DOE/ER-0485P

# Summaries of FY 1990 Engineering Research

U.S. Department of Energy

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

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UC-402

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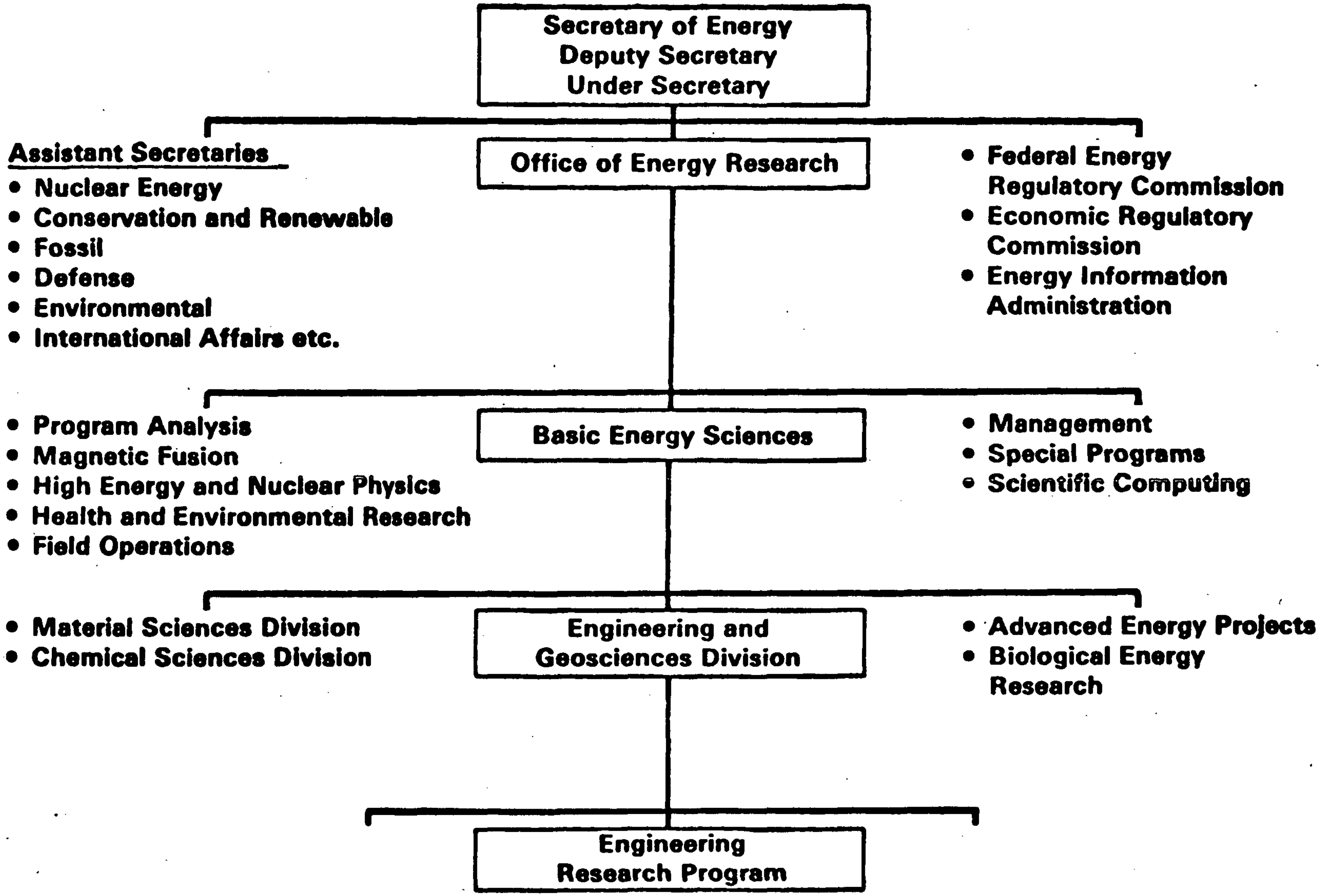
Washington, D.C. 20585

# Foreword

This report documents the BES Engineering Research program for fiscal year 1990; it provides a summary for each of the program projects in addition to a brief program overview. The report is intended to provide staff of Congressional committees, other executive departments, and other DOE offices with substantive program information so as to facilitate governmental overview and coordination of Federal research programs. Of equal importance, its availability facilitates communication of program information to interested research engineers and scientists. The organizational chart for the DOE Office of Energy Research (OER) on the next page delineates the six Divisions within the OER Office of Basic Energy Sciences (BES). Each BES Division administers basic, mission oriented research programs in the area indicated by its title. The BES Engineering Research program is one such program; it is administered by the Engineering and Geosciences Division of BES. Dr. Oscar P. Manley is technical manager of the Engineering Research program; inquiries concerning the program may be addressed to him, in writing or by phone at (301) 353-5822.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1990. 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 1990.

The projects are numbered sequentially for individual identification in the indexes. Each project entry begins with an institutional–departmental heading. The project number precedes the capitalized project title. The names of investigators are listed immediately below the title. The funding level for fiscal year 1990 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., 88–). 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, and modeling of combustion processes for engineering application.

These areas contain the most critical elements of the four topics enumerated above; as such they are of importance to energy technologies both in the short and long term, and therefore of immediate programmatic interest. It should be noted that other areas of basic research important to engineering are monitored elsewhere in BES. For instance, separation sciences and research on thermophysical properties are among the responsibilities of the Chemical Sciences Division, while microscopic aspects of fracture mechanics are in the domain of the Material Sciences Division. As resources permit, other high priority areas are being added to the Engineering Research Program. Thus as a result of 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 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. The research opportunities in this area of interest to the DOE Engineering Research Program have been identified in a workshop held in November, 1983. Proceedings of the workshop entitled "Research Needs in Intelligent Machines" are available from the Center for Engineering Advanced Systems Research, Oak Ridge National Lab, Post Office Box X, Oak Ridge, TN, 37830.

Secondly in FY 1985 there started a collaborative research effort 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)

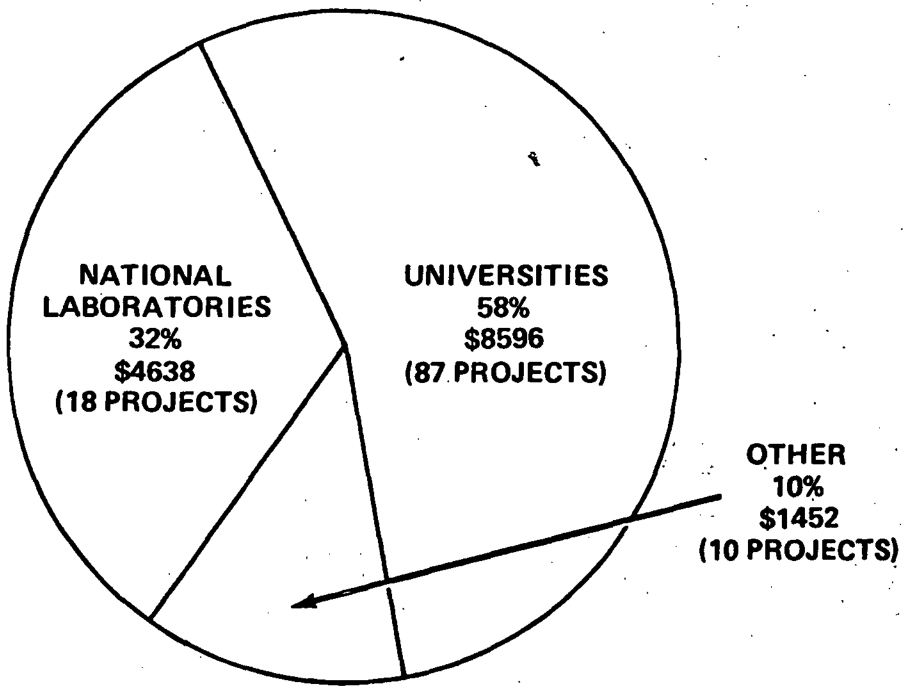
Two additional workshops were held during 1988. The first dealt with possible research opportunities in the field of novel devices using the new high temperature superconductors. The second addressed research needs for bioprocessing of fuels and energy related wastes. Reports of both workshops have been published.

It should be mentioned too, that some very limited support is available for research on large scale systems. A report of a Workshop on Needs, Opportunities, and Options in this field is available from Professor G.L. Thompson, Graduate School of Industrial Administration, Carnegie-Mellon University, Pittsburgh, PA 15213.

Research projects sponsored by the BES Engineering Research Program are currently underway at universities, private sector laboratories, and DOE national laboratories. In fiscal year 1990 the available program operating funds available amounted to about $14.7 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 proposals for competitive grants. Proposals which anticipate definite results in less than two years are usually referred to the appropriate DOE technology program for consideration. All those interested in submitting a proposal are encouraged to discuss their ideas with the technical program manager prior to submission of a formal proposal. Such discussion helps to establish whether or not a potential project has a reasonable chance of being funded. The primary considerations for possible support are the technical quality of the proposal and the professional standing of the principal investigators and staff. An effort is made to attract first rate, younger research engineers and energy oriented applied scientists. A high technical caliber of research is maintained by requiring that the projects supported have potential for a significant contribution to energy related engineering science, or for an initial contribution to a new energy relevant technology. Sponsored projects are selected primarily for their relevance to DOE mission requirements; the contribution to energy related higher eduction is an important but secondary consideration. Thus projects sponsored at universities are essentially limited to advanced studies both theoretical and experimental usually performed by faculty members, staff research scientists, and doctoral candidates.

## ENGINEERING RESEARCH PROGRAM

# FY '90 BUDGET ($000's) BY INSTITUTIONAL TYPE




## ENGINEERING RESEARCH PROGRAM

# FY '90 BUDGET BY TECHNICAL AREAS

| | ($000 s) | % | NUMBER OF PROJECTS |
|---|---|---|---|
| MECHANICAL SCIENCES | 4357 | 30 | 43 |
| SYSTEMS SCIENCES | 4993 | 34 | 25 |
| ENGINEERING ANALYSIS | 5336 | 36 | 47 |

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## University of Alabama

**Department of Mathematics** **$44,547**
**Tuscaloosa, AL 35487** **01-C**
**90-1**

**Linear and Nonlinear Stability Topics in Physico-Chemical Hydrodynamics**
***A.L. 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.

## Ames Laboratory

**Institute for Physical Research and Technology** **$254,388**
**03-B**
**Ames, IA 50011-3020** **88-3**

**New Ultrasonic Imaging and Measurement Techniques for NDE**
***D.O. Thompson, D.K. Hsu***

The objective of this project is to develop new knowledge and techniques for the nondestructive detection and characterization of flaws in materials and structures and the measurement of selected material properties that are important in obtaining materials reliability and structural integrity. In order to achieve this goal, efforts are made to develop new and novel ultrasonic NDE capabilities and to characterize emerging materials. Use is made of a multiviewing system previously developed in this work and quantitative elastic wave theories in the interpretation of results as well as microfocus radiography and eddy current techniques. Three major thrusts are being pursued:

1) Nondestructive material characterization methods are being explored for high transition temperature superconducting ceramics using three types of probing fields: x-ray, eddy current, and ultrasound. Efforts are aimed at nondestructive measurements that can be used to monitor material processing techniques.

2) Novel techniques have been developed that allow the fabrication of ultrasonic transducers that have fundamentally important wave propagation properties of engineering significance. Two such transducers, a Gaussian beam transducer and a Bessel beam transducer, have been developed. The Gaussian beam is field and the Bessel beam can potentially lead to diffraction-free elastic waves.

3) New techniques for ultrasonic computed tomographic imaging (reconstruction) are being explored that utilize elastic wave scattering models and the multiviewing instrumentation. This is an important innovation in that images so obtained are expected to be free of distortions due to effects of material anisotropy and complex surfaces encountered in some current imaging techniques.

## Argonne National Laboratory

**Materials and Components Technology Division** **$127,194**
**Argonne, IL 60439** **01-A**
**87-3**

**Bounds on Dynamic Plastic Deformation**
***C.K. Youngdahl***

Analytical studies are being performed to develop load correlation parameters which can be used in 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 load correlation parameters based on various weighted integrals of the time-space load distributions which can be used to characterize the effects of the load without resorting to detailed numerical analysis. These load correlation parameters have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events. The dynamic plastic deformation of some basic structural configurations will be analyzed for loadings which vary both in magnitude and region of application with time. Load correlation parameters will be hypothesized and their usefulness in predicting final plastic deformation will be determined. The analyses will be based initially on a rigid, perfectly plastic material model and small deformation response, but will be extended to include strain hardening, an initial elastic response period, and large deformation interactions.

## Arizona State University

**Mechanical & Aerospace Eng.** **$53,000**
**Tempe, AZ 85287** **01-A**
**88-4**

**Continuum Damage Mechanics II**
***D. Krajcinovic***

The efforts in the first two years of this research program were focused on the development of a micromechanically inspired continuum damage mechanics model. Specifically, the objective was to formulate a rigorous micro-to-macro transition along with the conditions which must be satisfied for this transition to be valid. For example, it was demonstrated that the change in elastic compliance is a proper choice for the thermodynamic macro-flux since it represents an orientation weighted volume average of micro-fluxes. The corresponding affinity is the energy release rate integrated along the crack perimeter and averaged across its surface. The macro-potential is subsequently determined as an inner envelope of the micro-potential. The corresponding damage surface is a convex piecewise smooth hypersurface possessing the normality property. The ensuing computations clearly indicate the simplicity and accuracy of the proposed model in several illustrative examples.

The micro-to-macro transition is, however, proven to be valid only as long as the application of the effective continua theories is justified. In other words, the macro flow potential cannot be proven to exist when the influence of the direct interaction of micro-defects on the deformation becomes significant.

One of the most important aspects of the analyses of brittle deformation processes is the determination of failure which is, obviously, associated with a critical microcrack density. However, the analytical modeling of the so-called cooperative phenomena, characterized in the considered case by a disorder of the material microstructure and the interaction of many defects of random geometry, distribution and orientation represents a serious problem. This class of problems, being inherently nondeterministic in nature, is seldom if ever addressed in continuum mechanics. A promising strategy, to be explored in the continuation of this research program, is to consider the application of the so-called percolation theory. One of the two main problems is to make a transition between the lattice and continuum percolation theory and recover the damage micro-flux (Budiansky-O'Connell variable) and enable mapping between the two models. The other problem is that the disorder is introduced into the percolation model traditionally by a bimodal distribution which might be to restrictive for real materials having a richer hierarchy of strengths on the micro-scale. Nevertheless, it is felt that the percolation theory offers a viable framework for the studies of the brittle deformation processes in the vicinity of the percolation thresholds (which are different that those associated with transport phenomena). The application of the percolation theory is important since it enables studies of estimates which the local fluctuations of stresses (hot-spots) and strengths (weak-links) have on the failure of the material.

## Battelle

**Mechanics Department** **$90,083**
**Columbus, OH 43201-2693** **01-A**
**90-3**

**An Investigation of the Effects of History Dependent Damage In Time Dependent Fracture Mechanics**
***F.W. Brust***

The demands for structural systems to perform reliably under severe operating conditions continues 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. Analytical techniques for predicting crack growth and failure under these conditions will be critically examined by direct comparison to experimental data developed here. Appropriate constitutive relations will be utilized in a finite element approach to determine parameters which characterize time and history dependent damage during crack nucleation and growth. It is hoped that methods developed may then be used by practicing engineers to enhance the life of high temperature structural systems during the design phase. This is the first year of this research effort.

## Boston University

**Department of Chemistry** **$66,650**
**Boston, MA 02215** **06-C**
**89-3**

**Transport In Porous/Disordered Materials**
***T. Keyes***

The aim of this project is the construction of theories of the transport processes-diffusion, fluid flow, electromagnetic wave propagation, etc. -in materials where strong interactions or disorder cause a near stoppage of the transport. Of special interest are materials with percolation thresholds, where the disorder blocks transport altogether, and systems near a glass transition. The research is broadly based and a wide range of theoretical and computational techniques are employed. Progress along three fronts was made in the past year.

Harmonic normal mode analysis is routinely applied to stable solids, but is not normally considered useful for fluids. We have developed a new method for fluid dynamics, based upon normal mode analysis, in which transport is governed by the unstable modes of the system. The method worked extremely well for supercooled liquids and is now being applied to suspensions of spheres.

Glass ceramics are composed of irregular crystallites in a glassy matrix. The propagation of light through these disordered materials was studied. The structure of the crystallites was related to the properties of the scattered light in a completely new scheme which requires the intensity statistics, but no knowledge of optical properties.

High intensity light will break chemical bonds and cut material. A fairly comprehensive model of this very nonlinear process was constructed and solved, with qualitative agreement with several observations. Computer simulation of the phenomenon was begun, with an eye to the study of laser-induced shock waves and to sorting out the "energy bookkeeping" -the ultimate destinations of the laser energy.

## Brown University

**Division of Engineering** **$117,000**
**Providence, RI 02912** **06-C**
**90-1**

**Two Studies of Nonlinear Processes in Irreversible Thermodynamics**
***J. Kestin***

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

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

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

The present task is to examine the qualitative effects of nonequilibrium on the general flow characteristics and on critical flow. In particular, a combined numerical and analytic study has re-interpreted the well-known Moby Dick experiments suggesting, at this stage provisionally, that critical flow was not reached in the throat but at the end of the experimental channel. This possibility may lead to a revision of our views on choking in two-phase flow.

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

Good success has been achieved with the formulation of an elementary theory of fracture in cooperation with Professor G. Herrmann of Stanford University which resulted in two joint papers.

## University of California, Berkeley

**Dept. of Electrical Engineering and Computer Sciences** **$89,775**
**06-C**
**Berkeley, CA 94720** **90-3**

**Self-Generated Stochastic Heating in an RF Discharge**
***A.J. Lichtenberg, M.A. 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, Los Angeles

**Mechanical, Aerospace, & Nuclear Engineering Department** **$75,760**
**School of Engineering and Applied Science** **01-C**
**Los Angeles, CA 90024-1597** **89-3**

**Basic Studies of Transport Processes in Porous Media**
***I. Catton***

This project is an ongoing study of single- and two-phase convective processes in porous media. The objective of this work is to develop physical understanding of the governing phenomena and models of the transport processes by theoretical and experimental means.

The effective thermal conductivity of single and binary particle size packed beds saturated with stagnant gas was determined numerically. Engineering correlations were developed for binary mixtures with various particle sizes, solid/gas conductivity ratios and gas pressures. Forced convection in a packed tube with axial dispersion is being modeled to further test our hydrodynamic dispersion model. The effect of dispersion on the onset of natural convection in a porous layer with volumetric heating is presently under investigation. The effects of the dispersion on finite amplitude behavior including bifurcation of the initial flow will be studied.

Steam injection into a uniform downward water flow in a porous channel has been studied both experimentally and theoretically. Conditions for oscillation of the resulting steam-water interface have been delineated and its effect on heat and mass transfer augmentation has been measured. Steam bubble size and shape, surrounding water temperature field, and pressure drop at the injector have been measured. A more extensive study of the oscillatory behavior of the bubble will follow. In the theoretical studies, steam zone shape, steam and water flow and temperature fields, local condensation rate, and average Nusselt number have been found by solving the continuity, momentum, and energy equations for both water and steam using a hodograph transform and an integral method for Darcy flow. Numerical modeling of the onset of bubble oscillation will be investigated for non-Darcy flows.

## University Of California, Los Angeles

**Mechanical, Aerospace, & Nuclear Engineering Department** **$27,485**
**06-B**
**School of Engineering & Applied Sciences** **90-1**
**Los Angeles, CA 90024-1597**

**Studies in the Combustion and Breakup of Transverse Liquid Jets and Fuel Droplets**
***A.R. Karagozian***

The present studies are concerned with analytical modeling of the processes of mass loss, breakup, and burning in liquid fuel jet streams injected transversely into a crossflow of air and in single liquid fuel droplets present in a convective environment. This multiphase flow study emphasizes the effect of the internal vortical structure of the liquid on important physical features of these reacting flowfields, i.e., 1) the incompressible vortex pair flowfield within the cross-section of the liquid transverse jet, and 2) the Hill's spherical vortex within the axisymmetric liquid droplet.

Since the inception of this grant, our efforts have focused on modeling of the deflection, mass loss, breakup, and burning of the liquid transverse jet in compressible crossflow, for a chemical reaction with fast kinetics. Inviscid, compressible flow about the elliptical cross-section of the jet is solved analytically in the low subsonic regime and numerically for upstream Mach numbers above 0.3. External boundary layer analysis along the surface of the cross-section allows determination of an effective drag associated with the jet, which balances centripetal forces resulting from jet deflection. The presence of a diffusion flame in the boundary layer for upstream Mach numbers less than 0.3 is represented, and fuel mass loss due to evaporation as well as combustion is computed. Mass and momentum balances are then performed along the jet, so that fuel jet and flame trajectories, bow shock penetration (if present), and effective flame length may be determined. An approximate technique for predicting jet breakup location is also developed, based on a balance of stresses and a local sonic point (if present) adjacent to the deflected jet. Correspondence of these predictions with experimental results is quite favorable, especially in that the modeling contains no empirical correlations or adjustable parameters. Current efforts are focused on the representation of ignition in the liquid jet by accounting for finite rate chemistry.

Modeling of the processes of evaporation and combustion for a single, axisymmetric fuel droplet in a convective environment is also undertaken here. The influence of the internal flowfield on various flame characteristics is computed, and the predicted variation of droplet size in time is compared with experimental measurements. At present, fast chemistry is assumed, but future studies will include the incorporation of finite rate chemistry in order that ignition and other flame stabilization characteristics may be studied.

## University Of California, Los Angeles

**Mechanical, Aerospace, & Nuclear Engineering Department** **$84,283**
**06-C**
**School of Engineering & Applied Sciences** **89-3**
**Los Angeles, CA 90024-1597**

**Modeling of Energy and Particle Transport**
***G.C. Pomraning***

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

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

## University Of California, Los Angeles

**Department of Physics** **$73,000**
**Los Angeles, CA 90024** **06-C**
**90-3**

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

Nonlinear wave interactions in far off equilibrium systems are being studied with the goal of understanding the development of stochasticity and the formation of localized coherent structures. From the general theoretical point of view one long term goal is the determination of the probability distribution for a sea of nonlinear interacting waves. This problem is being approached via the extension of the Fokker-Planck formalism to include ultra long time scales and higher order correlations. From the practical point of view these ideas are being applied to the propagation and interaction of waves on the surface of a fluid that is strongly driven.

At high amplitudes, propagating waves can also form localized structures such as kink, breather and envelope solitons. These structures as well as recently discovered nonlinear domain walls are being studied from the theoretical as well as experimental perspective. The experiments are being carried out on fluids and nonlinear lattices and are subject to analysis by computer simulation. A long term goal of this aspect of the research includes the attempt to discover higher dimensional solitons.

The key concept of adiabatic invariance underlies the issue of integrability and stochasticity in dynamical systems. The extent to which the action variable is conserved is being calculated with the goal of predicting experimental arrangements in which the exponentially suppressed deviations from adiabaticity can be probed and compared to theory.

## University of California, San Diego

**Scripps Inst. of Oceanography** **$156,000**
**La Jolla, CA 92093-0402** **06-C**
**90-4**

**Signal Processing in Chaos**
***H.D.I. 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 in FY90 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, San Diego

**Institute for Nonlinear Science** **$20,000**
**La Jolla, CA 87545** **06-C**
**90-1**

**Lattice Gas Simulation of Fluid Flows**
***B. Hasslacher***

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

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

## University of California, San Diego

**Department of Applied Mechanics and Engineering Sciences** **$117,000**
**06-B**
**La Jolla, CA 92093** **90-3**

**Fuel Droplets Subject to Straining Flow**
***P.A. Libby, F.A. Williams***

This research involves a combined experimental and theoretical effort related to the behavior of fuel droplets. The experiments concern the determination by photographic means of the trajectories and under the circumstances involving mass loss, of the radius histories of individual droplets in well defined, nonuniform laminar streams. Initial research involved three such flows of increasing simplicity: a nonpremixed laminar flame in a counterflow configuration, isothermal counterflowing nitrogen streams, and a vertical Poiseuille flow. In the first two flows unexpectedly large lift forces are found to act on the droplets. The magnitude of the lift suggests that its cause is a rapid change in the direction of the relative velocity vector resulting in an unsteady normal force identified with lift. This conjecture is presently under experimental investigation in a fourth flow; involved is a horizontal laminar jet with a well defined, top hot velocity profile into which vertically dropping droplets are injected. Thus the droplets experience a sudden and well defined change in relative velocity. The data for various droplet sizes and jet velocities are presently being reduced. The general conclusion reached from these studies to date is that the usual engineering formulas for the forces on, and heat and mass transfer to, droplets lead to considerable errors under the severe conditions existing in these flows. The results for Poiseuille flow show that droplets injected downward off-axis experience small amounts of lift causing them to migrate toward the axis in qualitative accord with low Reynolds number theory of spheres in pure shear flows. Surprisingly large increments in drag over that for uniform flow at the same Reynolds number are found. The Reynolds number range of our data is from 0.7 to 10. Further experimental studies along these lines are planned including flows involving significant chemical kinetic effects. In our theoretical work the new model we developed for the combustion of droplets in a quiescent ambient involving water gas shift equilibrium at the flame has been combined with a detailed multicomponent description of diffusion. It is found that the predicted mass loss is little affected by either the chemistry or transport model but the position of the flame sheet and thus the detailed distributions of species are greatly influenced. Finally, our work on applications of the spray equation to a laminar flame propagating in a cloud of fuel droplets with a distribution of droplet sizes is continuing.

## University Of California, San Diego

**Inst for Nonlinear Science, R-002 — $171,916**
**La Jolla, CA 92093 — 06-C**
**89-3**

**The Stochastic Trajectory Analysis Technique (STAT) Applied to Chemical, Mechanical and Quantum Systems**
***K. Lindenberg***

A number of important physical problems are described by dynamical equations containing fluctuating parameters. Most theories have until recently assumed the fluctuations to be delta-correlated, thus restricting the scales of the spatial and/or temporal inhomogeneities to be much shorter than the response scales of the system. This assumption is often known to be quite unphysical, especially in nonlinear systems in which all scales are present. Of particular interest in this program are chemical reactions in dense media with fluctuations arising from spatial inhomogeneities and thermal effects.

A number of methods to deal with correlated fluctuations have been developed under this program. One involves an explicit construction of trajectories (STAT). This method has now been extended to some nonlinear systems and to smooth fluctuation processes with superimposed shot noise. Different methods have been applied to systems driven by correlated Gaussian fluctuations in the limits of short and long correlation times. The unification of existing theories for short correlation times has shown them to give equivalent results. Numerical simulations confirm that these results are useful over practical ranges of parameter values. At the other end of the spectrum, we have produced a theory valid at long correlation times.

We have begun to address the problem of chemically reacting systems in which spatial diffusion plays a role. Of particular interest have been open systems of A and B molecules that annihilate one another upon (suitably defined) contact. The molecules are replenished by external sources that are spatially and temporally random. There are numerous applications for such processes ranging from chemical reactions to electron-hole combination processes. In finite systems of dimension 2 or less there is spontaneous segregation of chemical species over macroscopic length scales; in infinite systems segregation is observed if the dimension is 3 or smaller. These are interesting examples of spontaneous pattern formation.

## University Of California, San Diego

**Department of Physics — $99,806**
**La Jolla, CA 92093 — 01-B**
**90-3**

**Traveling-Wave Convection in Fluid Mixtures**
***C.M. Surko***

While some progress has been achieved recently in the understanding of the dynamics of free convection occurring in single component fluids, much less is known about the phenomenology of convection in fluid mixtures. Yet in realistic situations it is the latter that play the important role. Examples of interest to engineering include stability of double-diffusive systems, e.g. solar ponds, solidification of metal alloy casts, convection in fuel droplets, and so on.

The proposed research addresses the interaction of traveling waves with convective motion in a binary fluid mixture. Preliminary results show that in a relatively simple experiment the behavior of the system is such that on varying one or two control parameters the whole gamut of states ranging from a laminar traveling-wave state to well developed turbulence can be traversed. Specifically the experimental setup consists of an annular channel with a large radius. In it a water-ethanol mixture is heated from below giving rise to free convection. However, under certain conditions, in addition to this expected phenomenon, there occur traveling-waves interacting in complicated ways with the patterns driven by natural convection. The resulting oscillatory convection seems to be prototypical of similar phenomena arising in many contexts, ranging from oceanic motion to instabilities in liquid crystals.

The proposed research will address three related topics: 1) weakly nonlinear traveling waves in one dimension; 2) nonlinear pulses in an annulus; and 3) measurement of concentration field.

## University Of California, Santa Barbara

**Department of Physics** **$121,000**
**Santa Barbara, CA 93106** **06-C**
**90-3**

**Bifurcations and Patterns in Nonlinear Systems**

***G. Ahlers, D.S. 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, Santa Barbara

**Department of Chemical and Nuclear Engineering** **$92,806**
**Santa Barbara, CA 93106** **01-C**
**88-3**

**Turbulent Structure in Liquid Streams Bounded by a Free Surface and a Solid Wall**
***S. Banerjee, G. Hetsroni***

This project is aimed at studying basic turbulence structure in a liquid which flows in a horizontal flume. The experimental techniques used in this study include a three-dimensional Laser-Doppler velocimeter, with a 50m measuring volume; and an oxygen bubble tracing technique with high speed videos and flash photography.

The oxygen bubble technique resulted in capturing of the detailed turbulence production at the solid wall and at the liquid-air interface. The details of the high speed-low speed velocity streaks at the wall, the coherent structures near the wall, and the turbulent bursts were visualized and measured. It was found that the turbulent coherent structures reach the interface and are visualized there as patches. These patches then have a profound effect on the heat and mass transfer at the interface.

High speed and low speed velocity streaks were also observed at the liquid-gas interface, when shear was applied on the liquid by the gas flowing cocurrent or countercurrent to the liquid. The coherent structures from the interface were then observed to be ejected downwards.

Waves, which were generated by a wave generating machine, were observed to have a profound effect on the frequency of ejections of the coherent structures at the wall. The effects of the wave amplitude and wave length on the frequency and strength of the turbulent bursts are now being analyzed.

These experiments were complemented by numerical computations. The full Navier-Stokes equations were solved by a pseudospectral method to provide quantities which are difficult to obtain by flow visualization and single-point velocity measurements. The numerical computations were shown to capture the basic physics which is associated with the turbulence generation due to shear.

The three-dimensional Laser-Doppler velocimeter was assembled, and the hardware and software were readied for the measurements. The measurements with the LDV will be complemented by visualization by means of the oxygen bubbles and high speed video.

## Carnegie Mellon University

**Chemical Engineering Department** **$146,786**
**& Graduate School of Industrial Administration** **03-A**
**Pittsburgh, PA 15213** **89-4**

**Integration of Redesign Methodologies for Chemical Processes**
***L.T. Biegler, I.E. Grossmann, G.L. Thompson, A.W. 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 processes 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) <u>Development of Efficient Optimization Algorithms for Discrete and Continuous Variables</u>. Efficient decomposition strategies for nonlinear programming have been developed for large-scale process optimization. These are currently being tailored to various problem types. G. Thompson has also been working on the solution of several large scale combinatorial optimization problems that frequently occur in chemical engineering applications, namely, travelling salesman, and set covering (and partitioning) problems. He has been

implementing previously devised algorithms on various sequential and parallel computers such as the CRAY YMP and the Butterfly.

2) Redesign of Multicomponent Separation Sequences. Short-cut analysis methods have been developed for complex columns configurations. For redesign, a two step approach first assesses the capability of existing equipment to accomplish all or part of the alternative separation tasks. Second a superstructure embedding these alternatives within existing and new equipment is created which allows for traditional, parallel and serial sequences to be discovered which will minimize annualized cost. These strategies are being tackled with a scenario approach as well as with mixed-integer nonlinear programming (MINLP).

3) Redesign of Energy Management Ssystems. New *mixed-integer nonlinear programming* (MINLP) models have been developed for both the 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. In addition the case of multistream exchangers has been considered.

4) Redesign for Flexibility, Controllability and Reliability. New measures are being developed that can integrate these different operability characteristics. A stochastic framework is being used to integrate flexibility and reliability. In addition,we are also focussing on the development of optimization-based control methods for constrained, nonlinear processes.

## Carnegie Mellon University

**Department of Electrical and Computer Engineering** **$94,814**
**Pittsburgh, PA 15213** **03-C**
**89-3**

**Research on a Reconfigurable Modular Manipulator System**
***P.K. 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

**Department of Chemistry** **$156,707**
**Chicago, IL 60637** **06-C**
**89-3**

**Topics in Finite-Time Thermodynamics**
***R.S. Berry***

The objective of this research is the analysis in thermodynamic terms of the performance of systems and processes subject to time or rate constraints. Part of the research deals with developing methods for conducting analyses, such as emerged from the introduction of a suitable metric in the space of thermodynamic variables and the evaluation of path lengths with that metric. The lengths so obtained have been shown to be directly related to the dissipation associated with the path. Another piece of recent work at this basic level just completed under this project is an attempt to introduce a variational formulation of irreversible heat transfer and diffusion, which is intended to apply in nonlinear as well as linear situations.

The other aspect of this research is the application of the general methods to the analysis of specific systems of current interest. During the initial period of the project, the stopping of a beam of atoms by absorption and remission of laser light was analyzed and the entropy changes in the process were evaluated. The reduction in entropy of the atomic beam due to cooling and stopping is compensated a thousandfold over by the increases in the entropy of the light due to randomization of the phase, the polarization and especially the propagation direction.

## University Of Chicago

**The Enrico Fermi Institute** **$141,750**
**Chicago, IL 60637** **06-C**
**90-3**

**Fundamentals and Techniques of Nonimaging Optics for Solar Energy Concentration**
***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 might 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.

## Clarkson University

**Dept of Chemical Engineering** **$56,816**
**Potsdam, NY 13676** **01-C**
**88-3**

**Droplet Motion in Numerically Simulated Turbulence**
***J.B. McLaughlin***

The primary goal of the research is to obtain information about the dispersion of aerosol size droplets and particles in a turbulent channel flow. It is assumed that the flow is vertical so that aerosols do not sediment onto the channel walls. The behavior of aerosols in the viscous wall region is of particular interest since it has been suggested that shear induced lift forces may be very significant in this region. The approach - involves numerical integration of the aerosol particle equation of motion to obtain the trajectories of the droplets or particles. In order to perform such calculations, the undisturbed (by the particles) velocity field of the fluid is needed and this is supplied by a direct numerical solution of the Navier-Stokes equation using pseudospectral methods. The fluid velocity is used to evaluate the Stokes drag force and the Saffman lift force in the aerosol particle equation of motion. By comparing runs in which the lift force is dropped with runs in which it is retained, one can obtain information about the importance of shear-induced lift on aerosol motion.

## University Of Connecticut

**Dept of Mechanical Engineering** **$47,804**
**Storrs, CT 06268** **01-A**
**88-3**

**Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding**
***E.H. Jordan***

The goal of this research is the development and verification of a model of the time and history dependent viscoplastic deformation behavior of polycrystalline metals. Single grain behavior has been derived by summing postulated slip behavior on crystallographic slip systems. Multi grain behavior will be obtained by summing deformation occurring in different grains while accounting for grain interaction through a self consistent micromechanics approach. The model will also represent grain boundary sliding through the use of a solution recently published by T. Mura.

High temperature experiments on Hastelloy-X will be used to verify the model. Single crystal properties used for input to the model are currently being determined. Using these properties the behavior of polycrystal Hastelloy-X will be predicted and then compared with polycrystalline experiments recently completed. Prediction of these tests constitute a critical test for the theory.

The model will not only predict the viscoplastic response of polycrystals but also will allow metallurgical findings usually stated in crystallographic terms to be more directly incorporated into the model. The explicit calculation of grain boundary sliding will help illuminate the role played by grain boundary sliding in the overall deformation during complex load histories. Grain boundary sliding deformation plays an important role in material damage and the model should be useful in life prediction under complex variable temperature conditions.

At present, the single crystal model is available and the self consistent model without grain boundary sliding has been derived and is being programmed.

This work is being done with the cooperation of Engineering Science Software, Inc. working under a related contract. Single crystal specimens have been provided by Pratt and Whitney, Inc.

## Cornell University

**Sibley School of Mechanical and Aerospace Engineering** **$97,952**
**01-C**
**Ithaca, NY 14853** **88-3**

**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 shearless "second order" mixing layer. Here various turbulence generating grids are designed so that large turbulent eddies on one side of the flow mix and diffuse with smaller eddies on the other side of the flow. The porosity of the grid is such that the mean flow remains constant across the grid and hence there is no mean velocity shear or turbulence production. Thus, the spreading rate in the mixing region is determined solely by turbulence-turbulence interactions. This flow, although in some respects more fundamental than the turbulence mixing layer with shear, is poorly understood. The flow is unusual in that it is homogeneous in the mean but has large scale intermittence and the turbulence is inhomogeneous. Scalar dispersion from the thin thermal line source placed in the center of the flow is also being studied.

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.

The negative buoyancy causes the heat flux to decay (and in some cases reverse sign) and there is a complex interaction between the various components of turbulent kinetic energy and the potential energy. 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** **$110,461**
**Hanover, NH 03755** **01-C**
**88-3**

**Two Phase Potential Flow**
***G.B. 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 Geurst'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

**Mechanical Engineering and** **$65,000**
**Materials Science Department** **01-C**
**Durham, NC 27706** **90-3**

**Analytical and Experimental Study of Instabilities in Buoyancy-Driven Convection in Porous Media**
***J.G. 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: (i) porous media saturated with pure fluids, and (ii) 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.

## Engineering Science Software, Inc.

**Smithfield, RI 02917** **$46,048**
**01-A**
**A Micromehanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding** **88-3**
***K.P. Walker***

The aim of the project is to develop a viscoplastic constitutive model, with accompanying FORTRAN software, to model the deformation behavior of polycrystalline metals comprised of an aggregate of fcc single crystal grains whose crystallographic axes are oriented at random. The single crystal grains are assumed to be spherical and are modeled with an anisotropic viscoplastic theory based on crystallographic slip along the octahedral and cube slip directions of the fcc metal. The overall response of the polycrystalline aggregate is assumed to be isotropic and is deduced from the single crystal response by means of a self-consistent method. The effect of grain boundary sliding between the grains is being modeled in the self-consistent formulation to assess the importance of including this mechanism in the overall response of the polycrystalline material.

Experimental tests on single crystal specimens of the superalloy Hastelloy-X are being run at the University of Connecticut to determine the material constants in the single crystal constitutive model. The overall response of the self-consistent model of the polycrystalline aggregate will then be theoretically determined and compared with experimental results from isotropic specimens of polycrystalline Hastelloy-X.

The FORTRAN software will allow metallurgical and micromechanical work reported in the literature to be easily embedded in a constitutive (stress-strain) framework for analyzing the overall deformation response of polycrystalline metal aggregates under thermomechanical loading conditions.

## University Of Houston

**Dept of Mechanical Engineering** **$122,163**
**Houston, TX 77204-4792** **01-C**
**88-3**
**Comparative Study of the Vorticity Field in Turbulent Flows: Theory, Experiments, Computations**
***A.K.M. Hussain***

This is a unified research effort involving experimental, numerical and theoretical works to address the basic mechanisms of turbulence phenomena in shear flows via studies of its vorticity field. Experiments are being performed in jets and wakes to educe the coherent structures on the basis of the instantaneous vorticity maps obtained by one or multiple rakes of X-wires. Through an eduction algorithm developed by us, vorticity patches are aligned through cross-correlation and ensemble averaged: whatever survives the ensemble average is the 'coherent structure' (CS) and the remainder of each realization is 'incoherent turbulence'. Using coherent vorticity, production and Reynolds stress we discuss the topology and dynamics of CS in turbulent flows, in particular in elliptic jets and cylinder wakes. The same algorithm is applied to direct numerical simulations of turbulent flows and using spectral methods and the results are compared with experimental data. The simulation results provide spatial details of helicity, enstrophy and dissipative fields.

As an integral part of this project, we are also studying vortex dynamics using experimental, numerical and theoretical approaches. We have focussed particularly on vortex reconnection mechanisms. Experimental studies involve flow visualization and hot-wire measurements. Numerical studies of two anti-parallel vortex tubes have revealed three distinct stages of vortex reconnection: core deformation, bridging and threading. Their implications in turbulent flows are being explored. A second, high-resolution simulation has utilized symmetry to address higher Reynolds number as well as compressible vortex reconnection. A third study has considered collision of vortex rings. In these we have explored the mechanisms of enstrophy cascade, and helicity and dissipation fields. We have also started theoretical studies of how a blob of fluid in a rotational flow produces helicity outside it and how helicity fluctuations at a turbulent-nonturbulent interface affect entrainment. Another theoretical-numerical study has been begun on vortex chaos and thermodynamics of vortices.

Further studies will involve vorticity and helicity fields in laboratory flows with a 9-wire probe in conjunction with rakes of X-wires, and comparison with direct numerical simulation. We will also continue the studies of vortex reconnection, effects of compressibility on reconnection, and relation of helicity and vortex dynamics to turbulence.

## University of Houston

**Department of Mechanical Engineering $0**
**Houston, TX 77204-4792 01-B**
**90-1**

**High Flux Film and Transition Boiling**
***L.C. Witte***

The potential for altering the boiling curve through the effects of high subcooling and high velocity is being investigated. Liquid flowing upward in crossflow over 0.635-cm electric heaters is the configuration that is currently being used. As a part of the study, azimuthal temperature variations around the heater during nucleate and film boiling have been measured, the manner of onset of film boiling and vapor film collapse has been observed and photographed, and the effects of subcooling and velocity on $q_{min}$ and $q_{max}$ have been determined.

Experiments have been conducted at subcooling levels up to 58 C and at velocities up to 381 m/sec for Freon-113, and 95 C and 2.98 m/sec for water. With both, the $q_{min}$ to $q_{max}$ ratio was seen to be a stronger function of subcooling than velocity. Previous investigators have reported that the $q_{min}$ to $q_{max}$ ratio for Freon-113 increases from 0.083 for pool boiling to 0.303 for 6.8 m/sec at low subcooling levels. In Freon-113 experiments at 57 C subcooling and 3.53 m/sec, the ratio was found to be 0.77.

Discontinuities in measured wall temperatures were observed when the vapor film collapsed over certain portions of the heater prior to the entire heater being enveloped in nucleate boiling. These discontinuities are caused by film and nucleate boiling coexisting in near proximity of the location of thermocouples used to measure local heater temperatures.

It was also observed that the bottom of the heater underwent an unexpected temperature drop during nucleate boiling for high levels of subcooling. Such temperature drops were very repeatable. They resembled the "temperature overshoot" phenomena that have been observed in pool boiling experiments on a variety of heating surface and configurations. However, no observable significant increase in nucleation that is generally considered to be responsible for such behavior was found in our experiments.

An analysis of film boiling for constant wall flux conditions for the cylindrical heater yielded results that are consistent with experimental data. This analysis, based on a mass-energy balance, also predicts the point at which collapse of the vapor film occurs during transition boiling reasonably well.

## Idaho National Engineering Laboratory

**Biotechnology and Geosciences $100,087**
**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 Laboratory

**Applied Optics** $182,137
**Idaho Falls, ID 83415** 06-A
90-3

**In-Flight Measurement of the Temperature of Small, High Velocity Particles**
***J.R. Fincke***

Knowledge of in-flight particle parameters is fundamental to understanding particle/plasma interactions in the physical and/or chemical processing of fine powders. A measurement technique for simultaneously obtaining particle size, velocity and temperature has been developed. Particle size and velocity are obtained from a dual color combination laser Doppler velocimeter (LDV) and laser particle sizing system. The LDV system consists of a crossed beam technique while particle size is determined from the absolute magnitude of scattered laser light. The particle temperature is determined by a two color pyrometer technique. The spatial resolution is better than $1mm^3$ and allows the distribution of particle size, velocity and temperature to be mapped over laboratory scale flow fields. The influence of particle size, injection rate, torch power, etc., are currently being examined in typical flow fields.

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

## Idaho National Engineering Laboratory

**Materials Technology Group** $385,706
**Idaho Falls, ID 83415-2218** 01-A
90-3

**Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws**
***W.G. Reuter, W.R.Lloyd, J.S. 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.

## Idaho National Engineering Laboratory

**Energy and Systems Technology Group $0**
**Idaho Falls, ID 83415 06-A**
**90-3**

**Modeling of Thermal Plasma Processes**
***J.D. Ramshaw, C.H. 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 interaction between the plasma and a particulate phase. This research is directed toward the development of a comprehensive computational model of thermal plasma processes and plasma-particle interactions 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. LAVA uses a rectangular mesh with an excluded volume function to represent geometrical obstructions and volume displaced by particles. Simple highly vectorizable numerics are utilized, with rapid steady state and low-speed flow options. The plasma is represented as a multicomponent fluid governed by the transient compressible Navier-Stokes equations. Real gas physics is allowed for by temperature-dependent specific heats and transport properties. Multicomponent diffusion is calculated in a self-consistent effective binary diffusion approximation, including ambipolar diffusion of charged species. Both k-epsilon and subgrid-scale turbulence models are included. Dissociation, ionization, and plasma chemistry are represented by means of general kinetic and equilibrium chemistry routines. Discrete particles interacting with the plasma will be represented by a stochastic particle model similar to that previously used to model liquid sprays. This model allows for spectra of particle sizes, shapes, temperatures, etc., thereby capturing the important statistical aspects of the problem. It will include sub-models for the various plasma-particle and particle-particle interaction processes, including melting, evaporation, condensation, nucleation, agglomeration, and coalescence.

## Idaho National Engineering Laboratory

**Materials Technology Group $568,805**
**Idaho Falls, ID 83415-2210 06-A**
**90-3**

**Plasma-Particle Interactions**
***C.B. Shaw, Jr., T.L. Eddy, S.C. Snyder, L.D. Reynolds***

Plasma processing of materials saves energy and strategic materials, compared to other methods. The high temperatures and temperature gradients unique to plasmas make possible the synthesis or destruction of compounds not achievable by other means. However, for American industry to put this plasma technology to practical use, and thereby improve its competitive position in world markets, it is necessary to minimize the expensive trial and error scale-up from laboratory demonstration through pilot plant experimentation to full production. This goal requires creation of a rational basis for plasma torch design and operation, namely, a set of computer models (being developed at the INEL and at MIT) which have been fully validated by comparison of their predictions with experimental results of diagnostic measurements. The role of this task is to develop the necessary diagnostic methods, make the test results available to the modelers, and jointly determine what further features are needed in both the models and the diagnostics.

While a half dozen diagnostic methods have been developed and tested in this task, in FY 1990 attention centered on (1) a suite of emission spectroscopy measurements, interpreted by the generalized multi-temperature equilibrium model, to determine the significance of departure of thermal plasmas from the commonly assumed local thermal equilibrium; and (2) high resolution absolute intensity measurement of Doppler broadened and Doppler shifted laser radiation Rayleigh scattered by the atoms and ions of the plasma. The latter permits simultaneous determination of the true kinetic temperature, local mean flow velocity, and density of the scatterers.

## Idaho National Engineering Laboratory

**Materials Technology Group** **$480,000**
**Idaho Falls, ID 83415** **03-A**
**90-3**

**Intelligent Control of Thermal Processes**
***H.B. Smartt, J.A. 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 Massachusetts Institute of Technology.

## Idaho National Engineering Laboratory

**Nondestructive Materials Characterization Group** **$177,371**
**Idaho Falls, ID 83415-2209** **03-B**
**90-3**

**NonDestructive Evaluation of Superconductors**
***K. L. 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. In FY89 this project began identifying techniques that can determine critical superconducting properties on a local scale. This has resulted in the use of AC induced currents in conjunction with DC transport currents to determine critical currents and dissipation locally. The analysis of these measurements is being carried out with the aid of the London and "Critical State" models for supercurrent flow in these materials. These results are being correlated with material microstructure information and other measurement techniques.

## University Of Illinois

**Coordinated Science Laboratory** **$117,612**
**Urbana, IL 61801** **03-A**
**88-3**

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

This research program aims at a comprehensive study of some fundamental issues that arise in the modeling, control and coordination of deterministic and stochastic large scale systems. The research plan during the first phase has been to extend the relevant existing theories and methodologies in novel directions, covering areas such as (i) model simplification through decomposition and aggregation, (ii) temporal and spatial hierarchies, (iii) goal-orientedhierarchies and multiple decision layers, and (iv) control and coordination of large scale systems based on (probabilistic) multimodeling.

Some of the specific mathematical models that are being used in this context are Markov chains, stochastic teams, and deterministic and stochastic teams, and dynamic games, each one under a number of different information patterns. Following this first phase, research is being directed towards developing a new framework, to allow for distributed and interactive model building and control, where both structural and decision making hierarchies evolve over time. A unique characteristic of this approach is that the two independent tasks - modeling and control - treated heretofore independently, will now be designed to evolve in parallel and complementarily to each other.

## University Of Illinois

**Dept of Chemical Engineering** **$104,170**
**Urbana, IL 61801** **01-C**
**89-3**

**Gas-Liquid Flow in Pipelines**
***T.J. Hanratty***

Research is being conducted to obtain a better understanding of gas-liquid flow in horizontal and vertical pipelines. The goals are (1) to model slug flow and to predict when slugging will exist in horizontal gas-liquid flows, (2) to obtain improved predictive methods for horizontal and vertical annular flows, and (3) to develop models for the dispersion and deposition of drops and particles in a turbulent flow. Vertical flow 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 specifically designed platform whose angle can be controlled to within 0.01 degree. Droplet motion in turbulent flows is studied in a vertical 2 in. pipeline and in a supercomputer simulation for turbulent flow in a channel. A specifically designed facility that creates stationary slugs in a pipeline is also available.

Considerable progress has been made in developing a new mathematical framework for describing particle motion in horizontal turbulent fields, where gravitational settling can be important. This is being applied to understand droplet distribution in gas-liquid annular flows and sediment transport. A Lagrangian framework is used. The central problem, then becomes the description of the behavior of drops or particles originating from a source on the wall. To aid in modelling gas-liquid annular flows, optical techniques are being used to study droplet configurations and drop size.

A central problem in understanding the behavior of particles in a turbulent fluid is the prediction of the effect of flow inhomogeneities. This is being studied both in computer and laboratory experiments. Of particular interest are the discovery of a mechanism by which particles are trapped at the wall and of a relation of particle impaction on a wall to eddy structure.

In previous work necessary conditions for the existence of slugs were developed that viewed the front of a slug as a hydraulic jump and the tail as a Benjamin bubble. These are now being tested in special experiments which create stationary slugs in a downward inclined pipeline.

A comprehensive study of droplet distributions for gas-liquid annular flow in a 4 inch pipeline was completed. These gave the unanticipated result that a secondary flow can be initiated in the gas flow because of the presence of drops.

## University Of Illinois At Chicago

**Energy Resources Center** **$70,144**
**Chicago, IL 60680** **01-B**
**89-2**

**Heat Transfer to Aqueous Polymer Solutions**
***J.P. Hartnett***

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

a) Pool boiling behavior of aqueous solutions of several high molecular weight polymers, including hydroxyethyl cellulose, carboxymethyl cullulose (CMC) and polyacrylamide and a comparison with pool boiling performance of deionized water.

b) Forced convection behavior of viscoelastic fluids in laminar flow through rectangular channels.

To date the following results have been found:

a) High concentrations of the aqueous hydroxyethyl cellulose solutions yield higher values of the boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature difference. In contrast, aqueous polyacrylamide solutions yield lower values of boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature. A new series of measurements with another cellulose (CMC) is underway to determine if this family of polymers has special boiling properties. Detailed rheological properties are being measured to provide some insight into the boiling behavior.

b) The forced convection heat transfer performance of viscoelastic fluids in laminar flow through rectangular channels is considerably higher than predicted for purely viscous fluids, although the measured friction factor is in good agreement with the value predicted by the purely viscous analysis. Measurements of the dynamic properties including phase shift under oscillatory condition are shown to be related to observed heat transfer behavior.

## Jet Propulsion Laboratory

**California Institute of Technology** **$105,000**
**Pasadena, CA 91109** **03-C**
**89-3**

**Neural Learning Formalisms for Global Manipulator Redundancy Resolution Problems in Unstructured Environments**
***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** **$67,004**
**Baltimore, MD 21218** **01-C**
**89-3**

**Numerical and Physical Modeling of Bubbly Flow Phenomena**
***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 footing by comparing their results with those of direct numerical multi-particle simulations and rigorously-derived averaged equations.

Ensemble-averaged equations for the propagation of pressure waves in bubbly liquids have been derived correct to second order in the gas volume fraction. A new insight into the structure of the expansion and the role of bubble-bubble interaction and surface deformations is obtained from the work.

In a second study, by arranging *N* bubbles at random in a cubic cell and filling up the entire space with copies of this cell, the behavior of an infinite bubbly liquid has been simulated. For this situation two alternative definitions of added mass have been explored and the average viscous dissipation in the limit of large Reynolds number has been studied.

In another study, the propagation of pressure waves in a layer of bubbles has been considered. The novel feature of this work is the fact that the volume fraction is arbitrary and the wavelength can be comparable to the inter-bubble distance.

The last problem involves the flow of a "plug" of bubbly liquid in a conduit. For the time being the bubbles are arranged on the axis of the conduit, but will later be placed at random.

## Robert H. Kraichnan, Inc.

**303 Potrillo Drive** **$59,341**
**Los Alamos, NM 87544** **01-C**
**90-3**

**Turbulence Theory and Reduced Hydrodynamic Description**
***R.H. 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 two recent approaches to economical and meaningful description of turbulence. One is a systematic scheme for reducing the number of degrees of freedom ("decimation"). The other, developed only during the past year, is a method for distorting velocity fields with simple statistics into self-consistently determined approximations of actual turbulent velocity fields ("mapping closure"). Unlike traditional analytical methods for turbulence, mapping closure yields full probability distributions of velocity fields and contaminants carried by the turbulence. In particular, it can give meaningful estimates of the likelihood of extreme events. Currently, the application of mapping closure to the transport of passive contaminants by three-dimensional random velocity fields is being investigated. Previous work has shown the success of the method for predicting the probability distribution of velocity in Burgers' model of turbulence.

## Lawrence Berkeley Laboratory

**Accelerator & Fusion Res Div** **$123,250**
**University of California** **06-C**
**Berkeley, CA 94720** **90-3**

**Studies in Nonlinear Dynamics**
***A.N. Kaufman, R.G. 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.

## Lawrence Berkeley Laboratory

**Applied Science Division** **$194,242**
**University of California** **06-B**
**Berkeley, CA 94720** **87-3**

**Controlled Combustion**
***A.K. Oppenheim***

The principal objective of this project is to provide a fundamental background for the development of controlled combustion systems. Of particular interest in this respect are essential improvements of combustors for prime movers so that they will provide service not only as power sources, to which they are solely relegated today, but also as modern high-tech chemical reactors, where process instabilities and pollutant formation are adequately controlled by a micro-processor system. For automobile engines this offers the prospect of efficient and clean operation associated with relatively low exhaust temperature, devoid of the problems of knock and cycle-to-cycle variation and meeting practically all air pollutant emission requirements. The major technological constraints imposed upon the automotive industry, the octane number and the catalytic converter, could be therefore eliminated. Means to accomplish this task involve the utilization of a pulsed jet combustion system combined with prompt product recirculation, according to concepts developed on this project. Major laboratory apparatus for our studies consists of a cylindrical vessel with unobstructed optical insight, and a shock tube providing about 20 msec of test time at an elevated pressure (up to 50 atms) and high temperature (around 1000K), commensurate with conditions existing during combustion in engines. Its use is associated with laser-powered optical instruments, including in particular apparatus for megacycle-frequency schlieren cinematography and laser induced fluorescence imagery. In addition to experimental work, included in the program are numerical modeling studies of the fluid mechanic, thermodynamic, and chemico-kinetic phenomena influencing the processes of ignition and combustion in engines.

## Lovelace Medical Foundation

**Bioengineering Research** **$49,024**
**Albuquerque, NM 87108** **03-B**
**89-3**

**Two-Phase Flow Measurements by NMR**
***E. Fukushima***

We will use nuclear magnetic resonance (NMR) to study two-phase flows in model systems. Lovelace Medical Foundation (LMF) will carry out the experiments while Sandia National Laboratories (SNL) will provide the theoretical models of multiphase flows as well as help in running the labor-intensive NMR experiments. We will study steadily flowing nondilute solid suspensions by NMR to obtain the spatial distributions of the phases as well as the velocity distributions of each phase. Such determinations work best under moderately high concentrations of both phases, a case that is difficult for light and ultrasound scattering. Our exploratory studies for the coming year will include the following: f) Flow studies of suspensions (heavy particles in a Newtonian oil) in horizontal tubes to determine the dependence of flow properties on particle diameter, particle diameter to tube diameter ratio, mean particle concentration, particle shape and surface roughness, mean flow rate, and relative phase densities; 2) Measurement of the velocity and spatial distribution of a water/oil mixture in the annular region between counter-rotating, eccentrically-nested cylinders; and 3) Measurement of the simultaneous, time-averaged, axial velocity profiles for two immiscible liquids such as oil and water flowing in a horizontal tube.

## University Of Maryland

**Dept of Mechanical Engineering** **$49,999**
**College Park, MD 20742** **01-C**
**90-3**

**The Use of Stereo Optical Flow Fields in the Determination of Three-Dimensional Motion and Stereo Correspondence**
***J.H. 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** **$78,600**
**College Park, MD 20742** **06-C**
**88-4**

**Study of Magnetostatic Problems in Nonlinear Media with Hysteresis**
***I.C. 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: development of new generalized Preisach models of scalar hysteresis, study of new Preisach models of vector hysteresis, software implementation of the Preisach hysteresis models, extensive experimental testing and verification of hysteresis models, development of new techniques for the calculation of magnetic fields and eddy currents in media with hysteresis, application of Preisach type models to the description of superconducting hysteresis and evaluation of hysteretic losses in hard superconductors. It is hoped that, as a result of the ongoing research, the foundations of comprehensive theory of mathematical models of hysteresis will be established.

## University Of Maryland

**Electrical Engineering Department** **$76,091**
**Baltimore, MD 21228** **03-B**
**89-3**

### Pulse Propagation in Inhomogeneous Optical Fibers

*C. Menyuk*

Many systems, such as computers, sensors for intelligent machines, and high resolution graphics require ever increasing channel capacity to transfer information from one part of the system to another. Recent developments have shown that fiber optics offer a suitable medium to accommodate the growing need for large data rates. At present it is not clear how those rates are limited by the inevitable imperfections in the fibers. This is of particular concern to energy systems using this transmission medium because the presence of radiation and of other effects which may affect the integrity of essential communication links in those systems.

This research will study the effects of slowly varying inhomogeneities and localized imperfections in the fibers on their transmission properties.

Three topics are of particular interest:

1. Behavior near the zero dispersion point. This point denotes the frequency at which the wave propagation speed is independent of the wavelength - a point preferred for operating at the highest possible data rates because of the lowest power needs. The actual zero dispersion point depends on the material properties as well as on the geometry of the fiber. Small random variations in those properties along the length of the fiber will have a destructive effect on the integrity of the signal propagated by the fiber. At present it is not known how much of a limiting factor that is for a given statistical distribution of the slowly varying inhomogeneities.

2. Effects of a varying birefringence. As the material properties in the fiber change from point to point so does the fiber's response to the polarization of the electromagnetic wave. Under certain conditions that polarization may be changed enough by mixing to affect the properties of the transmitted signal. Again, while something is known about the effects of a single polarization mixing event on a pulse in the fiber, nothing is known about the effects of many such events and how they can be related to the properties of the fiber.

3. Bubbles and inclusions in optical fibers. Because such imperfections often focus the incident electromagnetic beam they are known to cause damage to the fiber itself. Previous studies have not taken into account the so-called ponderomotive forces, that is body forces arising from the interactions of the gradients in the properties of the fiber material with the incident electromagnetic fields.

This research will address the three topics enumerated above, first in the linear regime and then in the non-linear regime. While this effort is primarily theoretical, it will benefit from a close ties to related experimental work at Bell Labs, at NRL and at FDA.

## University Of Maryland

**Dept of Mechanical Engineering** **$64,244**
**and Systems Research Center** **03-C**
**College Park, MD 20742** **88-3**

### The Creation of Multi-Degree-of-Freedom Mechanisms for Robotic Applications

*L. Tsai*

This research is concerned with one of the most difficult stages of mechanical design, namely the conceptual synthesis of mechanisms. The objective is to develop a systematic methodology for the creation of multi-DOF (Degree-of-Freedom) gear trains for robotic mechanisms.

The concept of transmission lines has been introduced. Applying the concept, a new methodology for topological synthesis of articulated gear mechanisms has been established. All admissible structural matrices of three-DOF gear-coupled robotic mechanisms have developed.

Gear backlash introduces discontinuity, position uncertainty, and impact in mechanical systems which, in turn, makes control of a robot difficult. Backlash is a persistent problem due to natural clearances provided for prevention of mechanical interference. Traditionally, precision gears, spring-loaded split-gear assemblies, and precise mechanical adjustments have been used to overcome these difficulties. However, these techniques do not completely eliminate backlash and can further increase the cost of manufacturing.

In this study, a new and innovative concept for the control of backlash will be investigated. The concept utilizes redundant unidirectional drives to assure positive coupling of gear meshes at all times and, therefore, eliminates the backlash problem completely.

A methodology for systematic enumeration of RBR (Redundant-drive Backlash-free Robot) arms has been established and an atlas of admissible kinematic structures of two-and three-DOF, RBR arms has been developed. In order to establish a proof-of-concept, a planar two-DOF RBR arm has been constructed, and a controller based on computed torque technique has been designed. It is our plan to do a comparison study of the arm with and without redundant drives. This experiment will be a precursor to the investigation of advanced adaptive control strategies for redundant-drive backlash-free robotic arms.


## University Of Maryland

**Dept of Mechanical Engineering** **$122,163**
**College Park, MD 20742** **01-C**
**87-3**


### Comparative Study of the Vorticity Field in Turbulent Flows: Theory, Experiment, Computations


***J.M. Wallace***


This is a collaborative project with the City College of New York and the University of Houston. Fundamental studies of the vorticity field in a number of standard sheared and unsheared turbulent flows are being carried out. The research involves theoretical, computational and experimental investigations.

Theoretically, a mathematical derivation of a definition of 3-dimensional coherent structures superimposed on chaotic motion is being developed with an algorithm to educt these structures. The topological complexity of the vorticity field and its relation to the basic processes of spectral energy transfer, vorticity generation and intermittency will be mathematically described in physical space.

Numerically a full Navier-Stokes simulation code of the turbulent round jet as well as a high resolution code for box turbulence with periodic boundary conditions is being developed. With these codes the coherent structures definitions described above will be applied and a detailed study of energy transfer and helicity fluxes will be conducted.

Experimentally, the University of Maryland Turbulence Research Laboratory nine-sensor hot-wire probe for simultaneously measuring the instantaneous velocity and vorticity vector fields in turbulent flows has been further developed. Point measurements have been made in a turbulent grid, mixing layer, and boundary layer flows in order to obtain properties of the vorticity and helicity fields. Collaborative experiments on turbulent jets and wakes will soon be carried out at the University of Houston.

The results so far show that there is a higher probability for the velocity and vorticity vectors to align within the logarithmic region of the boundary layer and within the mixing layer than there would be for two uncorrelated vector fields. In the buffer layer of the boundary layer and in the grid flow there is virtually no increased probability for these vectors to align. These experimental results have important implications for the prospects of the much disputed conjecture that turbulence can be modelled as a Euler flow containing isolated dissipative regions.

## University Of Massachusetts

**Chemical Engineering Department** **$ 52,085**
**Amherst, MA 01003-0011** **06-A**
**88-3**

**Design and Synthesis of Reactive Separation Systems**
*M.F. Doherty*

The design and synthesis of chemical process flowsheets usually begins by breaking the problem down into three main sub-tasks. These are: synthesis of the reactor system, synthesis of the separation system and the development of an energy management system (i.e. heat integration). Although these tasks are not independent of each other, such a decomposition has the advantage of making a very difficult problem more manageable. The second stage of such a procedure then corrects for mismatches between the sub-tasks. The above view of flowsheet synthesis can be radically altered when the reactions occur in the liquid phase. In such circumstances, it is often possible to combine the reaction and separation tasks by using reactive separators. Fundamental studies on the phase behavior, design and synthesis of this class of problems are proposed. It is expected that this will lead to a systematic technique for inventing improved technology and that this will be of lasting value to the profession.

## University Of Massachusetts

**Chemical Engineering Department** **$111,746**
**Goessmann Laboratory** **03-A**
**Amherst, MA 01003-0011** **87-3**

**Screening Alternative Control Structures for Plant Control System**
*J.M. Douglas, M.F. 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

**Chemical Engineering Department** **$ 75,760**
**Goessmann Laboratory** **06-C**
**Amherst, MA 01003-0011** **88-3**

### Mixing of Viscous Fluids: Behavior of Microstructures and Chaos

***J.M. Ottino***

In spite of its universality and practical implications, the understanding of the fundamentals of mixing remains rather incomplete. This work focuses on basic experimental and computational studies along two main themes with the objective of establishing a framework capable of addressing mixing problems encountered in nature and technology: (1) investigations of chaotic mixing of single fluids in deterministic two- and three-dimensional flows, and (2) dynamics of microstructures in such flows (e.g., stretching, breakup, coagulation, etc.). Work in area (1) is underway and a clear picture is emerging. Experimental work is planned to address the problems listed under area (2). However, most of the results to-date are due to simulation which focused on coagulation of point particles in chaotic flows. The particles are convected without diffusion and allowed to coagulate with probability one when their mutual distance is less than their diameters. The most significant finding is that under "well mixed" conditions the system behaves as if the particles were moved by Brownian motion and a simple kinetic model describes the main results. The poorly mixed case is considerably more complex. In this case spatial inhomogeneities result from competition between the rate of coagulation and mixing, and trapping and leaking of clusters due to KAM surfaces.

## Massachusetts Institute Of Technology

**The Energy Laboratory** **$124,057**
**Cambridge, MA 02139** **03-B**
**91-3**

### Metal Transfer in Gas Metal Arc Welding

***T.W. Eagar, J. H. Lang***

The present research is part of a cooperative program among faculty at MIT and staff at Idaho National Engineering Laboratory to develop sensing and control methods which can be used to automate the gas metal arc welding processes.

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

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

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

## Massachusetts Institute Of Technology

**Department of Materials Science and Engineering** **$123,110**
**Cambridge, MA 02139** **06-A**
**91-1**

**High Temperature Gas-Particle Reactions**
***J.F. Elliot, P.P. Bolsaitis***

The purpose of the research is to examine the physico-chemical behavior of individual inorganic particles for conditions simulating those to which particles are exposed during thermal plasma processing. The particle is suspended in a closed chamber by an electrostatic field, and it is heated by a pulsed laser beam. The composition of the gas in the reactor can be controlled, and the temperature of the particle can be measured with a time resolution as short as two-tenths to one millisecond. Equipment for optical imaging of the particle during processing is being developed.

Study is in progress of melting, vaporization, and solidification of particles of ceramic materials (alumina, zirconia), metals (Al-Ni alloys, aluminum), and carbides (silicon carbide, WC-Co, and hard facing materials). Methods and procedures for improving the accuracy of single- and two-color temperature measurements during rapid heating and cooling of the particles have been developed. Measurements have been made of the evaporation of oxide particles while they are heated and cooled.

This work is closely connected with the experimental program on plasma processing at the Idaho National Engineering Laboratory, and other plasma processing studies in the Department of Materials Science and Engineering at MIT. The combination of data from this investigation, the data base from INEL on plasma spraying, and results of modelling of plasma spraying by Professor Szekely's group (MIT) will provide much more complete understanding of plasma processing of materials than has been available heretofore.

## Massachusetts Institute Of Technology

**Energy Laboratory** **$101,329**
**Cambridge, MA 02139** **03-A**
**91-3**

**Synthesis of Heat and Work Integration Systems for Chemical Process Plants**
***L.B. Evans***

The goal of this research is to investigate and develop improved methodologies for the synthesis of heat and work integration systems in process plants. This is an important problem in the design of new plants and in the retrofitting of existing plants for energy conservation.

In a typical process plant, such as a petroleum refinery, a petrochemical plant, or a paper mill, many process streams must be heated or cooled in heat exchangers. The heat integration system recovers heat from streams that must be cooled and transfers it to streams that must be heated. A plant also requires energy in the form of work to drive pumps and compressors and to provide mechanical energy needed. This work must be supplied externally, such as by purchasing electricity from a utility, or generated internally within the plant. The goal of work integration is to identify process modifications that can reduce the cost of energy in the form of both heat and work.

This project aims to combine powerful mathematical programming techniques with principles of artificial intelligence and include improved energy integration methodologies so as to develop a user-friendly prototype system for heat and work integration in process plants. With this objective in mind, fundamental research is being conducted so as to understand the important parameters involved and their interactions. Algorithms and heuristics are being developed to synthesize that heat and work integration system having minimum total cost.

The net result of this research will be improved understanding of the nature of the problem of energy integration in process plants. The prototype system being developed will help engineers solve realistic industrial problems.

## Massachusetts Institute Of Technology

**Dept of Mechanical Engineering** **$94,668**
**Cambridge, MA 02139** **01-C**
**89-3**

**Dryout In Horizontal and Almost Horizontal Heated Tubes**
***P. Griffith***

Fluidized bed combustors, waste heat, heat exchangers and combined cycle gas turbine-steam turbine power plants all use horizontal heated tubes with hot gas on one side as the heat source. Because the gas side heat transfer coefficient is so low, excessive heat transfer and burnout is never a problem.

The most important problem is dryout where thermal fatigue or excessive corrosion due to repeated quenching occurs. Dryout can always be eliminated by increasing the mass velocity in the tube but this increases the operating expense so it is important to know exactly where the dryout limit is.

Previous work has shown that periodic washing and dryout of the tubes in the intermittent (slug flow) flow regime is the most limiting condition. The primary goal of this project is to determine whether dryout is due to drainage, evaporation or bubble nucleation at the wall. Depending on which mechanism is dominant, a method for predicting dryout in non-uniformly heated, high pressure, large (2") diameter pipes will be developed and tested. The results will be cast in the form of appropriate boundary conditions for a two fluid model of heat transfer in a heated, horizontal pipe.

## Massachusetts Institute Of Technology

**Laboratory for Manufacturing & Productivity** **$152,467**
**03-B**
**Cambridge, MA 02139** **91-3**

**Multivariable Control Of The Gas-Metal Arc Welding Process**
***D.E. 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 non-linear 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 non-linear 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 (HAZ). 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 the solution of an inverse heat transfer problem. Surface temperature measurements match the predicted values. 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 proceeding.

## Massachusetts Institute Of Technology

**Dept of Mechanical Engineering** **$66,290**
**Cambridge, MA 02139** **01-D**
**89-2**

**The Development of a Friction Model Predicting the Sliding Behavior of Material Pairs, Especially at Low Temperatures**
***Y. Iwasa***

The principal objectives of this research program are 1) to develop a friction model which predicts correctly whether a system sliding at low speeds will give steady or unsteady sliding behavior and 2) to advance basic understanding of the friction process.

The program consists of experimental and analytical studies. Experimental work includes collection of data on creep properties of the two contacting materials, namely bulk creep behavior in tension and interface creep data in shear. The interface creep takes place when one material is pressed against the other by a constant force and a shear force insufficient to produce gross sliding is applied. The extent to which the bulk creep properties determine the interfacial creep behavior both at room temperature and at cryogenic temperatures will be determined, and this knowledge should lead to better models of the friction process. In turn, such knowledge will contribute to a more reliable operation of superconducting magnets.

## Massachusetts Institute Of Technology

**Dept of Mechanical Engineering** **$188,453**
**Cambridge, MA 02139** **01-A**
**91-3**

***Modeling and Analysis of Surface Cracks***
***D.M. Parks, F.A. 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.

## Massachusetts Institute Of Technology

**The Energy Laboratory** **$127,845**
**Cambridge, MA 02139** **01-A**
**91-3**

**Energetics of Comminution**
***C. Peterson***

This program is aimed at developing an understanding of the behavior of particle beds under compressive loading and, in particular, the fracture of individual particles within the bed. The ultimate purpose is to develop tools to permit the design of much more efficient comminution devices.

Research is proceeding on four parallel tracks: analytical and experimental explorations of both particle bed and single particle behaviors. The centerpiece of the program is a computer simulation of a two-dimensional bed of three-dimensional spherical particles, subject to various moving boundaries and including particle fracture. This simulation is now deemed satisfactory as a quasi-static design tool and examination of potentially improved concepts will begin. This simulation determines forces on and motion of all particles, and, in accordance with appropriate failure criteria, simulates particle fracture by replacing the failed sphere by several smaller spheres. The simulation will be expanded to include fluid dynamic drag on spheres as a means to move material through the crushing zone.

Experimental work included measurement of force and energy requirements to crush individual small glass spheres (.05 to 1.5 mmin diameter) and particle bed studies using roughly 2 mm spheres. Simulated bed behavior compares favorably to experimental observations.

Experimental and analytical work on the fracture of large (1 inch) spheres subjected to multiple point loads has been completed to determine the appropriate failure criteria for use in the simulation. There was some concern that many loads might induce an hydrostatic stress state that would inhibit fracture, but this proved not to be the case, at least for brittle materials. In anticipation of the need for modelling deep elastic cracks, an efficient 2-D finite element was developed that models crack growth as an internal parameter within 1%, without re-meshing. Inhibition from multiple loads may be of concern for plastic materials, however, and plastic behavior is of practical significance when considering very small particles of any material.

Future work will include preliminary design work on a novel crusher concept that integrates crushing and material transport actions, expansion and application of the simulation as a design tool, more detailed quantitative experimental work on bed behavior, and further studies of plastic particle behavior.

## Massachusetts Institute Of Technology

**Dept of Mechanical Engineering** **$107,508**
**Cambridge, MA 02139** **01-C**
**89-3**

**Rheological and Flow Characteristics of Dense Multiphase Slurries Employing a Bimodal Model**
***R.F. 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 Institute Of Technology

**Department of Materials Science and Engineering** — **$92,806**
**Cambridge, MA 02139** — **06-A**
**91-2**

**Mathematical Modelling of Transport Phenomena in Plasma Studies**
***J. Szekely***

The purpose of this investigation is to develop a comprehensive mathematical representation of heat flow, fluid flow and mass transfer phenomenon in thermal plasma systems and to compare the theoretical predictions with experimental measurements.

A general formulation of the problem has been developed and an extensive set of computed results has been generated, describing the velocity profiles, temperature profiles and concentration profiles in a variety of non-transferred arc systems. The theoretical prediction were found to be in good agreement with measurements reported by researchers at the Idaho National Engineering Laboratory and in two University Laboratories. More recent work is concentrating on plasma-particle interactions and on transport phenomena inside plasma torches. This latter work is very promising in providing a rational science base for plasma torch design.

## Massachusetts Institute Of Technology[1]

***Dept of Chemical Engineering*** — ***$52,820***
***Cambridge, MA 02139*** — ***06-C***
***88-3***

## Los Alamos National Laboratory[2]

**Design Engineering Division** — **$98,600**
**Los Alamos, NM 87545** — **06-C**
**88-3**

## Sandia National Laboratories[3]

**Fluid & Thermal Sciences Dept** — **$98,600**
**Albuquerque, NM 87185** — **06-C**
**88-3**

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

This research aims to establish a link between a statistical knowledge of the microstructure and the macroscopic behavior of dispersed systems, such as suspensions of particles in liquids. Because current capability to predict the behavior of multiphase systems is limited, this fundamental knowledge of suspensions will benefit a host of technologies, especially related to geothermal energy production, petroleum production and refining, and synfuels processing. Current empirical design procedures in these technologies are deficient in understanding how overall system behavior is related to the system's micromechanics.

The approach to enhancing this understanding - involves a novel combination of experiments, numerical calculations, and theory. Real-time radiography, high-speed video, and image processing are being used to observe and record the motions of spheres as they settle through suspensions of particles. Measurements of the average and higher moments of the position and velocity distributions of the tracer sphere will provide the boundary conditions for computer simulations of the flow fields in the continuous phase surrounding individual particles. This statistical knowledge of the mechanical response of both disperse and continuous phases will then be the basis for the development and verification of a new theory for predicting overall macroscale mechanical response of multiphase systems.

To date, experimental measurements of the three-dimensional position versus time of tracer spheres settling in quiescent suspensions have shown that the settling velocity varies more in the direction parallel to the fall than in the perpendicular direction. Therefore hydrodynamic dispersivity must be represented as a tensorial rather than scalar quantity. A theory has been developed to relate the average velocity of a tracer to the macroscopic viscosity of a suspension, including effects of container boundaries. Finally, both the finite element and boundary element methods have been used to model the hydrodynamic interactions of up to 25 suspended particles.

## University Of Minnesota

**Dept of Mechanical Engineering** **$113,676**
**Minneapolis, MN 55455** **01-B**
**87-4**

**The Impact of Separated Flow on Heat and Mass Transfer**
***R.J. Goldstein***

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

## University Of Minnesota

**Dept of Aerospace Engineering and Mechanics** **$ 68,000**
**01-C**
**Minneapolis, MN 55455** **90-3**

**Stability Studies of Core-Annular Flows**
***D.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 and 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** **$129,723**
**Minneapolis, MN 55455** **06-C**
**88-3**

**Thermal Plasma Processing of Materials**
***E. Pfender***

For measuring temperature and velocity fields in plasma systems used for thermal plasma processing, enthalpy probes have been developed and tested in this laboratory. The validity of measured enthalpy and velocity profiles has been checked by performing energy and mass flux balances in an argon plasma jet operated in argon atmosphere.

Ceramic powders of carbides, aluminum nitride, oxides, solid solutions, magnetic and non-magnetic spinels, superconductors, and composites have been successfully synthesized in a Triple DC Torch Plasma Jet Reactor (TTPR) and in a single DC Plasma Jet Reactor. All the ceramic powders with the exception of AlN were synthesized using a novel liquid injection method developed to overcome the problems associated with solid injection, in particular for the single DC plasma jet reactor, and to realize the benefits of gas phase reactions.

Equilibrium calculations based on the standard technique of minimization of the system total Gibbs free energy are not adequate for predicting the yield and the proper composition of the products from thermal plasma systems. This is due to domination by nucleation kinetics, a non-equilibrium effect. Therefore, total Gibbs free energy minimization calculations using a quasi-equilibrium modification have been applied to, for example, AlN, ZrC and $MgAl_2O_4$ reactions. The modeling results agree well with experimental data in terms of product yield and composition.

## National Institute Of Standards And Technology

**Chemical Eng Science Division — $104,170**
**Center for Chemical Technology — 01-C**
**Boulder, CO 80303-3328 — 89-3**

**Convection and Dispersion in Coarse-Packed Beds**
***M.C. Jones, J.D. Wolfe***

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 And Technology

**Thermophysics Division — $509,486**
**Gaithersburg, MD 20899 — 03-B**
**Boulder, CO 80303 — 90-5**

**Thermophysical Property Measurements in Fluid Mixtures**
***R.F. Kayser, J.M.H. Levelt-Sengers***

The project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multiphase, fluid mixtures containing hydrocarbons. The research is being done jointly by two research groups within the Thermophysics Division of the NIST Center for Chemical Engineering. One group is located at the Gaithersburg, MD laboratories and the other at the Boulder, CO laboratories. The properties involved are PVT (pressure-volume-temperature), PVx (pressure-volume-composition), phase equilibria (liquid-vapor and liquid-liquid equilibria), phase behavior in interfaces, and transport properties (viscosity, thermal conductivity, and diffusion coefficient). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (800K) and high pressure (30 MPa and in some cases 70 MPa). Also under study are methods for evaluating supercritical solvent mixtures and related fluid mixtures.

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

## National Institute Of Standards And Technology

**Superconductor & Magnetic Measurements Group** **$94,700**
**Electromagnetic Technology Division** **06-C**
**Boulder, CO 80303** **89-3**

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

The purpose of this project is to fabricate and characterize high-$T_c$ superconductor/semiconductor contacts. Developing a method for optimizing the current capacity of such contacts will extend the application of high-$T_c$ superconductors to hybrid superconductor-semiconductor technologies. These technologies include integrated circuit interconnects (both on-chip and package) and proximity superconductor/semiconductor/superconductor SNS Josephson junctions. Presently, these are among the most promising high-$T_c$ superconductor applications, but an essential first step is the development of reliable, stable, ohmic contacts between semiconductors and the high-$T_c$ oxide superconductors.

The initial phase of this program is to determine the compatibility of various metals and alloys (Au and Al alloys and W, for example) as contact materials for superconducting YBCO and other high $T_c$ materials. Once a good combination has been established, patterned YBCO\normal metal contacts will be deposited onto semiconductor wafer surfaces. We have purchased a sputter co-deposition system for YBCO thin films and have adapted three other vacuum systems for contact deposition including two sputtering systems and an evaporator.

## The City University of New York

**The City College** **$162,982**
**The Benjamin Levich Institute** **01-C**
**for Physico-Chemical Hydrodynamics** **90-3**
**New York, NY 10031**

**The Rheology of Concetrated Suspensions**
***A. Acrivos***

This research program aims to investigate the flow of concentrated suspensions from a fundamental point of view. Earlier studies by the principal investigator and his associates have uncovered two effects which exert a major influence on the rheology of such systems even under conditions when the particle Reynolds numbers are vanishingly small, specifically: a) the shear-induced migration of particles from regimes of high shear to low, and from regions of high concentration to low, and b) the resuspension of a settled bed of particles when subjected to shear.

Both these effects are currently being studied experimentally in a double-gap Taylor-Couette apparatus where it is has been found that a settled bed of glass beads in a viscous fluid resuspends under the action of shear. In fact, the settled bed completely resuspends and particles are seen to migrate from the chamber having the lower shear rate to the other, in quantitative agreement with an existing theoretical model.

## The City University Of New York

**The City College** **$122,163**
**The Benjamin Levich Institute** **01-C**
**for Physico-Chemical Hydrodynamics** **87-3**
**New York, NY 10031**

**Comparative Study of Vorticity Field in Turbulent Flows**
***E. Levich***

The purpose of this project is to study - theoretically, numerically, and experimentally coherence in vorticity field. During the last year the following results have been obtained.

The analysis of the build up of coherence in numerical isotropic turbulence has been performed. Large fluctuations of helicity and the growth of helicity at low scales been has detected in 128 x 128 x 128 simulations of decay turbulence.

The comparative study of symmetry breaking in turbulence has been considered. It has been shown that in order to preserve statistical invariant the continuous growth of coupling H(k) H(k') is inevitable. Laboratory experiments with two different systems - water past the grid and air past the grid - support this observation. In both experiments helicity spectrum has been measured and the build up of coherence was observed.

A theoretical model of the phase coherence in turbulence observed in numerical simulations of turbulence and laboratory experiments has been constructed. A stationary driven turbulence, was reduced to a 4-D equilibrium system.

The study of the linear stability of incompressible turbulent fluids with respect to coherent perturbations which give a nonzero mean flow has been performed. It was shown that there is no instability, in marked contrast to the compressible case, where the reflectional asymmetry of the basic turbulence rendered certain helical perturbations unstable.

A method of creating initial field for simulations of decaying turbulence has been developed which enables creation of Gaussian velocity field with given energy and helicity spectrum. It has been shown in numerical experiments that strong helicity slows down the cascade of energy and the buildup of enstrophy at all later times.

## The City University Of New York

**The City College** **$60,750**
**Department of Chemical Engineering** **01-C**
**New York, NY 10031** **87-3**

**Periodically Structured Multiphase Flows and Hydrodynamic Instabilities in Narrow Channels**
***C.M. Maldarelli***

The goal of this research effort is to understand the hydrodynamics and stability of fluid particle multiphase flows in capillaries (e.g., the movement of foams, emulsions, and gas and liquid slugs). Particularly encouraging and significant progress has been obtained on the influence of surface active agents on these flows.

Surfactant molecules adsorb onto a fluid particle surface, and are convected to the back end of the particle. If the desorption and bulk diffusion of the surfactant away from the surface is slow compared to the convective rate of transport to the back end, surfactant accumulates and creates Marangoni stresses which retard the surface velocity. In the context of the movement of fluid particles in narrow pores, the immobilization of the particle interface increases the pressure drop required to move the flow regime and thus lowers the mobility of the particle phase.

By undertaking experiments on a particular slug flow regime in a capillary, this investigation has identified non-retarding polyethoxy surfactants. These surfactants have in common two characteristics: First, their desorption kinetics is fast. Second, at elevated bulk concentrations, they form micelles which can quickly exchange with monomer in free solution. This latter characteristic increases the rate of bulk diffusion of monomer away from the surface as the micelles act as monomer "sinks." Since the transport away from the surface is unhindered, these surfactants do not collect at the back end of the particle, and no Marangoni stresses develop.

This investigation has also demonstrated how nonretarding surfactants can be used to remobilize a surface previously retarded by the adsorption of a surfactant impurity unavoidably dissolved in the bulk phase. When the fluid particle phase is formed, the polyeythoxy surfactant, present at high concentration in the bulk, preferentially adsorbs onto a surface, not allowing adsorption of the impurity and maintaining a mobile interface. This concept of remobilization has applications in many areas, particularly in microgravity separations where thermocapillary induced migration can be reduced considerably by the presence of surfactant impurities which retard the surface mobility, and in foam drive oil recovery where the use of remobilizing surfactants can lead to greater control on the mobility of foam in rock pores.

## The City University Of New York

**The City College** **$94,700**
**The Benjamin Levich Institute** **06-C**
**of Physico-Chemical Hydrodynamics** **87-3**
**New York, NY 10031**

**Topics in Physico-Chemical Hydrodynamics**
***G.I. Sivashinsky***

The objective of this project is a unified theoretical approach to the description of large-scale spatio-temporal structures spontaneously emerging in a variety of physico-chemical systems.

The significant difference between the characteristic scales of the primary and secondary structures suggests the method of multiple scale asymptotic analysis as a natural technique for solving the relevant mathematical problems. This approach enables one to reduce the study of complex physico-chemical systems governed by strongly nonlinear, three-dimensional and highly coupled sets of partial differential equations to the incomparably more simple weakly nonlinear evolution equations of lower space dimensions. These equations are then easily tractable either analytically or numerically. With all their relative simplicity the reduced equations proved rich enough to capture many nontrivial features of physical systems which hitherto resisted analytical description by any other means. Specifically, in this study multiple-scale methods are applied to the mathematical modelling of curved nonsteady flames propagating in gaseous combustible mixtures. A nonlinear geometrically invariant dynamic equation for the flame front evolution is derived on the assumption that the curvature of the flame is small. The equation generalizes the corresponding weakly nonlinear equation obtained previously near the stability threshold. The new equation is capable of describing the evolution of complex geometric flame configurations such as those frequently observed in a strongly turbulent gas flow.

A theory of chaotic, hexagonal and polyhedral spinning flames is developed. Effects of acceleration on flame propagation in horizontal, vertical and rotating channels are analyzed.

The concept of turbulent flame speed based on invariant renormalization group approach is proposed. A consistent mathematical theory of premixed flame propagating in large-scale homogeneous turbulent flow-field is elaborated. An equation for turbulent flame speed as a function of the turbulent flow-fieldintensity is derived.

The study is presently in progress of spontaneous formation of large-scale structures in thin liquid films, in interfaces under directional solidification, and in viscous flows performing periodic motion at small scales.

## North Carolina State University


**Department of Mechanical and Aerospace Engineering** **$91,859**
**Raleigh, NC 27695-7910** **06-A** **89-4**


**Transport Properties Of Disordered Porous Media From The Microstructure**
***S. Torquato***

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

Both theoretical and computer-simulation techniques have been employed to quantitatively characterize the microstructure and compute the transport properties of disordered media. Statistical-mechanical theory has been used to obtain n-point distribution functions and to study percolation phenomena in continuum random-media models. This has led to accurate predictions of transport properties of realistic models of isotropic as well as anisotropic heterogeneous media. An efficient computer-simulation methodology has been developed to exactly yield effective transport properties in which the transport process is governed by a steady-state diffusion equation. Hence, the algorithm, which is based upon simulating the Brownian motion of a diffusing particle, can be applied to determine the conductivity, dielectric constant, magnetic permeability, diffusion coefficient, and the trapping rate associated with diffusion-controlled reactions among sinks.

## Northwestern University


**Department of Civil Engineering** **$80,921**
**Evanston, IL 60208** **03-B** **89-3**


**Effects of Crack Geometry and Near-Crack Material Behavior on Scattering of Ultrasonic Waves for QNDE Applications**
***J.D. 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

**Department of Engineering Sciences and Applied Mathematics**
**Evanston, IL 60208**

**$ 0**
**01-B**
**89-3**

### Thinning And Rupture of a Thin Liquid Film on a Horizontal Heated Solid Surface

***S.G. Bankoff, S.H. Davis***

A thin liquid film on a horizontal heated plate can become unstable and rupture, exposing dry areas of the plate.

For a volatile liquid we analyze the consequences of evaporation on the layer, incorporating the effects of viscosity, surface tension, vapor recoil, thermocapillarity and long-range molecular (van der Waals) forces in a nonlinear stability theory for the film. We have also extended the theory to include the effects of a non-volatile solute on the stability of the evaporating film. Quite general forms of the viscosity-concentration function can be employed.

If the liquid is non-volatile, and a two-dimensional heating strip is inlaid in the plate, thermocapillarity creates a dimpled interface. As the heat flux to the strip increases, the dimple deepens until dryout occurs. A nonlinear theory for this steady state and its instabilities is given, in which we include the effects of viscosity, surface tension, thermocapillarity and van der Waals forces.

In the latter case we examine experimentally the dimpling of an oil film and compare quantitatively the interface profiles measured and predicted, giving the temperature profiles sensed with thermocouples. Excellent agreement is obtained, giving the first experimental confirmation of lubrication theory applied to these films.

When the heated plate is tilted with respect to the horizontal, a heated falling film is created. The former theory is generalized to examine the interplay between the bulk flow and evaporative effects. Wavebreaking, sideband instabilities, and thinning to the point of dryout are studied, using asymptotically-correct approximations.

For viscous liquids the temperature dependence of viscosity may also be important, leading to another dimensionless parameter. It is shown that, by rescaling, the new results can be expressed in the same form as the Williams-Davis equation. The theory is generalized to the case of a two-component liquid simultaneously evaporating and draining on a horizontal spinning disk, as in photolith production. A region of transient stability is found, especially for poor solvents of high volatility, which can lead to frozen-in surface waves in the finished polymer film.

## Northwestern University

**Department of Engineering Sciences and Applied Mathematics**
**Evanston, Illinois 60208**

**$49,007**
**01-C**
**88-3**

### Attenuation of Waves in Partially Saturated Porous Solids

***M.J. Miksis***

This project will be concerned with investigating the dissipation of energy associated with the motion of fluid in a partially saturated material. An understanding of this process is important in explaining the attenuation of waves (compressional and shear) in a partially saturated porous material. It is also important in understanding how two immiscible fluids (e.g. oil and water) displace one another in a porous media. On the microscopic scale we will allow the fluid to dissipate energy by viscosity and by the movement of the contact line of the gas/liquid/solid intersection. There are two parts of this project. The first concerns an investigation of the fluid mechanics associated with contact line movement, while the second concerns using these results in either existing or modifications of existing macroscopic theories of wave propagation in a porous material.

The first phase of this project is currently underway. A macroscopic theory of wave propagation in partially saturated porous media which includes the effects of contact line movement has been developed. There are several limitations on this model but it does show that there can be considerable error in attenuations if contact line movement is neglected especially for low frequency waves. The motion of the fluid in this model was solved for analytically by matching. In order to better understand this model and the effects of the contact line motion on the fluid motion we are currently developing a numerical code to solve the microscopic moving boundary problem. Initially a lubrication model is being investigated. Next we plan to consider the complete equations of motion and to systematically incorporate these results into a macroscopic model of waves in partially saturated porous materials.

## University Of Notre Dame

**Department of Chemical Engineering $49,194**
**Notre Dame, IN 46556 01-C**
**88-3**

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

The objectives of the work are to develop an understanding of the fundamental behavior of interfacial waves which occur in separated gas-liquid flows. Interfacial waves influence significantly pressure drop, transport rates, atomization and flow regime stability; however, accurate methods for predicting this behavior are not presently available.

The primary focus this year has been flow conditions very close to neutral stability. This was chosen because specific aspects of wave behavior are easily identifiable. Experiments show that a mode corresponding to the linearly most unstable wavelength grows first followed immediately by one or more overtones. Because the overtones are linearly stable and are coherent in phase with the fundamental mode (as determined from bicoherence spectra) they are probably generated by nonlinear interaction with the fundamental mode. This net energy transfer to stable modes is the primary mechanism by which linearly unstable modes saturate at finite amplitudes. If the fundamental mode saturates at a sufficiently large amplitude, it is possible for energy to be transferred to the first subharmonic. Also observed are side band interactions, which promote transfer of energy to low frequency modes (of possible importance in slug formation), and emergence of disturbances transverse to the flow direction. To interpret the measurements, a set of weakly-nonlinear waves approach is reasonable because experiments indicate that waves usually saturate with wave slopes less than 1/50.

It is expected that identification of the generic behavior close to neutral stability will aid in interpretation and prediction of wave spectra at more highly-sheared conditions.

## Oak Ridge National Laboratory

**Engineering Physics $1,270,878**
**and Mathematics Division 03-C**
**Oak Ridge, TN 37831 87-5**

**Center for Engineering Systems Advanced Research (CESAR)**
***R. Mann***

The Center for Engineering Systems Advanced Research (CESAR) conducts interdisciplinary, long-range research and concept demonstration related to intelligent machines. CESAR provides a framework for merging concepts from the fields of artificial and machine intelligence with advanced control theory. There are two primary themes: (1) robotics systems for identification, navigation, and manipulation in unstructured environments, and (2) multi-purpose plant management for maintenance.

Illustrative FY 1990 research initiatives resulting in archival publications have included: (1) Concurrent Simulation: Development and Testing of a Learning Expert system for an Autonomous Robot, (2) Autonomous Mobile Robot Navigation and Learning, (3) Asynchronous Production Systems for Control of an Autonomous Mobile Robot, (4) HERMIES-III: A step Toward Autonomous Mobility Manipulation and Perception, and (5) Treatment of Systematic Errors in the Processing of Wide Angle Sonar Sensor Data for Robotic Navigation.

In addition, CESAR organized a national workshop and published Proceedings of the 1989 Workshop on Human-Machine Symbiotic Systems. Finally, the HERMIES-III robot assembly has been completed and quality assurance/safety procedural testing is underway.

## Oak Ridge National Laboratory

**Chemical Technology Division** **$98,600**
**Oak Ridge, TN 37831** **06-A**
**89-3**

**Bioprocess Engineering Research for Energy Applications**
***C.D. 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) advanced bioreactor concepts, (3) innovative bioseparations approaches.

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** **$63,733**
**Columbus, OH 43210** **03-B**
**88-3**

**Physics of Cellular Automata and Coherence and Chaos in Many-Body Dynamical Systems**
***C. Jayaprakash, F. Hayot***

This program deals with the dynamics of non-linear systems. It concerns two significant areas of research:

(i) the study of automata both as microscopic models underlying the macroscopic physics embodied in partial differential equations, and, in their own right, as simple, non-linear dynamical systems exhibiting complex behavior.

(ii) the study of spatial coherence and temporal chaos in systems with many degrees of freedom: as model systems, couple maps on d-dimensional lattices will be investigated.

## University Of Pennsylvania

**Electrical Engineering Department $104,312**
**Philadelphia, PA 19141 03-B**
**88-3**

**Interaction of Radiation with Surface Microstructures**
*J. Zemel*

Recent theoretical and experimental studies have shown that the basic approach leading to the conventional views about the nature of black body radiation fails when the size of the cavity is comparable with the wavelength of the incident radiation. Such a situation can arise when light interacts with periodic microgrooves inscribed on a surface. The detailed nature of such an interaction may be studied by means of spectral, angular, polarized emittance (SAPE).

Preliminary results show that SAPE allows the measurement of the effects of thermally excited standing waves in the microgrooves on the scattering of the incident radiation. It was found that indeed there are standing waves in the interior of the microgrooves, or slots. Those waves couple efficiently to the incident radiation as well as to the surface plasmons. The measured dependence of the latter coupling onthe depth of the slot cannot be accounted for fully by the existing theory. Measurements of the radiation scattered by the microgrooves shows that spontaneous emission is inhibited in some directions. It is possible that this unusual behavior may find eventually practical applications in electro-optic devices.

This research program call for determining how the geometry of the microgrooves affects the interaction between the incident radiation and the standing waves inside the slots; determining the role played by the material properties of the micromachined surfaces on the polarized, angular emission; and determining the necessary corrections to the Stefan-Boltzman radiation law necessitated by the small size of the scattering cavities.

## Physical Optics Corporation

**2545 W. 237th Street, Suite B $148,674**
**Torrance, CA 90505 03-B**
**89-3**

**Nonuniform Liouville Transformers for Quasi-Homogeneous Optical Fields**
*J. Jannson*

In this program, Nonuniform Liouville Transformers (NLT) are proposed for an important class of quasi-<R>homogeneous optical fields containing those emitted by thermal (Lambertian) and other convectional sources, as well as by the majority of multi-mode high-energy ($CO_2$, Nd:YAG, Excimer, X-ray, etc.) lasers and semiconductor lasers (including laser diodes (LD), which are important sources in local area networks (LANs)). These NLTs are nonuniform, nonimaging beam-shaping systems acting on the basis of the general energy transport equations for the phase-space density (related to the generalized Liouville theorem) and the power flux vector. The proposed theoretical model is more general than those based on geometrical optics (including Winston's nonimaging optics), yet less general than those based on either the scalar diffraction or electromagnetic theory. The fundamental goal of this program is to find a theoretical and engineering solution for highly efficient (close to 100%) beam shaping/concentration/ collimation of weakly spatially coherent and quasi-uniform large-aperture optical fields (so called quasi-homogeneous fields, which are more general than Lambertian ones), using an optimized higher-hierarchy architecture of longitudinal and transversal, imaging and nonimaging optical elements (nonimaging cones, lenses, diffusers, holographic optical elements (HOEs)). The proposed theoretical model holds for the quasi-homogeneous radiation emitted by the state-of-the-art of the majority of high energy and coherent and noncoherent electromagnetic sources.

## Physical Sciences Inc.

**20 New England Business Center $118,375**
**Andover, MA 01810 06-A**
**88-4**

**Experimental and Theoretical Studies of Condensation in Multicomponent Systems**
***M.B. 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 used in practical applications such as turbo-machinery. Experimentally, condensible vapors mixed with a carrier gas are cooled in a supersonic nozzle to obtain high nucleation rates. The nozzle is designed to ensure that steady-state nucleation occurs and to give satisfactory spatial resolution of the temperature profile. Laser light scattering and interferometry are used to detect the "onset" of condensation and to monitor subsequent droplet growth.

Experiments on condensing water vapor have shown that the number density of water droplets falls sharply after an initial rapid increase. This previously unobserved behavior appears to be due to polydispersity of the droplet size distribution which favors growth of larger droplets at the expense of smaller ones. Theoretical calculations of the droplet size distribution along the flow axis support this interpretation. The calculated size distribution broadens rapidly; large numbers of large droplets (9 nm radius) are already present at the observable onset of condensation. The rapid growth in number and size of these large droplets is responsible for the latent heat release that disturbs the gas flow. These results contradict the conventional view of condensation in nozzles. In that view, onset is attributed to the rapid nucleation of a monodisperse cloud of very tiny microclusters (0.4 nm radius) which then grow in a number-conserving fashion. This work shows that nucleation and condensational growth do not occur in separate stages beginning at onset, and it establishes both the presence and importance of large droplets at the onset of condensation.

## Princeton University

**Department of Mechanical $91,859**
**and Aerospace Engineering 06-B**
**Princeton, NJ 08544 90-3**

**Mechanisms and Enhancements of Flame Stabilization**
***C.K. Law***

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

A theoretical analysis has been conducted on the structure and extinction of diffusion flames with flame radiation. The structure analyzed consists of a thin reaction zone embedded within a thicker radiation zone which in turn is situated within the O(1) diffusive-convective flow field. Using droplet combustion as a model problem, the recent analytical results exhibit a dual extinction behavior in that flame extinction occurs not only for sufficiently small droplets due to reduced residence times, as is well established, but it also occurs for sufficiently large droplets as a result of excessive heat loss from the correspondingly large flame. Consequently there exist systems for which steady combustion is not possible for all droplet sizes.

A theoretical and experimental investigation has been performed for the effects of flame curvature on diffusion flame extinction by using opening of the Burke-Schumann flame tip as the model problem. Asymptotic analysis of the flame structure in the tip region shows that increasing the extent of the flame curvature facilitates near-complete reaction and thereby enhances the burning intensity. Consequently, for unity Lewis number flames, increases in the flow velocity tend to inhibit tip opening because of the corresponding decrease in the radius of the flame tip. Experimental results agree with the theoretical prediction, and further show that tip opening is possible by using a sub-unity Lewis number fuel stream of hydrogen and carbon dioxide.

In the third project, a chemical kinetic criterion of flammability limits is proposed. The criterion is based on defining a flammability exponent, which measures the sensitivity of a crucial termination reaction to the corresponding branching reaction, and identifying the flammability limit as the state at which this exponent becomes unity. Application of this criterion to the carbon-hydrogen-oxygen system shows extremely close agreement with the experimental data, for both the lean and rich limits. The study further shows that the $H + O_2$ ----> $0 + OH$ is the dominant branching reaction for all lean and rich limits, that $H + O_2 + M$ ----> $HO_2 + M$ is the dominant termination reaction for all lean limits, and that the dominant termination reaction for rich limits can be mixture specific.

## Purdue University

**School of Mechanical Engineering** **$86,196**
**West Lafayette, IN 47907** **01-C**
**90-3**

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

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

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

## Purdue University

**School of Nuclear Engineering** **$100,000**
**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 (Kocamustafaogullari) 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

**Department of Mechanical Engineering, $ 0**
**Aeronautical Engineering & Mechanics 01-B**
**Troy, NY 12180-3590 89-4**

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

This study is directed toward the thermal-hydraulic behavior of water and aqueous mixtures, flowing in plain tubes and in tubes with enhancement devices, at very high heat fluxes. The mode of heat transfer is subcooled nucleate boiling, and the limiting phenomenon is the critical heat flux (CHF). Very large heat fluxes can be accommodated on a steady basis with pure water by use of large subcoolings, high velocities, small tube diameters, and short tubes. It is expected that simultaneous use of several enhancement techniques will extend the maximum heat flux to at least $5x10^8$ W/m$^2$, which would be higher than 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 has been designed to systematically investigate the effects of subcooling velocity, tube geometry, and enhancement techniques on CHF, the boiling curve, and the pressure drop. The CHF's will be correlated as a function of flow and geometrical variables. The experiments will be complemented by mechanistically based models for CHF under normal and enhanced conditions.

The experimental facility has been modified to permit data acquisition under extreme conditions of flow and heat flux. CHF data have been obtained with pure water flowing in plain tubes to describe the main parametric trends. A complementary data base of results from the literature is being assembled for the correlation development.

## Rensselaer Polytechnic Institute

**Dept of Mechanical Engineering, $122,541**
**Aeronautical Eng & Mechanics 01-A**
**Troy, NY 12180-3590 88-3**

**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 AISI Type 304 Stainless Steel 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.

For the experiments, an MTS servohydraulic axial/torsion test system is available together with an MTS Data/Control Processor. Induction heating (10 kHz) frequency), MTS biaxial grips and an MTS biaxial extensometer are available together with a reversing direct current potential drop facility. It is intended for early monitoring of damage during cyclic loading. It has been tested out at room temperature.

Uniaxial and torsional ratchetting experiments showed considerable strain accumulation at room temperature and they demonstrate that ratchetting is due to viscous effects. Surprisingly, insignificant ratchetting and rate sensitivity were observed at 550, 600 and 650°C for uniaxial tests. This unexpected finding was attributed to strain aging in the stainless steel. A finite deformation theory of viscoplasticity based on overstress (VBO) is being developed and is being implemented into a finite element computer program. To simulate the complex hardening behavior of AISI Type 304 Stainless Steel during non-proportional loading, new hardening rules are under investigation and are being implemented into the small deformation VBO theory developed previously.

## Rensselaer Polytechnic Institute

**Department of Nuclear Engineering and Engineering Physics** **$117,428**
**Troy, NY 12180-3590** **01-C**
**89-4**

**The Continuum Modeling of Two-Phase Systems**
*R.T. Lahey, Jr., D.A. 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** **$80,495**
**Troy, NY 12180-3590** **01-C**
**89-3**

**Microcomputer Enhanced Optical Investigation of Spreading and Evaporation Processes in Ultra-Thin Films**
*P.C. 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 will be studied. During the first year microscopic image-processing equipment, procedures, and related computer programs will be developed to improve data resolution and automate data acquisition. First, the image processing equipment will be developed and used in conjunction with an interferometer designed to study the transient film thickness in draining films in an inclined cell. The glass cell will be designed to optimize temperature control, cleanliness and simplicity. The optical data will be obtained using a video camera attached to a microscope through which the interference fringes will be recorded. Transport processes in polar and non-polar fluids, with and without heat transfer, will be experimentally studied and analyzed. Using the results of these studies, an ellipsometer with a complementary interferometer will be designed for construction and use in subsequent years. The long term objective is to determine the heat transfer characteristics of evaporating ultra-thin liquid films. The near term objective is to develop microscopic image-processing equipment and a complementary heat transfer cell.

## University of Rochester

**Dept of Physics and Astronomy** **$63,594**
**Rochester, NY 14627** **06-C**
**89-3**

**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 with various values of applied magnetic field. I-V characteristics and resistivity were computed and related to vortex structure. Preliminary work on the behavior of flux line lattices in three dimensional networks has begun.

This research will greatly enhance our fundamental understanding of pinning and flux flow resistance in 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/generators.

## University of Rochester

**Dept of Physics and Astronomy** **$86,218**
**Rochester, NY 14627** **06-C**
**90-3**

**Coherence Effects in Radiative Energy Transfer**
*E. Wolf*

The conventional approach to radiative transfer rests on the premise that geometrical optics is a valid approximation to the exact solutions of the wave equations arising in electromagnetic theory. While that may be a correct assumption in the case of propagation in homogeneous media, it may not be so in the case of random media with relatively short correlation lengths. For in that instance account must be taken of the coherence properties of the propagated radiation, an aspect of optics outside of geometrical optics.

The proposed research will examine the limits of validity of the theory of radiative transfer and radiometry. At the same time the degree to which coherence affects energy distribution in a source will be examined.

More specifically, some problems with known solutions obtained by conventional means will be reexamined from the point of view of coherence theory. Here the effects of randomness of the medium in which the propagation takes place will be taken into account explicitly. It is expected that this exercise will clarify the conditions under which the conventional radiative transfer approach must be replaced by coherence theory.

Further, the trade-offs between coherence and intensity distribution at a radiation source will be examined with a view to determining the resulting effects on radiance distribution in the far field. Recent theoretical results confirmed by experiments suggest that such effects may lead to the design of more energy-efficient sources of electromagnetic radiation, for instance for illumination purposes.

Finally, the effects of the interplay between the statistical properties of the incident light and the statistical properties of the scattering medium will be examined. Recent novel and unexpected results show that under some conditions such interactions may lead to a shift in the spectrum of the observed light.

## The Rockefeller University

**Department of Physics** **$78,032**
**1230 York Avenue** **06-C**
**New York, NY 10021** **88-3**

**Some Basic Research Problems Related to Energy**
***E.G.D. Cohen***

The present project is concerned with the following problems. 1) The approach to thermal equilibrium of dynamical systems with relatively few degrees-of-freedom is studied. This is of interest not only for the foundations of statistical mechanics but also for chemical and other problems. The question is: when does equipartition of energy and other thermal equilibrium properties hold? Computer as well as theoretical calculations will be used. 2) An investigation of Lorentz lattice gas cellular automata with independent particles moving on a lattice occupied by randomly placed scatterers is carried out. Two goals are a closer study of (a) the abnormal diffusion found in strictly deterministic models and, (b) the connection with polymer statistics. Computer and analytic approaches will be employed. This investigation is also expected to elucidate the connection between particle motion in lattice gas cellular automata and the hydrodynamic behavior of fluids in general. 3) A possible relation between the transport coefficients of a fluid in ordinary space and the Lyapunov exponents of the same system in phase space will be investigated using computer simulations as well as theory. 4) A newly discovered analogy between the structural relaxation found in dense atomic fluids and that in concentrated solloidal suspensions will be further explored. Laboratory experiments, computer simulations as well as analytical methods will be used.

## Sandia National Lab

**Fluid, Thermal, and** **$29,580**
**Structural Sciences Division** **03-B**
**Albuquerque, NM 87185** **89-1**

**Two-Phase Flow Measurements by NMR**
***R. Givler***

We will use nuclear magnetic resonance (NMR) to study two-phase flows in model systems. Lovelace Medical Foundation (LMF) will carry out the experiments while Sandia National Laboratories (SNL) will provide the theoretical models of multiphase flows as well as help in running the labor-intensive NMR experiments. We will study steadily flowing nondilute solid suspensions by NMR to obtain the spatial distributions of the phases as well as the velocity distributions of each phase. Such determinations work best under moderately high concentrations of both phases, a case that is difficult for light and ultrasound scattering. Our exploratory studies for the coming year will include the following: 1) flow studies of suspensions (heavy particles in a Newtonian oil) in horizontal tubes to determine the dependence of flow properties on particle diameter, particle diameter to tube diameter ratio, mean particle concentration, particle shape and surface roughness, mean flow rate, and relative phase densities; 2) measurement of the velocity and spatial distribution of a water/oil mixture in the annular region between counter-rotating, eccentrically-nested cylinders, and 3) measurement of the simultaneous, time-averaged, axial velocity profiles for two immiscible liquids such as oil and water flowing in a horizontal tube.

## Sandia National Laboratories

**Combustion Research Facility** **$138,040**
**Thermofluids Division** **06-B**
**Livermore, CA 94550** **90-3**

**Mixing and Phase Change During Combustion**
***A.R. 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 substationally 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** **$138,040**
**Thermofluids Division** **06-B**
**Livermore, CA 94551-0969** **87-3**

**Nonlinear Analysis of Ligament and Droplet Breakup**
***B.R. Sanders, H.A. Dwyer, D.S. Dandy***

The objective of this research program is to study the nonlinear fluid dynamics and transport processes which govern the deformation and breakup of liquid ligamentsand large droplets. In particular, finite-volume computations will be used to study the time evolution of surface disturbances on a three-dimensional liquid element as it deforms and breaks up under the influences of variable-property interfacial tension, aerodynamic forces, liquid circulation, heat transfer between phases, and vaporization. Since the three-dimensional analysis provides all surface force components, the drag coefficient will also be characterized for a family of non-axisymmetric liquid elements as they experience the highly nonlinear transport processes mentioned above. The scope of this research proposal is limited to computational studies, however this research is closely tied to experimental research efforts at Sandia and elsewhere. Two spray combustion experiments are beginning at Sandia's Combustion Research Facility, one with a pulsed spray and one with a steady spray. Data from these experiments will aid in verification of breakup criteria predicted by the model under development.

## Stanford University

**Dept of Mechanical Engineering** **$160,000**
**Stanford, CA 94305-3030** **01-B**
**89-3**

**Heat Transfer in Three-Dimensional Turbulent Boundary Layers**
***J. Eaton***

The objectives of this research are to identify, understand, and model the effects of three dimensionality on turbulent boundary layer heat transfer. Early work on this project examineddistortions of a 2D boundary layer with embedded longitudinal vortices. Experiments showed that two-dimensional similarity laws are violated and that new modelling concepts are needed to correctly represent embedded vortex flows. The next set of experiments examined an initially 2D boundary layer which was skewed laterally resulting in strong three dimensionality. Rapid distortion of the turbulence structure was observed but this apparently had a minor effect on the heat transfer behavior. A vector enthalpy thickness was defined which extends standard correlations to this new area.

Two experiments are presently ongoing. The first examines the interaction of an embedded longitudinal vortex with a three-dimensional boundary layer. The results were surprising in that the vortex was attenuated about one order of magnitude more rapidly in a 3D boundary layer than in a similar 2D layer. The boundary layer distortion is strongly dependent on the sign of the vortex. These results appear to have considerable significance to flow control applications of vortex generators. The second experiment is being developed to study the three-dimensional boundary layer on a rotating disk at a tip Reynolds number of approximately 1 million. The disk apparatus is complete and a new laser Doppler anemometer is being installed. A heat transfer measurement disk is also being developed.

## Stanford University

**Dept of Mechanical Engineering** **$161,000**
**Stanford, CA 94305-3030** **01-A**
**86-4**

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

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

During the past year we have developed a computational routine capable of computing the energies of, and forces on dislocations in layered anisotropic media, which are important configurations of interest in modern integrated circuit technology. The theory of interfacial (Stoneley) waves in bonded piezoelectric half-spaces has been fully developed, as has also the theory and computations of so-called zero curative extraordinary transonic states in anisotropic elastic media. Orientations and elastic constant restriction admitting Type 3 transonic states have been delineated for five of the eight anisotropic crystal classes. Color computer graphics is now being used to produce three-dimensional views of slowness surfaces in anisotropic elastic and piezoelectric solids; this work has also led to the production of faster algorithms for determining the limiting speed which defines the first transonic state. In the coming year we intend to improve these graphics capabilities to include rotations and slicing, and to extend our elastic studies to deduce the behavior at interfacial crack tip singularities in anisotropic elastic and piezoelectric media.

Problems of composite materials consisting of single inclusions or two inclusions have been solved using a "circle theorem" developed previously and a "two-circle theorem" discovered in the past year. The latter theorem is now being used to study inclusions with either bonded or "slipping" interfaces. Using Noether's theorem, conservation laws based on non-classical transformations are being examined for their application to fracture and defect mechanics. Finally, our previous work on isothermal thermodynamics of stressed solids as applied to theories of damage in brittle solids is being extended to non-isothermal conditions.

## Stanford University

**W.W. Hansen Lab of Physics** **$252,549**
**Stanford, CA 94305-3030** **03-B**
**90-3**

**Nondestructive Testing**
***G.S. Kino***

The object of this research is to determine the usefulness of new optical methods, including photoacoustic and photothermal measurements as novel techniques in solidstate research, notably for high critical temperature superconductivity.

The proposed research deals with the development of nondestructive techniques for characterizing the new high temperature superconducting materials. Those materials are difficult to characterize because they are polycrystalline, brittle, highly anisotropic, and inhomogeneous. The noncontacting photoacoustic and photothermal techniques developed in the preceding phase of this project can provide important information on the nature of the microstructure and grain boundaries which influence the superconducting properties.

## Stanford University

**Department of Civil Engineering** **$98,497**
**Environmental Fluid Mechanics Lab** **01-B**
**Stanford, CA 94305-4020** **90-3**

**Fluid Mechanics of Double Diffusive Systems**
***J.R. Koseff, R.L. Street, S.G. 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

**High Temperature Gasdynamics** **$198,870**
**Stanford, CA 94305** **03-B**
**88-4**

**Diagnostics for Plasma Chemistry**
***C.H. Kruger, M.A. 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 electron density and temperature. The methods under study 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.

## Stanford University

**Department of Chemistry** **$ 0**
**Stanford, CA 94305** **06-C**
**89-3**

**Reduction of Dissipation in Combustion and Engines**
*J. Ross*

Research is concerned with the issue of the enhancement of power output in thermal and chemical engines by means of external perturbations of constraints coupled to nonlinearities of the mechanism of the engine. The theoretical possibility of an increase in power output of a thermal engine driven by a chemical reaction by means of external periodic variations of reactant influx has been confirmed in a series of experiments. The power output of an engine is necessarily accompanied by dissipation due to irreversible processes essential for power production. Hence an increase in power output by means of external perturbations usually implies a decrease in dissipation but may also come about due to a change in the final state of the system. Increases in efficiency can be achieved for a particular range of frequencies and amplitudes of external perturbations which yield resonance effects and appropriate phase shifts of fluxes and forces. Theoretical and experimental studies are in progress on optimization of efficiency by choices of functional forms of external perturbations. A variational theory has been constructed which gives limits of improvements in efficiency by external perturbations.

## Stanford University

**Dept of Mechanical Engineering** **$80,218**
**Design Division** **03-A**
**Stanford, CA 94305** **88-3**

**Monotonicity Analysis and Geometric Programming in Mechanical Shape Optimization**
*D.J. Wilde, S.D. Sheppard*

This theoretical and computational research intends to bring the theory and practice of Monotonicity Analysis and Geometric Programming to bear on finite element optimization problems related to mechanical component shaping. Better analysis, approximation and computation methods would contribute to the design of lower weight, more energy efficient vehicles and machines. Since for existing methods each iteration requires a computationally intensive finite element analysis (FEA), these innovations are intended to reduce the number of FEA iterations.

This approach has been applied successfully to the shaping of a planar cantilever support for minimum weight. Three zones: (1) the fillet near the support, (2) an interior zone free of stress concentration, and (3) one near the load -- were modeled approximately by classical solid mechanics and more precisely by FEA. Monotonicity analysis of the classical approximation identified as critical the shear stress near the load and the bending stress in the fillet and interior zones. This immediately determined the optimal shape of the interior and load zones. It also gave the differential equation of the fillet shape as a function of its variable curvature, initially unknown. FEA-predicted deviations of fillet stress from the desired value generated a new curvature function whose integration produced a much better shape. Only three iterations were needed for convergence. The idea is also proving practical for deflection- and vibration-limited cantilever situations. A connecting rod vibration study has shown remarkably large shape improvement in a single iteration.

## Stevens Institute Of Technology

**Dept of Physics and Engineering** **$64,077**
**Hoboken, NJ 07030** **06-C**
**87-4**

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

The transition from order to chaos in dynamical systems of few degrees of freedom are studied, using theory, numerical computation and a laboratory experiment as tools of this investigation. This work is nearly completed and we are tooling up to study more complex systems with many degrees of freedom.

We have determined the dynamics of transition from Hamiltonian to dissipative systems in the chaotic regime. As the Hamiltonian limit is approached, strange attractors disappear in an orderly fashion as dissipation is reduced. There exist a set of universal Jacobians Jn' where the 2n piece strange attractors disappear. This phenomenon is universal as we have proven using renormalization calculations, in the vicinity of the universal Hamiltonian function T*. In fact we have shown that all phenomena possess a universal scaling in the K-J parameter space, where K is the strength parameter and J is the Jacobian.

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

Physical systems that produce two dimensional maps are of course different from the universal ones. We have found recently that such systems exhibit extremely rapid convergence to the universal sequence of Jn values. Among the systems studied were the driven damped pendulum, the bouncing ball, and the particle in the standing wave field. All systems studied exhibited the rapid convergence to the universal system as predicted. The fundamental theory of dissipative dynamical systems, represented by two dimensional maps has been established.

## Syracuse University

**Dept of Mechanical Engineering and Material Sciences** **$57,572**
**Syracuse, NY 13244** **01-C**
**90-2**

**Numerical and Physical Modeling of Bubbly Flow Phenomena**
***A. Sangani***

The ultimate purpose of this study is to put the widely used engineering averaged-equations models of multi-phase flows on a firmer footing by comparing their results with those of direct numerical multi-particle simulations and rigorously-derived averaged equations.

Ensemble-averaged equations for the propagation of pressure waves in bubbly liquids have been derived correct to second order in the gas volume fraction. A new insight into the structure of the expansion and the role of bubble-bubble interaction and surface deformations is obtained from the work.

In a second study, by arranging *N* bubbles at random in a cubic cell and filling up the entire space with copies of this cell, the behavior of an infinite bubbly liquid has been simulated. For this situation two alternative definitions of added mass have been explored and the average viscous dissipation in the limit of large Reynolds number has been studied.

In another study, the propagation of pressure waves in a layer of bubbles has been considered. The novel feature of this work is the fact that the volume fraction is arbitrary and the wavelength can be comparable to the inter-bubble distance. The last problem involves the flow of a "plug" of bubbly liquid in a conduit. For the time being the bubbles are arranged on the axis of the conduit, but will later be placed at random.

## University Of Texas At Austin

**Ctr for Studies in Statistical Mech** **$94,700**
**Austin, TX 78712** **06-C**
**88-3**

**The Behavior of Matter Under Nonequilibrium Conditions: Fundamental Aspects and Application in Energy-Oriented Problems**
***I. Prigogine***

This research aims at new fundamental developments in the area of non-equilibrium phenomena, as well as at various applications to disciplines in which complex systems giving rise to instabilities and bifurcations are of current and primary concern. Special emphasis is being placed on three principal directions: 1) Continuation of the study of self-organization on the microscopic scale, as exemplified in the early stages of matter-radiation interaction. 2) Investigation of the onset of coherent temporal behavior and spatial pattern formation at the microscopic level, by means of molecular dynamics: a) Approach to equilibrium starting from initial nonequilibrium spatial distributions. Preliminary results show that equilibrium structures are produced by nonequilibrium processes, involving long-range and long-living correlations. b) Observation of sustained stable rhythmic phenomena in a model involving 3 chemical intermediates undergoing binary collisions. Preliminary results show agreement with macroscopic reaction-diffusion theory, for a homogeneous system. The onset of stable spatial chemical patterns (Turing instability) is currently under investigation. The important conclusion is that dissipative structures are the outcome of dynamical processes at the microscopic theories which are based on phenomenological assumptions. 3) Molecular dynamics computer experiments testing the limits of validity of macroscopics physics: The traditional formulation of macroscopic physics rests on the strict applicability of the local equilibrium assumption. Most of the familiar phenomena of non-linear physics, such as hydrodynamical and chemical instabilities, turbulence, combustion etc. are direct manifestations of this hypothesis. For gas-phase exothermal chemical reactions, significant deviations from the usual equilibrium theory have recently been measured through molecular dynamics. The origin of these deviations can be explained by the perturbation of the local Maxwellian distribution through reactive collisions. Quantitative agreement with a theory taking account of this effect have been established.

## University Of Texas At Austin

**Department of Physics** **$139,209**
**Austin, TX 78712** **06-C**
**87-5**

**Complex Temporal and Spatial Patterns in Nonequilibrium Systems**
***H.L. Swinney***

Dynamical systems methods are being developed and used to characterize nonequilibrium processes and to address outstanding unresolved questions regarding bifurcations and chaos, especially in reaction-diffusion systems. An information-theoretic property, the mutual information, is being examined as a means for detecting and quantifying spatiotemporal chaos. The work has demonstrated that information on dynamics deduced from noisy data can be used to reduce the noise in those data. These tools from dynamical systems and information theory are being applied to data obtained in laboratory experiments on homogeneous systems and on extended systems. A novel unstirred chemical reactor has been designed for studies of the development and evolution of chemical spatial patterns, and experiments with this reactor have yielded the first sustained chemical spatial patterns in a controlled laboratory environment. These laboratory experiments and numerical and analytic studies of models should provide general insights into spatiotemporal patterns in nonequilibrium systems.

## Tufts University

**Dept of Mechanical Engineering** **$53,978**
**Medford, MA 02155** **01-A**
**88-3**

**Effective Elastic Properties of Cracked Solids**
***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 Research Center

**Propulsion Science Laboratory** **$175,217**
**East Hartford, CT 06108** **06-A**
**89-3**

**Laser Diagnostics Of PACVD Processes**
***W.C. Roman, S.O. Hay, F.A. Otter, A.C. Eckbreth***

The objectives of this research are to perform a comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process applicable to hard face coatings. Based on its superior erosion resistance, TiB2 was selected as the initial coating for deposition onto a titanium alloy substrate (Ti-6A1-4V). In task I, novel non-intrusive laser diagnostic techniques (e.g. Laser Induced Fluorescence Spectroscopy (LIFS), and Coherent Anti-Stokes Raman Spectroscopy (CARS)) are being used to determine, in situ, the reactive plasma composition, temperature, and species concentration and distribution in the gas phase. Coupled with these experiments will be modeling of the plasma chemistry process. The second task includes use of Auger Electron Spectroscopy (AES), Ion Scattering Spectroscopy (ISS), Secondary Ion Mass Spectroscopy (SIMS) and other complementary techniques for detailed coating characterization. These are being combined with physical measurements of coating surface smoothness, hardness (state-of-the-art nanoindenter apparatus) and adherence (UTRC custom built pin-on-disc apparatus). These combined tasks will allow a correlation of the PACVD parameters with their required coating properties, thus providing a predictive capability that is severely lacking in the present science base of advanced protective coatings. Results to date include: 1) fabrication of a 5 kW rf PACVD reactor system integrated with a completely oil-free, high vacuum system; 2) exploratory spectral emission surveys for major molecular band and atomic line identification; 3) development of a colinear, scanned, narrowband CARS system; 4) implementation of a ultramicrohardness tester and adhesion test apparatus; 5) initial characterization of TiB2 and diamond coatings; and 6) first time CARS measurement of several key species (e.g. B2H6).

## Washington University

**Department of Systems Science and Mathematics** **$69,957**
**03-A**
**Saint Louis, MO 63130** **90-3**

**Dynamical Systems with Internal Structure: A New Approach to the Problem of Analysis and Robust Design of a Time Varying System**
***B.K. 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 agood 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 differmorphism 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** **$66,290**
**Pullman, WA 99164-2920** **01-B**
**89-2**

**Particle Dispersion by Ordered Motion in Mixing Layers**
***T.R. Troutt***

The primary goal of this research is to determine the role organized vortex motions play in the dispersion of particles by free shear flows. This research goal has been pursued using analytical, numerical and experimental techniques to examine the particle dispersion process in plane mixing layers and wakes. The results of these studies have shown that the character of the particle dispersion process in free shear flows is a function of a time scale parameter formed between the ratio of the particle aerodynamic response time and the time scale of the organized vortex motion. For intermediate time scale ratio particles two types of dispersion mechanisms have been recently 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 plane wakes, where large scale vortex mergers are not a dominant feature, intermediate scale particles are "focussed" into highly concentrated regions near the vortex boundaries. The resulting order of the self-organized particle dispersion patterns for both mixing layers and wakes can be quantified using the fractal correlation dimension. This quantity is found to be a strong function of particle time scale ratio. Current research efforts are aimed at further exploring these dispersion mechanisms and developing improved strategies for predicting and controlling particle dispersion in free shear flows. New design concepts for multiphase mixing systems are a highly plausible application of these results.

## University Of Wisconsin

**Mechanical Engineering Department** **$99,869**
**Madison, WI 53201** **01-C**
**90-3**

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

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 onthe 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** **$104,170**
**Madison, WI 53706** **03-A**
**89-3**

**The Development of Process Design and Control Strategies for Energy Efficiency, High Product Quality, and Improved Productivity in the Process Industries**
*W.H. Ray*

The process industries are having great difficulty competing in the world market because of high energy costs, high labor rates, and old technology for many processes. This project is concerned with the development of process design and control strategies for improving energy efficiency, product quality, and productivity in the process industry. In particular, (i) the resilient design and control of chemical reactors, and (ii) the operation of complex processing systems, will be investigated. Major emphasis in part (i) will be on two important classes of chemical reactors: polymerization processes and packed bed reactors. In part (ii), the main focus will be on developing process identification and control procedures which allow the design of advanced control systems based on limited process information and which will work reliably when process parameters change in an unknown manner. Specific topics to be studied include new process identification procedures, nonlinear controller designs, adaptive control methods, and techniques for distributed parameter systems. Both fundamental and immediately applicable results are expected. The theoretical developments are being tested experimentally on pilot scale equipment in the laboratory. These experiments not only allow improvements in theoretical work, but also represent real life demonstrations of the effectiveness of the methods and of the feasibility of implementing them in an industrial environment. The new techniques developed in this project will be incorporated into computer-aided design packages and disseminated to industry. Therefore, it is expected that the work will have an impact on industrial practice.

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# Principal Investigators



*U.S.G.P.O:1991-281-714:40039

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