest Research Institute

6220 Culebra Road **$99,912**
San Antonio, TX 78228-0510 **03-B**
91-3

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

The project objective is to study the effects of neutron embrittlement and biaxial stress on signals from various magnetic measurement techniques in steels. It is expected that interaction between experiment and modeling will lead to design of efficient magnetic measurement procedures for monitoring neutron embrittlement and biaxial stress.

Magnetic measurement techniques to be assessed are: (1) magnetic hysteresis loop measurement of properties like coercivity and permeability; (2) magabsorption, which measures the impedance of an rf coil brought close to a magnetic sample: (3) Barkhausen noise analysis; (4) magnetically induced velocity change (MIVC) of an ultrasonic wave; and (5) harmonic analysis of an ac magnetic hysteresis loon. The model of Sablik et al for magnetic hysteresis and uniaxial stress effects on magnetic properties will be extended to conditions of biaxial stress and neutron embrittlement. The effects of these conditions on magnetic probe signals (1) - (5) will be modeled and compared to experiment. In the case of neutron embrittlement, measurements will be made on steel samples characterized by Charpy tests after previous exposure to various neutron fluences.

Project research is important for safety monitoring in the nuclear power and gas industries. Preliminary results on neutron-embrittled samples will be presented at the QNDE Conference in San Diego in July 1992.

Stanford University

Dept of Mechanical Engineering **$98,695**
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 a flat surface against diffusional perturbations and the stress concentration caused by surface roughness.

The surface morphology of materials will be studied by using a unified perturbation procedure based on the notion of thermodynamic forces and the energy momentum tensor. The thermodynamic forces on material inhomogeneities such as interfaces and inclusions are a measure of the rate at which the total energy varies with the configurational change of these inhomogeneities. Within the general methodology, any type of material and loading condition can be studied as long as the proper forces can be identified. By using corresponding material conservation laws discovered previously, a systematic analysis of surfaces of piezoelectric solids can be made. Preliminary studies have shown that under sufficiently large stresses, surfaces of materials become unstable against a range of diffusional perturbations bounded by two critical wavelengths. Even a slight undulation such as micro-level bumps and troughs can result in a substantial stress concentration along a material surface. These concentrations may lead to mechanical failures along the surface and may have more consequences for piezoelectric materials where the deformation is coupled to an applied electric field.

In the past year we have also developed a simple analytical solution to a special class of surface roughness characterized by a cycloidal profile. Surprisingly we find that the cycloidal rough surface is subjected to the same stress singularity and stress intensity factor as an array of periodically spaced semi-infinte cracks. Application of fracture mechanics would predict that these two brittle structures fail at the same bulk stress level, even though there is no apparent "crack size" associated with the rough surface! The full significant of this solution is being investigated.

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 the mechanics of solids defects such as inclusions or holes may undergo rearrangements or changes of form; the energy changes associated with such rearrangements play a preponderant role in characterizing the gross response of solids under load to these "transformations". To this end, the heterogenization techniques developed with DOE support proves most useful. The method has been extended to provide a number of universal formulae valid for the average stresses between two holes or inclusions, for inclusions with imperfect interfaces, and for stresses in cylindrical and plane layered media. A new methodology to establish conservation laws for dissipative systems has been advanced, and a theory of stressed solids prone to damage has been formulated based on the Gibbs free energy.

Another portion of our research has as its objective the development of further understanding of subsonic and supersonic surface waves and interfacial and bulk waves in anisotropic linear elastic solids. In the past year we have completed a reasonably thorough study of the existence of triply degenerate acoustic axes in these solids, including a delineation of restrictions on elastic stiffnesses and orientations in crystals of isotropic, cubic, hexagonal, trigonal, and tetragonal symmetry which allow for such acoustic axes to occur. Our previous discovery (last year) of the existence of "one-component surface waves" (which are necessarily supersonic) is being used to develop numerical and theoretical methods for finding the space of simple reflection in generally anisotropic solids, and to study the connection of this space with supersonic surface waves (both leaky and pure). New investigations of so-called "generalized surface waves" and Stoneley waves in pre-stressed anisotropic bimaterials have also been undertaken.

Stanford University

W.W. Hansen Lab of Physics **$134,678**
Stanford, CA 94305-3030 **03-B**
90-3

Optical Techniques for Superconductor Characterization
G. Kino

The aim of this project is to develop a photothermal microscope for non contact testing of materials. Techniques of this kind are particularly well suited to the determination of thermal parameters, and anisotropy of small samples.

One example of the work is the measurement of high temperature superconductors over a range of temperatures from room temperature through the critical temperature T_c down to 20°K. A modulated laser beam, focused to less than I m diameter, impinges through a sapphire window onto a sample of Bi-Ca-Sr-Cu-O in a helium cryostat and periodically modulates its temperature. This process excites a thermal wave, which can be detected by the variation in reflected signal amplitude of a second focused laser beam, due to the change of refractivity with temperature. The sample can be rotated under the beams and the thermal diffusion coefficient, its anisotropy and its magnitude can be measured from the phase delay of the thermal wave. By measuring the amplitude of the thermal wave, material phase changes associated with superconductivity can be measured. A pronounced peak in amplitude is seen at the critical temperature T_C. Even stronger effects of this type are observed with charge density waves in a variety of materials.

Stanford University

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

Fluid Dynamics of Double Diffusive Systems
J. Koseff, R. Street, S. Schladow

This project is focused on processes that occur in a double-diffusive system subject to external forcing, using a combined experimental and numerical approach. In particular it addresses a water body that is continuously stratified in both temperature and salinity. The forcing is provided by a combination of a lateral heat flux and a surface shear. Double-diffusive instabilities and mixed layer deepening occurs in response to this forcing, resulting in changes to the vertical and horizontal fluxes of heat and salt. The goals are to (1) understand the initiation and evolution of the double diffusive instabilities, (2) quantify the effects on the vertical fluxes, and (3) compare observations of the mixed layer deepening to the existing data for singly stratified systems. The experimental component has to date concentrated on the effects of lateral heating. A new 4.0 m long and 0.8 m wide experimental tank, together with appurtenant facilities for controlling the initial stratification, has been commissioned. The end wall of this tank is uniformly heated using a radiant source. Fast response thermistor and conductivity probes are used to provide vertical profiles, and flow visualization is provided by video imaging of dye in illuminated planes. Initial findings suggest that the nature of resulting convective intrusions is a function of two dimensionless stability parameters. The numerical component involves using a finite volume formulation of the non-linear Navier-Stokes, conservation of mass, and conservation of species equations in three space dimensions and in time. The experimental results suggest that the high resolution required to satisfactorily represent the intrusion interfaces will make a conventional modeling approach very difficult, with the number of grid points required to resolve the interfaces excessive, even in the context of modern supercomputers. For this reason work on implementing an adaptive gridding procedure has been commenced.

Adaptive gridding allows the grid to be selectively refined only in those areas where high resolution is required, thus facilitating large savings in both computational time and memory requirements.

Stanford University

Mechanical Engineering Dept **$441,508**
Stanford, CA 94305 **03-B**
92-4

Advanced Diagnostics for Plasma Chemistry
C. Kruger, M. Cappelli

This research is concerned with optical diagnostics for plasma chemistry and plasma processing, with an emphasis on methods which allow for departures from local thermodynamic equilibrium -- such as finite chemical reaction rates, nonequilibrium electron densities and temperatures, and radiation loss effects. Laser and other optically based methods are being developed for measurements of plasma parameters including species concentrations and temperature. The methods under study include Laser Induced Fluorescence and Degenerate Four Wave Mixing, and are designed to be applicable whether or not the plasma is in local thermodynamic equilibrium, and indeed to assess the importance of nonequilibrium effects under conditions of interest in plasma chemistry.

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

To apply this approach to diagnostics to a realistic and promising form of plasma processing, we have undertaken experiments on diamond synthesis on substrates in the test section of the induction torch. Diamond crystals and films have been grown at rates that are at least one order of magnitude greater than those characteristic of low-pressure diamond synthesis.

Recent measurements in the diamond synthesis environment show that Degenerate Four Wave Mixing is a very pomising diagnostic for the intensely luminous environments of plasma chemistry. Current measuremtns show a sensitivity for CH radical concentrations of a few ppm, with a submillimeter spatial resolution.

Stanford University

Dept of Chemistry **$142,000**
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. Work is planned on the formulation of thermodynamics of nonlinear (auto-catalytic) 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

A need exists for *in situ* noninstrusive diagnostics for probing trace and highly reactive radical intermediates in nonequilibrium plasma used for chemical vapor deposition. We propose applying a novel nonlinear spectroscopic technique, degenerate four-wave mixing (DFWM). The DFWM signal is a coherent scattered beam at frequency which is generated by the nonlinear response of the medium to the interaction of three incident waves at the same frequency. The signal is enhaced by a reasonant transition and offers a form of Doppler-free spectroscopy with extremely high spectral, spatial, and temporal resolution. Signal detection is remote and does not suffer from background interference from the bright plasma source. In addition, the phase conjugate nature of the signal eliminates optical aberration. The environment we propose to study is an atmospheric-pressure rf-inducively-coupled plasma and the target radicals include CH, CH_2, C_2, C_2H, and CH_3 that are important in plasma synthesis of diamond thin films. The spatial sensitivity of DFWM will be used to study the coupling of gas-phase and gas-surface chemistry by measuring temperature and concentration profiles. The proposed research will advance diagnostic techniques for plasma environments and provide a better understanding of the plasma chemistry of diamond synthesis.

Stevens Institute Of Technology

Dept of Physics and Engineering $66,932
Hoboken, NJ 07030 06-C
92-3

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

This project focuses on the application of dynamical system (chaos) theory to problems occurring in nature and technology. The approach is computational as well an analytical.

The mechanism of generation of terrestrial and solar magnetic fields is still not understood. It has been recently proposed that the chaotic flow in a conductive fluid can lead to a fast dynamo, where an initially small magnetic field increases exponentially with time. Several artificial chaotic systems have been studied computationally, and claims have been made of the presence of fast dynamo action in these systems. In this work the question of fast dynamo action in naturally occurring systems is studied. A fluid heated from below gives rise to Rayleigh-Bernard instability generating chaotic flow regions. First this flow (the Arter flow) is studied to determine the dependence of chaotic regions on the instability parameter, the location of stagnation points and invariant manifolds. This work is analytical as well as computational. Next a computational study is undertaken to determine whether such flows can generate fast dynamo action.

Another area of study involves the mixing of polymers. Such mixing involves time dependent externally driven, incompressible chaotic flows. The question of which parameter regions produce large chaotic domains and hence the best mixing is being studied. So far excellent agreement has been found between these computational studies and experimental results reported in the scientific literature.

University Of Texas At Austin

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

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

This proposal, which is a continuation of previous work deals with the behavior of matter under non-equilibrium conditions in terms of microscopic description. A theoretical framework for integrating "non-integrable" large Poincare systems will be applied to the study of a number of interesting situations. (1) Application to interacting fields, including classical and quantum electrodynamics: The method permits the representation of radiation damping as part of the complex spectrum of the Liouville operator, and avoids the well-known difficulties of the classical and quantum radiation damping theory. (2) Numerical validation of the approach: Numerical experiments will be pursued in order to verify the quantum formulation. Especially, the collapse of the wave function and the appearance of an equilibrium statistical distribution, as predicted by the theory, will be verified. (3) The present work, already well advanced for the definition of unstable particles in the frame of a complex spectral representation, will be continued. Unstable particles with decaying modes cannot simply be identified, since decaying modes, taken separately, do not carry energy. (4) The theory gives the possibility to derive new criteria for the transition to classical chaos by studying the complex spectrum of the Liouville operator in a form that is appropriate to mapping problems. (5) The theory goes beyond the non-Markovian master equation and permits a new approach for the study or transport processes (diffusion, viscosity, etc.). (6) Irreversibility appears to be of special interest in high-energy problems, and especially to transitions from virtual to real particles.

University Of Texas At Austin

Dept of Physics **$152,496**
Austin, TX 78712 **06-C**
87-5

Complex Temporal and Spatial Patterns in Nonequilibrium Systems
H. Swinney

Dynamical systems methods are being developed and used to characterize the formation and evolution of temporal and spatial patterns in systems maintained far from equilibrium. In particular, experiments and analyses are considering electrodeposition of fractal metallic clusters, pattern formation in reaction-diffusion systems, and instabilities in convecting fluids. Novel reactors have been developed to search for chemical patterns (i.e., spatial variations in the chemical composition), and sustained patterns have been found in several different one- and two-dimensional geometries. Bifurcations in these patterns are studied by varying control parameters, e.g., the concentrations of the feed chemicals or the temperature. The observed two-dimensional chemical patterns range from the stationary patterns, similar to those predicted by Turing in 1952 but not observed until 1990, to chemical turbulence, which is characterized by large numbers of defects and a rapid decay of spatial correlations. Much needs to be done, both experimentally and theoretically, to characterize and understand these spatiotemporal patterns. These laboratory experiments together with numerical and analytic studies of models should provide general insights into the formation and evolution of patterns in nonequilibrium systems.

Tufts University

Dept of Mechanical Engineering **$59,798**
Medford, MA 02155 **01-A**
88-3

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

The knowledge of effective elastic properties of solids with cracks appears to be of increasing engineering importance. Extensive microcracking in structural elements working under conditions of high temperatures or irradiation, and microcracking in composite materials under fatigue conditions may noticeably reduce the stiffness of the material and make it anisotropic. Understanding and prediction of these changes are essential for proper design and strength and lifetime assessments. A new approach to many cracks problems based on interrelating the average tractions on individual cracks is introduced. Its advantages are that it yields simple analytical results which are quite accurate up to very high crack densities and that it can be applied to crack arrays or arbitrary geometry. Relation between deterioration of elastic properties and "damage" is discussed.

United Technologies Res Center

Propulsion Science Lab **$179,995**
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 measurement 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)
9) formulation of chemical kinetic models to account for spectral observations
10) adapted of pyrolysis mechanism to photoinitiated pyrolysis and comparison with experimental results
11) proposal of surface species and heterogeneous reaction mechanism for the growth of boron from diborane plasma

Washington University

Department of Systems Science and Mathematics — **$75,664**
Saint Louis, MO 63130 — **03-A**
90-3

Dynamical Systems with Internal Structure: A New Approach to the Problem of Analysis and Robust Design of a Time Varying System
B. Ghosh

The main objective of the proposed project is to study design problems for linear time-varying control systems leading to a robust design via an adaptive controller. Specifically, for autoregressive moving average systems with time-varying coefficients, it turns out that a good design strategy is to adaptively assign the parameters of the closed loop system by a judicious choice of a time-varying compensator. The parameters of the compensator which assign a specified set of coefficients in the closed loop satisfy a nonlinear recursion. We propose to study these recursions in details. For specific cases, we show that the proposed recursion is an Anosov diffeomorphism on a three-dimensional torus. In particular, such a dynamic is chaotic. We feel that our design should try to avoid chaotic dynamics.

In order to analyze and design a compensator for a time-varying system it is important to be able to estimate the trend, i.e., predict future values of the parameters of the system. An important part of our project is to assume that the parameters change in accordance with an internal structure viz. a time series. Our goal is to estimate the parameters of the internal structure.

Thus we propose to investigate in this project an identification scheme with internal structure together with recursive coefficient assignment in real time in order to generate a desirable performance in the closed loop.

Washington State University

Dept of Mechanical Engineering — **$72,000**
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. Two types of previously unknown particulate dispersion processes have been identified. In mixing layers, where large scale vortex mergers occur regularly, intermediate scale particles are concentrated into sheet like patterns which undergo stretching and folding operations. For bluff body wakes where large scale vortex mergers are not a dominant feature intermediate scale particles are focussed into thin regions of high particle concentrations near the vortex boundaries.

Current research efforts are directed towards exploring the effects that two-way momentum, mass and energy coupling have on the multiphase dispersion processes previously uncovered. These efforts involve analytical, numerical and experimental investigations. Recent analytical and numerical results indicate that momentum coupling effects can significantly alter the global stability and potentially the large scale features of the multiphase flow field. These multiphase coupling effects may have significant importance with regard to predicting the performance of many energy conversion systems.

University Of Wisconsin

Mechanical Engineering Dept **$107,708**
Milwaukee, WI 53201 **01-C**
90-3

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

The objective of the research program is 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 local void fraction, interfacial area concentration, fluid particle size distribution and flow patterns in vertical two-phase flow systems are studied in detail. For the purpose of understanding the dynamic behaviors, the interfacial velocity, wave characteristics and coalescence and disintegration of fluid particles are investigated. Special emphasis is placed on developing the four-sensor and five-sensor resistivity probe method and improving the double-sensor resistivity probe method. A second emphasis is on the system size and entrance effects on the interfacial characteristics described above. The changes in the interfacial structures and flow regimes as a function of an axial location are measured experimentally. This information together with the local measurements from the probe method are used to study the mechanisms of flow regime transitions. This research is part of a joint program between Purdue University (Ishii) and the University of Wisconsin-Milwaukee. The research program is expected to lead to a) local instrumentation methods for detailed interfacial characteristics, b) data for local interfacial area, void fraction, relative velocity and wave propagation velocity, and c) phenomenological models for interfacial area and interfacial structural changes.

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-C

01-D

03-A

03-B

03-C

06-A

06-B

06-C

Principal Investigators

UNITED STATES
DEPARTMENT OF ENERGY
WASHINGTON, D.C. 20545

OFFICIAL BUSINESS
PENALTY FOR PRIVATE USE, $300

ER-15