DOE/ER-0436

Summaries of FY 1989 Engineering Research

1989

U.S. Department of Energy

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

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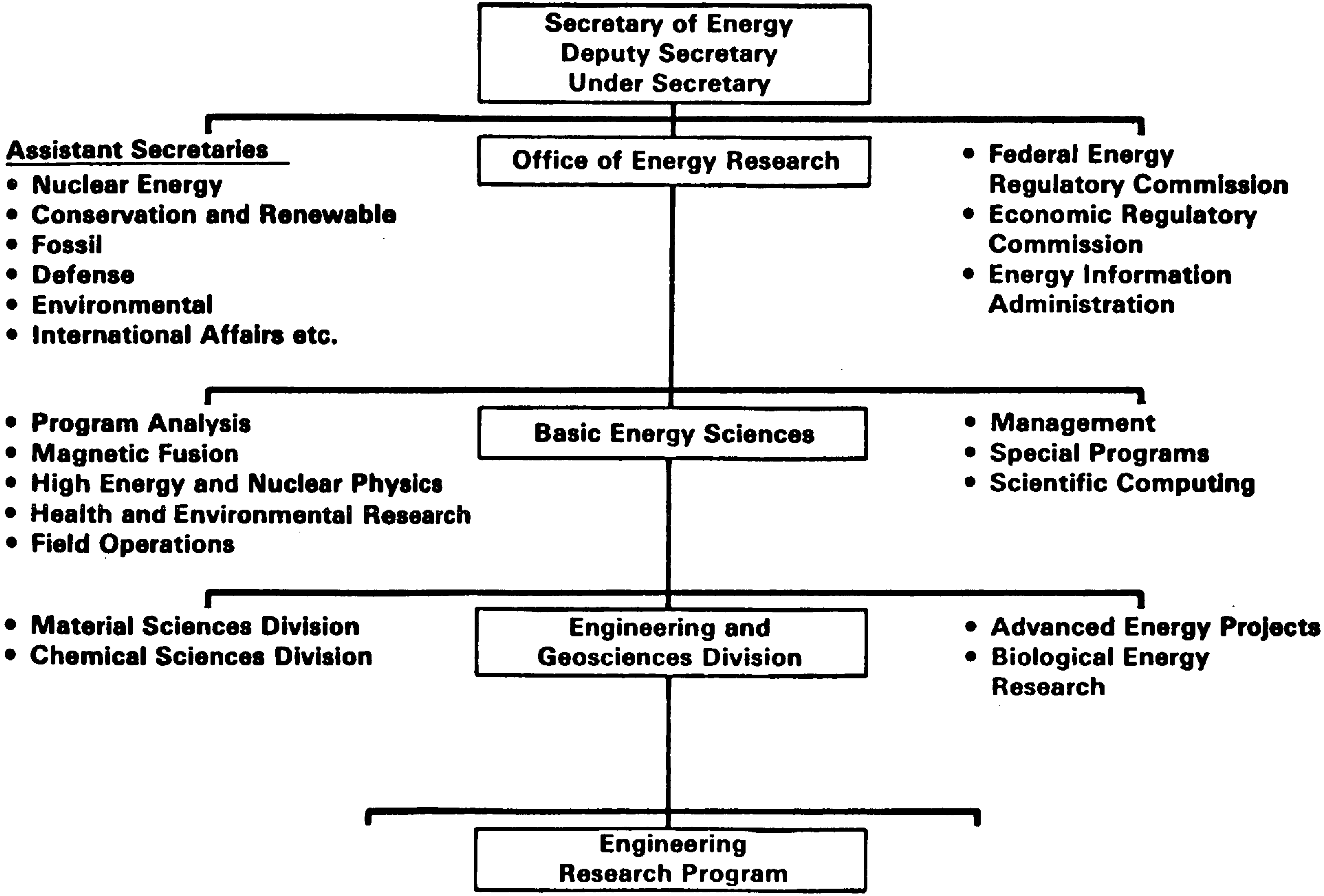
Washington, D. C. 20545

Foreword

This report documents the BES Engineering Research program for fiscal year 1989; 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 1989. 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 1989.

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 1989 appears to the right of title; it is followed by the budget activity number (e.g.,01-A). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The 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 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 and crack propagation in 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 crack propagation).

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. Proceeding 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.

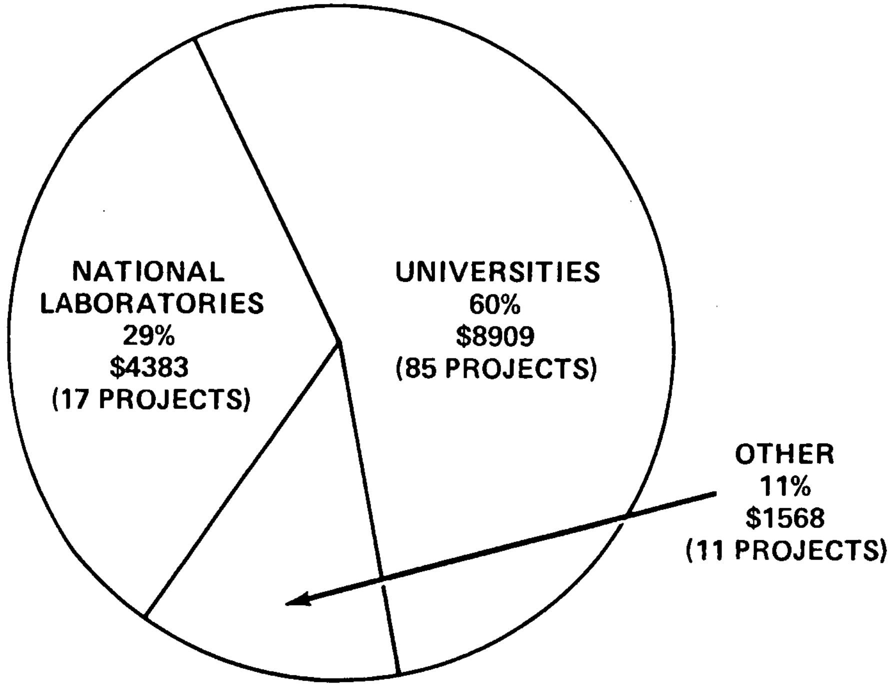
In the expectation of a future modest growth of this Program, two International Workshops on Two Phase Flow Fundamental were held one in September 1985 and the other in March 1987. The meetings were used to identify basic research needs in the field of two phase flow and heat transfer; summary reports 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 1989 the available program operating funds available amounted to about $14.9 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 '89 BUDGET ($000's)
BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '89 BUDGET (EST.)
BY TECHNICAL AREAS

	($000 s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	4894	33	43
SYSTEMS SCIENCES	4428	30	22
ENGINEERING ANALYSIS	5538	37	48

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Ames Laboratory

Institute for Physical Research and Technology	**$258,000**
Ames, IA 50011-3020	**03-B**
	87-3

1. 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 particularly desirable for inspection in the near 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

Argonne, IL 60439	**$100,000**
	01-C
	87-3

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

The research program is a joint effort by the members of the University of Wisconsin-Milwaukee and Argonne National Laboratory. The objective of the research program is to develop instrumentation techniques, a data base and predictive methods for describing the interfacial structure of horizontal and vertical two-phase flow, such as flow pattern transitions, interfacial area concentration and interfacial wave structure. The special emphasis will be placed on developing local interfacial area concentration measurement techniques, and two-phase flow-pattern transition criteria. The latter include 1) scaling criteria in terms of systems size and fluid properties 2) entrance geometry and developing flow effects, and 3) rational procedure and design criteria for predicting these effects.

To achieve the objectives, the technical approach is divided into three parts. The first part deals with theoretical modeling of the interfacial area and flow-pattern transitions based on physical mechanisms. The second part is concerned with designing and performing horizontal and vertical two-phase flow experiments to generate benchmark data using flow visualization and objective measurements. Finally, the third part deals with incorporating the results of theoretical and experimental studies to examine and verify the validity of proposed flow-pattern transition mechanisms and interfacial area concentration modeling.

The results of this research program will provide information in horizontal and vertical two-phase flow fundamentals and information critical to the design of advanced two-phase flow systems.

Argonne National Laboratory

Materials and Components Technology Division — **$138,000**
Argonne, IL 60439 — **01-C** — **86-3**

3. Theoretical/Experimental Study of Stability Control
T.M. Mulcahy, E.L. Reiss (Northwestern University), S.P. Vanka

Theoretical and experimental studies are aimed at enhancing the understanding of stability phenomena involving fluids, solids, and their coupling. The objective is to develop methods of controlling, delaying, and/or avoiding instability in engineering components. Currently fluid elastic instabilities caused by flow leaking between closely spaced bodies are being investigated.

To interpret and present the experimentally observed fluid-structure interaction at the slip-joint region of telescoping tubes conveying fluids, a mathematical model of the unsteady, one-dimensional flow in a narrow, finite length channel, which includes a piecewise linear variation in channel width and several sharp-edged constrictions, has been solved for harmonic perturbations in the channel width. Model problem parameter variations are being investigated to identify spatial distributions of flow resistance which produce negative flow-damping and dynamic instabilities for the fundamental vibration mode of the tubes. Observed phenomena not explainable using one-dimensional flow models will be investigated using computational fluid mechanics techniques.

Another model problem, consisting of two different, infinitely long, uniform, and parallel flow channels that interact through a common wall, has been formulated to study linear and nonlinear responses and to develop mathematical techniques. In particular, spatially periodic bifurcation and secondary bifurcation solutions for the three channel walls, modeled using nonlinear von Karman plate theory, are being investigated for steady, one-dimensional viscous flow modeled by Darcy's law. Also sought is justification for the use of Darcy's law as an approximation to the Navier Stokes equations.

Argonne National Laboratory

Materials and Components Technology Division — **$129,000**
Argonne, IL 60439 — **01-A** — **87-3**

4. 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

Department of Mechanical and Aerospace Engineering — **$62,000**
Tempe, AZ 85287-6106 — **06-B** — **87-3**

5. Combustions and Heat Transfer in Porous Media
R.E. Peck, T.W. Tong

A study of combustion and heat transfer of premixed, gaseous fuel-air mixtures in inert porous media is underway. The objective is to generate fundamental information about flame propagation and heat release behavior in porous materials.

A theoretical model of the combustion and multimode heat transfer processes in planar porous media as a function of the relevant factors has been developed. The model includes finite-rate reaction kinetics and the equation of transfer for describing radiative heat transfer in porous media. Calculations revealed a unique spatial variation in elevated, stable flame speeds that was unique spatial variation in elevated, stable flame speeds that was linked to the relative importance of radiative and conductive heat fluxes. Parametric studies demonstrated the influence of porous material properties (optical depth, scattering albedo, and thermal conductivity), stoichiometry, convective coupling and heat sink temperature and reflectively on the burning rate and external radiant output when the porous matrix was used as a porous radiant burner.

Experimental are underway to obtain flame speed, product species concentration and temperature profiles, and energy output data under various operating conditions for comparison to theoretical predictions. Results for ceramic foam of low optical depth have confirmed the existence of two stable combustion zones, one in the upstream half of the porous material and the other at the downstream edge. Measured flame speeds and radiant output are also in close agreement with predicted values.

The findings will be useful for applying the relatively unexploited technology of porous radiant burners to industrial heating systems, yielding potentially large savings in energy consumption and operating costs. The results will also provide a scientific basis for understanding combustion and heat transfer in other energy technologies including catalytic combustors and combustion in packed beds and geological systems.

Boston University

Department of Chemistry **$70,380**
Boston, MA 02215 **06-C**
89-3

6. 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 the complicating presence of significant disorder and/or nonlinearity. Of special interest are materials with percolation thresholds, where the disorder blocks transport altogether and nonlinear effects become particularly pronounced. 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.

Porous solids may be modeled as fixed, overlapping or non-overlapping, hard spheres; these models may show percolation. The Repeated Ring kinetic equation accurately describes diffusion in these systems, but is difficult to solve. Novel methods were applied to this difficulty. Stochastic computer simulations were obtained which provide exact solutions in an intuitively appealing format. A self-consistent modeling of the kinetic operators also appears promising.

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 highly nonlinear process was constructed and solved in qualitative agreement with several observations. Computer simulation of the phenomenon was begun,with a particular eye to the study of laser-induced shock waves.

Brown University

Division of Engineering **$124,200**
Providence, RI 02912 **06-C**
87-3

7. 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 thermodynamics 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 explicity 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. Hermann of Stanford University which resulted in two joint papers.

University Of California, Berkeley

Department of Mechanical Engineering **$68,000**
Berkeley, CA 94720 **01-B**
87-3

8. The Turbulent Transport of Heat Within a Longitudinal Vortex/Boundary Layer Interaction
P.A. Eibeck

The physical processes that govern the transport of heat in turbulent, three-dimensional flows are not well understood, yet successful predictions of local convective heat transfer in most practical engineering flows require this information. Scalar transport in these complex flows is controlled by turbulent diffusion coupled with advection introduced by organized flow motions. The objective of this research program is to experimentally and computationally study the contribution of both mechanisms to the thermal transport in a boundary layer containing longitudinal swirl.

Three different flows are being studied; the single vortex embedded in a turbulent boundary layer, the trailing legs of a horseshoe vortex, and flow downstream of a spanwise row of obstacles. The single vortex is the simplest of these flows, such that detailed thermal transport measurements will isolate the influence of swirl from other flow complexities.

The trailing legs of a horseshoe vortex, located downstream of a stream-lined obstacle, have been observed close to the wall by our mean velocity measurements. This flow will have thermal transport influenced by both the swirl of the vortices and the wake effects.

The flow downstream of a spanwise row of obstacles presents the most complex flow configuration. Each obstacle will be rectangular with a height roughly equal to the boundary layer thickness. In addition to horseshoe-type vortices that will be generated at the leading edge, separation of the flow over the elements and reattachment downstream will lead to very large levels of turbulent mixing. The coherent vortical motions may still remain present, but their convective influence on local heat transfer may be less significant than the turbulent transfer of heat.

The experimental results of this study will be used to develop a phenomenological model for the predominant heat transfer mechanisms in turbulent flow containing swirl. We expect that a turbulent heat flux model incorporating both gradient-type diffusion (caused by the small-scale turbulence) and bulk convective transport (induced by the large-scale motion) may be appropriate for these flows. Computational predictions of the local Stanton numbers will be made utilizing the heat transport model.

University Of California, Berkeley

Department of Electrical Engineering and Computer Sciences **$95,000**
06-C
Berkeley, CA 94720 **87-3**

9. Self-generated Stochastic Heating in an RF Discharge
A.J. Lichtenberg, M.A. Lieberman

The purpose of the project is to study electron heating mechanisms in plane parallel, radio frequency (r.f.) discharges. These discharges are used extensively by industry for surface modification of electronic and mechanical materials. The energy deposition in these discharges is not well understood. In addition to the usual r.f. ohmic heating in the plasma interior, stochastic heating at the plasma surface is believed to play a major role.

The stochastic electron heating arises from successive decorrelated reflections of electrons with the oscillating sheath near the surface of the discharge. By examining the dynamics of the electron collisions with the sheath, a mapping is derived that describes the electron motion. For high frequency (frequency exceeding 50 MHz), the electron motion is found to be stochastic rather than adiabatic and heating occurs. A

Fokker-Planck equation is used to calculate the electron energy distribution, which is shown to be non-Maxwellian. A simulation model of the discharge, using self-consistent physical constraints gives results in agreement with the analytical theory. Elastic collisions will extend the stochastic heating to lower frequencies.

Power is deposited in a radio frequency discharge by three mechanisms: (1) ohmic heating of electrons; (2) stochastic heating of electrons by reflection from moving sheaths; and (3) acceleration of ions through sheaths and out of plasma. We are measuring the importance of each of these mechanisms in an argon discharge of a range of pressures, powers, and r.f. frequencies. A typical discharge has pressure 3 mTorr, power 100 watts, and frequency 13 Mhz. In this regime, we predict that 95% of the electron heating occurs stochastically.

University Of California, Irvine

Department of Mechanical Engineering **$83,800**
Irvine, CA 94720 **01-B**
89-1

10. Radiation in Particulate Systems
C.L. Tien

A combined analytical and experimental program investigates the effects of intraparticle interactions on the radiative properties of densely-packed particulate systems. The classical theory of radiative transfer in participating media, which assumes the particles respond to radiation independently of one another, is not valid for densely-packed systems. Examples of systems where dependent theory must be used include fluidized-bed combustors, catalytic reactors, packed-bed combustors, microsphere insulation, spray combustors, and furnaces laden with soot conglomerates.

Simple expression that include dependent effects have been developed for the radiative properties of random homogeneous systems, randomly oriented agglomerates, and for the effective diameter of agglomerates. Predictions from these expressions are in agreement with experimental data. This analysis has been applied to the problem of thermal radiation in packed and fluidized beds and to radiative heat transfer in porous media.

Continuing research focuses on three new topics involving radiative heat transfer: diffraction effects on radiative heat transfer; the influence of internal-field radiation on liquid droplet combustion; and the radiative properties of thin-film high-temperature superconductors. Again, both analytical and experimental work is being undertaken. Experiments will be carried out using a newly-acquired Fourier Transform Infrared Spectrometer and an existing conventional optical bench.

University Of California, Los Angeles

Mechanical, Aerospace and Nuclear **$80,000**
Engineering Dept. **01-C**
School of Engineering and Applied Science **89-3**
Los Angeles, CA 90024-1597

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

The research covers two broad areas: 1) single-phase convection in porous media, and 2) two-phase convection in porous media. The objective of this study is to develop physical understanding of the governing phenomena and models for prediction of transport processes by theoretical and experimental means.

The validity of stochastic models for single-phase flow through randomly packed beds was established by demonstrating that the predicted dispersive enhancement of the axial "effective" transport coefficient agrees with measurements found in literature of both heat and mass transfer. The role of this dispersive component on the heat transfer was considered in the porous Benard problem. This work will be continued by application of the Augmented Power Integral to Benard convection in the porous media. Numerical modeling of conduction in a bed of particles of one diameter has been shown to yield very good predictions of the bed conductivity if proper care is taken. This work will be extended to binary mixtures. Engineering correlations will be developed.

Steam injection in a porous channel is being studied experimentally and theoretically. In the experimental studies, the behavior of a steam-water interface in a porous channel will be measured with high speed movies. The pressure and temperature distributions will be measured along with flow rates of steam and water. The physical mechanisms causing the observed rapid oscillations of the interface between the two phase region and the subcooled water are being delineated. In the theoretical studies, critical conditions where a stationary of oscillatory steam zone will be established. Numerical modeling based on Darcy flow will yield the steam zone shape and size, local condensation rate along the interface, flow fields for both steam and water and temperature distributions.

University Of California, Los Angeles

Department of Mechanical, Aerospace, and Nuclear Engineering
School of Engineering & Applied Sciences
Los Angeles, CA 90024-1597

$68,000
06-B
88-2

12. 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

Department of Mechanical, Aerospace, and Nuclear Engineering
School of Engineering & Applied Sciences
Los Angeles, CA 90024-1597

$89,000
06-C
89-3

13. 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
Los Angeles, CA 90024

$ 78,000
06-C
87-3

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

The goal of this project is to advance our understanding of the response of nonlinear elastic media driven far from equilibrium. Research efforts are focused on the competition between turbulence and localization and how these processes affect the fate of energy which is injected, into a continuous medium, in the form of wave motion.

Regarding turbulence in propagating waves an attempt is being made to determine the probability distribution function for the higher-order correlations as well as the cross-correlations of the various modes. This goal requires the development of a theory of stochastic response that is an extension of the Fokker-Planck approach to ultra-long time scales.

Recent research also indicates that the wave turbulent state also possesses organized structure manifested by the appearance of new propagating modes analogous to second sound. These new modes have been calculated for wind driven waves in a stormy sea.

In one and two dimensional systems high amplitude wave motion can self-focus into long-lived structures that are the physical realization of solitons. Present research has led to the experimental discovery of envelope solitons in flexing shells and kink solitons in vibrating fluids. Extensive measurements are under way to determine the extent to which these solitons persist at amplitudes which are so high that there is no corresponding theory.

University Of California, San Diego

Institute for Nonlinear Science **$90,000**
La Jolla, CA 87545 **06-C**
89-1

15. 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 reproducers 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 **$124,200**
06-B
La Jolla, CA 92093 **87-3**

16. Fuel Droplets Subject to Straining Flow
P.A. Libby, K. Seshadri, 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. Three such flows of increasing simplicity have been studied to date: a nonpremixed laminar flame in a counterflow configuration, isothermal counterflowing nitrogen streams and a vertical Poiseuille flow. In each case the equations of motion in the axial and radial directions and the known gas velocities are used to determine the lift and drag which must be operative on the droplet to account for the observed trajectory. 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 not the mechanism operative in the rectilinear motion of spheres along the streamlines of a pure shear flow. Rather it is conjectured that rapid changes in the direction of the relative velocity vector results in an unsteady normal force identified with lift. This conjecture will be examined in future studies. The general conclusion is reached from these studies 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. Because of the large deviations of the forces from those expected, our research to date has focused on those forces but future experimental work will deal in detail with the heat and mass transfer to droplets. The presently available results from droplets in the flame indicate significant chemical kinetic effects: if the droplet passes through the reaction zone slowly large rates of mass loss are observed while high speed passages through the same zone lead to small mass loss. 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 the theory of spheres in pure shear flows. Quantitative comparison with the existing low Reynolds number theory is underway. In our theoretical work a new model for the combustion of droplets in a quiescent ambient involving water gas shift equilibrium at the flame has been developed. The influence of multicomponent diffusion on the rate of mass loss from spherically symmetric droplets is being studied. Finally, as a preliminary to future applications of the spray equations which leads to a differential-integral formulation of the conservation equations we are studying the relatively simple case of a laminar flame propagating in a cloud of fuel droplets.

University Of California, San Diego

Institute for Nonlinear Science, R-002 **$ 90,769**
La Jolla, CA 92093 **06-C**
89-3

17. 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 system segregation is observed if the dimension is 3 or smaller. These are interesting examples of spontaneous pattern formation.

University Of California, San Diego

Institute for Nonlinear Science **$78,000**
La Jolla, CA 92093 **01-C**
87-3

18. Parameterization of Intermittent Turbulence and the Vorton Method

E.A. Novikov

This research project involves the study of a new type of parameterization of small-scale turbulence, which recognizes the important phenomena of intermittency. The parameterization is based on the theory of intermittent relative motion of fluid particles, which may be of independent interest. The method of three-dimensional vortex singularities (vortons) is used for the calculations of elementary events in the intermittent turbulence (breakdown, reconnection and double reconnection of vortex filaments). The vorton method may also have applications to some problems in aeronautics. Some vorton calculations, including cross instability of two perturbed antiparallel vortex filaments and merging subsequent splitting of vortex rings, have been presented at IUTAM (Symposium of Fundamental Aspects of Vortex Motion September, 1987, Tokyo, Japan).

University Of California, Santa Barbara

Department of Physics **$128,300**
Santa Barbara, CA 93106 **06-C**
87-3

19. 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 point where stochastic effects control to 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 **$98,000**
Nuclear Engineering **01-C**
Santa Barbara, CA 93106 **88-3**

20. Turbulent Structure in Liquid Streams Bounded by a Free Surface and a Solid Wall

S. Banerjee, H. Fenech, G. Hetsroni

This project is a continuation of an ongoing project aimed at studying turbulence structure in liquid which flows between a solid surface and a gas-liquid interface. The experimental techniques used in this study include three-dimensional laser-Doppler anemometry with a 30-micron spot size and oxygen-bubble tracing with high-speed videos and flash photography. The oxygen-bubble technique resulted in capturing of the detailed turbulent production at the solid wall, including visualization and photography of the coherent structures at the wall, and the turbulent bursts. It was found that the turbulent bursts reach the interface and affect the heat and mass transfer there. It was also found that similar turbulent structures can be observed at the liquid gas interface, providing shear is applied on the liquid by gas cocurrent or countercurrent flow. these experimental methods were complemented by a numerical approach in which the full Navier Stokes equations were solved by a pseudospectral method to provide quantities which ar difficult to obtain by flow visualization and single-point velocity measurement. Both the experimental and computational techniques resulted in very similar turbulent description, and the computer flow simulations were very close to the experimental observations.

The experiments with the LDA are being continued on a newly designed and constructed test section. Also, the effect of waves on the turbulence characteristics will be studied. A wave generating machine is now being readied to be installed in the test section.

Carnegie Mellon University

Chemical Engineering Department and Graduate School of Industrial Administration **$155,003**
03-A
89-4
Pittsburgh, PA 15213

21. 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 process and often do not apply. This project addresses the development of systematic design methodologies for the redesign of chemical processes. This integrated approach deals with a broad range of problems in process redesign. Here we discuss progress in the following areas:

1) Development of Efficient Optimization Algorithms for Discrete and Continuous Variables. Efficient decomposition strategies for nonlinear programming have been developed for large-scale process optimization. Their refinement relies on newly developed primal/dual LP and QP algorithms developed earlier. In addition, for discrete variable systems two new exact algorithms have been developed for set partitioning and set covering problems.

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. We are also examining the impact of column heat integration.

3) Redesign of energy management systems. New mixed-integer nonlinear programming models are being 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 is 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, mathematical models have been developed to characterize controllability through the speed of recovery of a process to disturbances.

Carnegie Mellon University

Department of Electrical and Computer Engineering **$100,125**
03-C
Pittsburgh, PA 15213 **89-3**

22. 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 **$81,000**
Chicago, IL 60637 **06-C**
89-3

23. 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 **$150,000**
Chicago, IL 60637 **06-C**
87-3

24. 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

Department of Chemical Engineering **$59,996**
Potsdam, NY 13676 **01-C**
88-3

25. 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

Department of Mechanical Engineering **$50,480**
Storrs, CT 06268 **01-A**
88-3

26. 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 **$103,434**
01-C
Ithaca, NY 14853 **88-3**

27. 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 main 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 linear 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 **$116,644**
Hanover, NH 03755 **01-C**
88-3

28. 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 for particles. Results were also obtained for the forces on particles and the effective Berrioulli 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. New links have also been established between this approach and Geurst's variational methods.

Experiments have been performed to measure the natural frequency of arrays of spheres in water and air. Results are compatible with predicted values of the exertia.

Future work will continue along the same lines. It is anticipated that there will be further exploitations of the velocity potential in the fluid and functions derived from it, such as the average of its derivative with respect to time throughout the fluid and over the surface of particles. During the next year it is expected that oscillating spheres tests will be completed, with a variety of boundary conditions, and new ones devised with free assemblies of spheres, for example in fluidized beds.

Engineering Science Software, Inc.

Smithfield, RI 02917 **$ 48,626**
01-A
88-3

29. A Micromechanical Viscoplastic Stress-strain Model with Grain Boundary Sliding
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

Department of Mechanical Engineering **$129,000**
Houston, TX 77204-4792 **01-C**
87-3

30. 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 **$75,000**
Houston, TX 77204-4792 **01-B**
88-2

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

The potential for altering the boiling curve through the effects of high velocity and high subcooling will be investigated in this study. This investigation is based on evidence that the transition region can be avoided when very cold liquids are boiled at high velocities. An experimental flow loop capable of circulating liquids up to 8-10 m/sec will be equipped with a chiller so that liquid temperatures down to 3-4 C for water and -32 C for Freons are achievable. Boiling data along with visual observations of water and Freon-113 boiling from a small electrically heated cylinder in crossflow will be obtained.

As a complement to the experiments, an analytical model for film boiling heat transfer that accounts for turbulent flow in the liquid and vapor layers flowing over the heater will be developed. Existing laminar flow models will be modified to include turbulence effects. There is some evidence that flow of high velocity, subcooled liquids degenerates into "froth" in the normal film/transition regions. Insight into the nature of these flows will be sought using high speed video, and, if possible, models will be developed to predict heat transfer during such flows.

Idaho National Engineering Laboratory

Applied Optics **$183,000**
Idaho Falls, ID 83415 **06-A**
87-3

32. 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 Imm3 and allows the distribution of particle size, velocity and temperature to be mopped over laboratory scale flow fields. The influence of particle size, injection rate, torch power, etc., are currently being examined in ty pical flow fields.

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

Idaho National Engineering Laboratory

Sensors and Diagnostics Group **$189,000**
Idaho Falls, ID 83415 **03-B**
87-3

33. Nondestructive Characterization of Fracture Dynamics and Crack Growth

J.A. Johnson, K. Telschow

The objectives of this research are: to develop instrumentation and models to measure and predict the emission and interaction of ultrasound from growing cracks in engineering materials.

To develop NDE techniques for measurement of properties of high T_c superconducting materials and devices.

A high speed digital acoustic emission (AE) data acquisition system is being developed and applied to fracture mechanics experiments that are part of the Elastic-Plastic Fracture Analysis program at INEL and the Modeling and Analysis of Surface Cracks program at the Massachusetts Institute of Technology. The AE detection system is capable of detecting and digitizing AE signals with a larger bandwidth and with less dead time than in conventional systems. This allows improved resolution in detecting the locations of the sources of emissions and in discriminating between types of sources. A source of acoustic emission is modeled using finite element techniques by changing boundary conditions and the ultrasonic fields that propagate from the source to a receiver are calculated. All mode conversions are automatically included in the numerical solution. Other work includes transducer design, transducer calibration, generalized ray theory analysis (Green's functions), source location algorithms, and inverse source identification algorithms.

Starting in FY1989 the use of electromagnetic probes to measure the transport critical current in superconducting coatings, films and wires as a function of position are being designed and tested. These probes are noncontacting and can be scanned over the surface of the materials to provide information about the homogeneity of the superconductor. Probes with a resolution of 10 microns are being designed. A cryostat with access for scanning has been designed and is currently being assembled.

Idaho National Engineering Laboratory

Materials Technology Group **$454,000**
Idaho Falls, ID 83415-2218 **01-A**
87-3

34. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws

W.G. Reuter, W.R. Lloyd, S. Graham

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

Materials Technology Group **$530,000**
Idaho Falls, ID 83415 **06-A**
87-3

35. Experimental Measurement of the Plasma/Particle Interaction

C.B. Shaw, S.C. Snyder, L.D. Reynolds

The objective of this research is to quantitatively describe the heat mass, and momentum transfer associated with metallic or oxide particles immersed in thermal plasma environments. In order to characterize the interaction between plasma constituents and particles, the development of new methods to determine plasma flow velocity and species compositions are being developed. Holographic interferometry is currently being considered for plasma flow velocity determination and planar laser induced fluorescence is being considered for compositional measurements adjacent to particle surfaces. Using these advanced techniques, temporal and spatially resolved distributions of the chemical and physical properties of the plasma/particle environment will be determined. Since this research is performed in collaboration with research at Massachusetts Institute of Technology, the resulting experimental data will be used to validate and correct theoretical models used for thermal plasma processing and for predictions relating to optimal torch and fixture design criteria. Experiments are currently being performed in two plasma torch designs, a constricted nozzle torch and an expanding nozzle torch. Input power dissipation levels ranging from 5 to 180 kW are being studied. These torch designs produce a representative plasma characteristic of those employed for industrial plasma processing.

Idaho National Engineering Laboratory

Materials Technology Group **$465,000**
Idaho Falls, ID 83415 **03-A**
87-3

36. Integrated Sensor Model Development for Automated Welding

H.B. Smartt, J.A. Johnson

Automation of an arc welding process is presently limited by an incomplete understanding of the process dynamics, lack of subsurface sensing capability, and need for more advanced control capability. Heat and mass transfer in arc welding is typically dominated by coupling between the electrical and thermal dynamics of the process. Critical physical events include the formation, detachment from the electrode wire, and transfer of a liquid droplet in a plasma column, followed by the interaction of the droplet with a substrate and the associated convective flow and solidification. These droplet events are nonlinear and may be either periodic or chaotic depending on the state of the process. This project is studying the droplet events with the goal of developing fundamental models of process dynamics suitable for use in control applications. The transition from periodic to chaotic behavior is related to changes in droplet transfer mode; desirable transfer mode depends on engineering applications. Signal analysis/pattern recognition techniques are being developed for in-process recognition of droplet transfer mode.

Subsurface sensing of the liquid/solid interface bounding the weld pool is being developed using noncontact transducers. A laser is used to generate sound in the weld pool. The sound is detected with an electromagnetic acoustic transducer (EMAT) or a confocal Fabry-Perot interferometer. The transmission and reflection of the ultrasound provides information about the geometry of the pool and about the potential for defect formation. Signal analysis/pattern recognition techniques are being developed based on a combination of statistical and AI methods for automated measurements.

A neural network controller is being developed suitable for application to welding control. The network builds two models, one of the process dynamics and the other of the control dynamics, and is capable of accomplishing multiple-input, multiple-output control. A major effort is presently aimed at understanding the relationships between process state, network structure and learning dynamics. This will be followed by optimization of the network for multisensor integration capability.

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

University Of Illinois

Coordinated Science Laboratory **$124,195**
Urbana, IL 61801 **03-A**
88-3

37. Model Building and Control of Large Scale Systems

T. Basar, P. Kokotovic

The research agenda laid out in this proposal aims at a comprehensive study of some fundamental issues arising 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 oriented hierarch and multiple decision layers, and (iv) control and coordination of large scale systems based on (probabilistic) multimodeling. Following this a new framework will be developed, to allow for distributed and interactive model building and control, where both structural and design making hierarchies evolve over time. Its unique characteristic is that the two independent tasks - modeling and control - treated heretofore independently, will now be designed to evolve in parallel and complementary to each other.

University Of Illinois

Department of Chemical Engineering **$110,000**
Urbana, IL 61801 **01-C**
89-3

38. 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 develop methods to predict when slug flow will exist in horizontal gas-liquid flows, (2) to obtain a better understanding of the interfacial wave patterns in stratified gas-liquid flows, (3) to obtain improved predictive methods for horizontal and vertical annular flows. Vertical flow experiments are being conducted in pipelines with diameters of 3/4 in., 1 1/2 in., and 2 1/4 in. The horizontal flow facility, which has pipelines of 1 in., 2 in., and 4 in., was completely renovated during the past year so that it can operate with a wide range of liquid viscosities and at inclinations of 2 degrees.Three mechanisms have been identified for the initiation of slug flow. Slugs can originate from the growth of infinitesimal long wavelength disturbances or form small wavelength disturbance which develops into large wavelength disturbances through a non-linear energy transfer process. The possibility of their initiation by entry disturbances can be predicted by the development of necessary conditions for the existence of slugs.Interfacial stress in stratified flows has been associated with large amplitude waves which are generated by a Kelvin-Helmholtz mechanism. In particular, it has been shown that the stress is uniquely related to the wave steepness for wide range of pipe diameters and liquid viscosities.Techniques have been developed to measure the rates of atomization and deposition in vertical annular flow. A theoretical understanding of these rate processes is being obtained through measurements of wave patterns and droplet motions. These measurements are being used to develop better predictive methods for entrainment. Previous measurements of entrainment for air-water flow in a horizontal one inch pipe have been extended to include 2 inch and 4 inch pipelines. It is found that an understanding of the effect of pipe diameter on entrainment depends on understanding the importance of the gravitational settling of drops.

University Of Illinois At Chicago

Energy Resources Center **$ 74,070**
Chicago, IL 60680 **01-B**
89-2

39. 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 the two high molecular weight polymers, hydroxyethyl cellulose and polyacrylamide and a comparison with pool boiling performance of deionized water.

b) Forced convection behavior of viscoelastic fluids in laminar and turbulent flows 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. Detailed studies of the bubble dynamics using high speed video equipment are being carried out to establish a rational basis for the observed behavior.

b) The forced convection measurements in the rectangular channel, taken together with earlier circular tube measurements, lead to the following conclusions:

1. The friction-factor and heat transfer behavior of purely viscous and viscoelastic fluids is the same under fully developed laminar pipe flow conditions.

2. The heat transfer performance of viscoelastic fluids in laminar flow through rectangular channels is considerably higher than predicted for purely viscous fluids, although the friction factor is predicted by the purely viscous analysis.

3. In turbulent flow through circular and noncircular channels many, but not all, viscoelastic fluids are drag reducing. In particular, aqueous Carbopol solutions are viscoelastic but show no drag reduction.

University Of Illinois At Chicago

Department of Civil Engineering, Mechanics and Metallurgy — **$56,000**
Chicago, IL 60680 — **01-A** — **88-4**

40. Continuous Damage Mechanics II
D. Krajcinovic

The current state of development of the theory dealing with the brittle response of solids is characterized by a substantial arbitrariness reflected in a host of conflicting analytical models. The main objective of this research is to formulate a comprehensible continuum damage theory based on the improvements in the understanding of the underlying phenomena gained through experiments and application of micromechanics. Even though they are very useful micromechanical models typically require manipulations of very large databases causing significant computational complexities and presenting potent discouragement for their application in engineering practice.

The proposed model should retain the simplicity of a continuum theory without loosing the physical insights provided by the micromechanical studies. Once the theory has been checked on some benchmark problems (for which the pertinent micromechanical data are available) it will be possible to study more complicated problems.

The principal tasks of the initial phase of the project are: to select representative fluxes and affinities, to formulate a reasonable damage and failure surfaces and investigate the applicability of the normality property. Initial effort will be focused on the perfectly brittle response of solids such as concrete, rocks and ceramics.

Illinois Institute Of Technology

Department of Chemical Engineering — **$82,800**
Chicago, IL 60616 — **03-A** — **87-3**

41. Vibrational Control of Chemical Reactors: Selectivity Enhancement, Stabilization and Improvement of Transient Behavior
A. Cinar

The objective of this project is to develop novel applications of the vibrational control theory to various types of chemical reactors. From the mathematical standpoint, the goal of this research is to analyze the effects of fast parametric oscillations on the dynamics of the systems studied. Research is focused on three areas of application:

1) Selectivity and yield enhancement in parallel reactions with desirable and undesirable products. The oxidation of ethylene over supported silver catalysts to ethylene oxide and carbon dioxide is used as a test reaction.

2) Stabilization of nonadiabatic and autothermal tubular packed-bed reactor operation at an otherwise unstable steady state. The CO oxidation reaction is used as a test reaction.

3) Improvement of transient behavior of nonadiabatic and autothermal tubular packed-bed reactors by relocation of system zeros using vibrational-feedback control.

The theoretical developments will be tested experimentally on pilot scale equipment in the laboratory. Vibrational control will be implemented by introducing forced periodic oscillations in the input concentrations and flow rates. The effects of multiple vibrating inputs will be analyzed and the contributions of the phase relationships between the forcing functions of various inputs will be investigated. This study will provide techniques for improving selectivity and yield in complex chemical reactions and for reducing the overall control effort in reactor configurations used in the industry.

Jet Propulsion Laboratory

California Institute of Technology **$111,000**
Pasadena, CA 91109 **03-C**
89-3

42. 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.

Jet Propulsion Laboratory

California Institute of Technology **$81,000**
Pasadena, CA 91109 **03-B**
87-3

43. Applications of Molecules as High Resolution, High-Sensitivity Threshold Electron Detectors

A. Chutjian, S.H. Alajajian, O.J. Orient

Measurements and theoretical calculations are carried out of electron attachment cross section $\sigma_A(\varepsilon)$ and rate constants in molecules at electron energies below 200 millielectron volts (meV). Measurements are carried out at extremely high energy resolution (5-8 meV, FWHM) using the krypton photoionization technique developed at JPL. This electron energy region is accessible by no other experimental technique, and previously-published JPL results have clearly shown the s-wave threshold behavior in which $\sigma_A(\varepsilon)$ diverges as $\varepsilon^{-1/2}$. The molecules c-C_5F_8 and c-C_6F_{10} have shown extremely narrow, delta-function like widths for attachment of zero-energy electrons. This feature makes them suitable as high sensitivity threshold electron detectors useful in, for example, obtaining threshold photoelectron spectra of atoms and molecules. Published experimental results in F_2, and theoretical calculations in $CFCl_3$ and CCl_4 have shown significant discrepancies with calculation and other experiments (flowing afterglow) as to energy dependence of the $\sigma_A(\varepsilon)$, and temperature dependence of the rate constants. Recent results in HI and DI have shown a strong temperature dependence for attachment in DI, because the process is slightly endothermic (by 35 meV). These properties have bearing on the plasma-assisted etching process, isotope separation, and on soot (and/or electron density) reduction in combustion plasmas.

Johns Hoplins University

Mechanical Engineering Department **$98,214**
Baltimore, MD 21218 **01-C**
89-3

44. Numerical and Physical Modeling of Bubbly Flow Phenomena

A. Prosperetti

The objective of this proposal is the assessment of the accuracy of available phenomenological models of bubbly liquids and the development of new models. The means by which this will be achieved is through a comparison of the predictions of these models with the results of direct numerical simulations. A special numerical and analytical technique developed by the proposers renders calcualtions involving 40-50 bubbles feasible without recourse to supercomputers. Larger systems (e.g., and unbounded bubbly mixture) can be simulated by the periodic repetition of a fundamental "cell" containing 20-30 randomly placed bubbles. Available experience indicates that the artificial periodicity thereby introduced does not effect the main features of the simulation, which are the only ones of engineering significance. A number of different situations will be studied, such as pressure wave propagation through bubble screens, scattering by bubble clouds, the flow of bubbly mixtures through nozzles and over a wavy wall, the motion of a cloud of bubbles in an unbound expanse of liquid, and others.

Lawrence Berkeley Laboratory

Accelerator and Fusion Research Division **$125,000**
University of California **06-C**
Berkeley, CA 94720 **87-3**

45. 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 situation 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 **$190,000**
University of California **06-B**
Berkeley, CA 94720 **87-3**

46. 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 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

47. 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. 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. 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

Department of Mechanical Engineering **$ 0**
College Park, MD 20742 **01-C**
87-2

48. The Use of Optical Flow Fields in Establishing Stereo Correspondence
J.H. Duncan

The major difficulty in the analysis of stereo images is establishing correspondence, i.e., finding features in one image that correspond to given features in the other image. For static stereo pairs, a number of methods have been developed to establish correspondence. These methods are time consuming and difficult to implement at the edges of objects where the range is discontinuous. In many applications, there is relative motion between the camera pair and the objects in the field of view. In these cases, it is possible to obtain an optical flow field in the left and right images. Since the relative motion between the cameras is known, equations can be derived relating the left and right image flow fields. One relation is obtained by subtracting the flow fields; the resulting equation for the rate of change of disparity is called the binocular flow equation. Preliminary calculations and experiments for rigidly attached, parallel camera-pair configurations have shown that this relation is promising as a guide for establishing correspondence: potential matches can be tested by substituting the measured positions and velocities of the features into the equation. In the present study, the binocular flow equation is being explored in detail to find the limits of its usefulness in establishing correspondence in terms of camera- pair motions and surface shapes.

University Of Maryland

Department of Electrical Engineering **$83,000**
College Park, MD 20742 **06-C**
88-4

49. 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 **$81,778**
Baltimore, MD 21228 **03-B**
89-3

50. 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

Department of Mechanical Engineering	**$ 0**
and Systems Research Center	**03-C**
College Park, MD 20742	**88-3**

51. 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 methodology for the creation of multi-degree-of-freedom (DOF) gear trains and to explore its application for the designof robotic mechanisms.

Structural characteristics associated with the function of multi-DOF gear trains have been analyzed. A computational algorithm, based on graph theory and combinatorial analysis, has been developed for the enumeration of the kinematic structures. As a result, an atlas of two-DOF gear trains has been established. Furthermore, a class of robotic wrist mechanisms, using these gear trains for power transmission, has been developed. summaries of this work has been published in several articles in the ASME and IEEE journals. Bevel-gear-type wrist has the advantage of compactness and light weight. We are now in a position to perform the feasibility study of several new designs from the kinematic and dynamic points of view.

Using gear trains for power transmissions, robotic arms can be configured with the most of its actuators ground connected. This has the advantage of reduced inertia. A class of geared robotic arms will be enumerated and the kinematic and dynamic characteristics of such arms will be studied.

Geared robotic mechanisms do have the inherent backlash problems. Gear backlash introduces discontinuity and impact in the mechanical system. These undesirable properties can cause the response of a mechanical system to deviate from the desired function. Up to date, backlash can not be completely controlled with the existing techniques. A new and innovative method, based on the concept of redundant drives, for the control of gear backlash will be studied and experiments will be conducted to prove the concept.

University Of Maryland

Department of Mechanical Engineering	**$129,000**
College Park, MD 20742	**01-C**
	87-3

52. 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 mathematically 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 furtherdeveloped. 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 — **$ 0**
Amherst, MA 01003-0011 — **06-A**
88-3

53. 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 subtasks. 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 — **$118,000**
Goessmann Laboratory — **03-A**
Amherst, MA 01003-0011 — **87-3**

54. Screening Alternative Control Structures for Plant Control System

J.M. Douglas, M.F. Malone

An interactive computer code that helps the user to develop a conceptual design of a petrochemical process has been completed, and a similar code that helps the user to retrofit has also been completed. A code that estimates the incremental costs associated with the steady state control of the process is currently being developed. That is, the code helps to identify the dominant disturbances, it checks to see if an adequate number of manipulative variables are available for control (and it calculates the costs associated with modifying the flowsheet to ensure that the process is controllable), it assess if equipment constraints are encountered when disturbances enter the process and manipulative variables are changed to compensate for these disturbances (and it estimates the costs required to remove these constraints), and it suggests control system alternatives that give close to the optimum operating costs.

We are also building approximate dynamic models of complete processes in orderto determine the effect of control system alternatives on the total operating costs of the complete process. We intend to use the results of these studies to develop short-cut procedures for screening control system alternatives. Some short-cut models have been developed, but these need to be tested against rigorous simulations.

University Of Massachusetts

Chemical Engineering Department — **$80,000**
Goessmann Laboratory — **06-C**
Amherst, MA 01003-0011 — **88-3**

55. 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 (for a general presentation of experimental and computational studies see J.M. Ottino, C.W. Leong, H. Rising, and P.D. Swanson, Morphological structures produced by mixing in chaotic flows, Nature, 333, 419-425, 1988). Experimental work is planned to address the problems listed under area (2). However, most of the results to-date are due to simulation; a computational study 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 d. 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 (F.J. Muzzio and J.M. Ottino, Coagulation in chaotic flows, Phys. Rev. A, 38, to appear Sept. 1988). Studies continue in this area.

Massachusetts Institute Of Technology

The Energy Laboratory **$131,000**
Cambridge, MA 02139 **03-B**
88-3

56. Metal Transfer in Gas Metal Arc Welding

T.W. Eagar

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 **$130,000**
Cambridge, MA 02139 **06-A**
88-3

57. High Temperature Gas-Particle Reactions

J.F. Elliot, P.P. Bolsaitis

The purpose of the research is to examine the physicochemical 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 form 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 **$107,000**
Cambridge, MA 02139 **03-A**
87-3

58. 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

Department of Mechanical Engineering **$99,967**
Cambridge, MA 02139 **01-C**
89-3

59. 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

Energy Laboratory **$181,000**
Cambridge, MA 02139 **06-C**
88-3

60. A Parity Simulator for Nuclear Power Plant Dynamics

K.F. Hansen

The simulation of the behavior of dynamic systems is an important part of the computer field. The great advances in digital electronics are such that most simulation is done digitally. However, problems unique to the use of digital computers, such as computer languages, numerical algorithms, and computer/user interfaces have made simulation of engineering systems difficult and/or awkward. This is particularly true with regard to transient analysis of nuclear power plants.

One area of analog simulation that has remained in widespread use is that of "breadboard" circuits to simulate electronic networks. Recent developments have led to a very flexible and convenient breadboard technique called parity simulation, where individual integrated circuits in the simulator behave as individual circuit elements. The system is also user friendly in that the analyst communicates in his own engineering language. It is well-known that electric analogs can be constructed to other physical systems such as mechanical, thermal, fluid, magnetic, or acoustic systems.

The research objective of this project is to study the applicability of the parity simulation concept to fluid-flow systems such as encountered in nuclear power plants. Work to date has led to the successful electronic modelling of plant components such as pumps, pipes, reactor cores, heat exchangers, etc. The IC elements constructed have been used to solve the conservation of mass, energy, and momentum in single-phase incompressible and compressible flow; as well as two-phase homogeneous equilibrium flow.

Massachusetts Institute Of Technology

Laboratory for Manufacturing and Productivity — **$161,000**
Cambridge, Massachusetts 02139 — **03-B**, **88-3**

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

Gas Metal Arc Welding (GMAW) is a complex process involving thermal, geometric, and metallurgical transformations. Our work has been addressing the use of multivariable control methods to develop a comprehensive process control methodology for this and potentially other fusion welding processes. We have so far progressed on two independent fronts: measurement and control of geometric properties of the weld and measurement and control of weldment properties via thermal history control.

For the latter we have analyzed the process to develop a 3 input -3 output process model. The inputs include arc power, arc speed and high frequency arc motion (used to distribute the arc power along the weld line). The outputs comprise heat affected zone width, centerline cooling rate and overall weld cross sectional area. A full non-linear numerical simulation for this process has been developed and equivalent non-stationary linear transfer functions were used to explore the real-time control problem based on surface temperature measurement. It was found that because of the vast parameter variations present in welding the adaptive control methods are necessary for stable regulation. An adaptive control to regulate two output variables (heat affected zone width and cooling rate) was implemented and used to successfully demonstrate stable regulation of this non-linear, dynamically coupled system.

As for geometry control, we have concentrated on both bead contour measurement methods and on control models for the process. Off-line measurements using a standard structured light approach have been made, but these have proven to be insufficient for high bandwidth real-time control. Accordingly we have begun development of a enhanced system based on strobe light and gated CCD camera technology. Using these sensing system we have identified transfer function relating bead width and reinforcement height to process inputs of wire feed rate and torch speed. These functions have as well proven to be non-stationary and control approaches will again require adaptive methods.

Massachusetts Institute Of Technology

Department of Mechanical Engineering — **$70,000**
Cambridge, MA 02139 — **01-D**, **89-2**

62. 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

Department of Mechanical Engineering **$199,000**
Cambridge, MA 02139 **01-A**
88-3

63. 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 determining parametric limits of applicability of the "dominant singularity" formalism of nonlinear fracture mechanics in these crack configurations as they are influenced (principally) by material strain hardening, load magnitude, and crack geometry. When such single-parameter dominance is obtained, correlations of crack response with J-integral or related measures may be justified. The analysis requires detailed finite element computations which are too costly for routine applications, so further development of simplified analytical models such as the so-called "line-spring" model is underway.

To date, detailed non-linear three-dimensional finite element studies of surface cracks under predominant tension show that the asymptotic HRR stress fields of power law hardening materials typically dominate for nominal stress levels up to 75% of yield strength, with a rapid loss of dominance at higher load levels. Calculated crack front deformations are in good agreement with experimental measurements made at the Idaho National Engineering Laboratory. The line-spring has been generalized to include elastic/power law behavior, and resulting solutions are within a few percent of corresponding continuum solutions requiring more than an order of magnitude more computation.

Detailed three-dimensional studies of through-cracks in "thin" sheets have accurately quantified the stress intensity variation through the thickness, as well as the boundary layer structure near the intersection of the crack front with the free surface. Three-dimensional elastic plastic analysis of the plane strain/plane stress plastic zone transition in a through-cracked thin ductile plate has quantified the loss of dominant singularity constraint.

Prior work at the Idaho National Engineering Laboratory has shown that cracks growing laterally in the slant-mode may transform to cleavage even above the temperature usually regarded as safe in practice. These transitions have been found to show cleavage island ranging in size from a few grains to the specimen thickness. Tests of medium-sized specimens and numerical analysis of plastic crack growth are in progress as a basis for pressure vessels an improved assurance of safety. Related statistical modelling of cleavage transitions is also being performed.

Massachusetts Institute Of Technology

The Energy Laboratory **$135,000**
Cambridge, MA 02139 **01-A**
88-3

64. 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 such 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 mm in 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 "appropriated 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 2-0 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

Department of Mechanical Engineering **$113,525**
Cambridge, MA 02139 **01-C**
89-3

65. 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 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 biomodal, 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 **$ 98,000**
06-A
Cambridge, MA 02139 **88-3**

66. 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 based for plasma torch design.

Massachusetts Institute Of Technology[1]

Department of Chemical Engineering **$55,900**
Cambridge, MA 02139 **06-C**
88-3

Los Alamos National Laboratory[2]

Design Engineering Division **$100,000**
Los Alamos, NM 87545 **06-C**
88-3

Sandia National Laboratories[3]

Fluid and Thermal Sciences Department **$100,000**
Albuquerque, NM 87185 **06-C**
88-3

67. 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

Department of Mechanical Engineering **$120,060**
Minneapolis, MN 55455 **01-B**
87-4

68. 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

Department of Aerospace Engineering **$ 72,000**
and Mechanics **01-C**
Minneapolis, MN 55455 **87-3**

69. Lubricated Pipelining
D.D. Joseph

This project has as its aim the understanding and control of water lubricated pipelining of viscous crude oils, coal-oil dispersions and other viscous materials. The basis for this work is that there are domains of parameters in which water lubricated transportation of viscous materials is stable. The lubricated configurations can introduce enormous savings of energy in the form of reduced pressure gradients for enhanced transport. The studies underway are theoretical and experimental. The experimental studies are on the transportation of coal oil dispersions, on the properties of emulsified solutions at large shear, and on stable wavy interfaces arising from nonlinear interactions. The problem of coal-oil dispersions is to know if the coal can be made to stay in the oil under conditions of lubricated transport. Stability calculations underway are designed to identify the windows of parameters in which core annular flow is stable and to calculate maximum growth rates for unstable flow. Future studies will concentrate on extensions to include effects of oil wetted walls, gravity and nonlinear mechanisms.

University Of Minnesota

Department of Mechanical Engineering **$ 0**
Minneapolis, MN 55455 **06-C**
88-3

70. Thermal Plasma Processing of Materials
E. Pfender

The objective of this research project is a combined experimental and analytical study for thermal plasma processing of materials including the production of fine ceramic powders.

A new Triple Torch Plasma Reactor (TTPR) has been used for the synthesis of fine AlN powders. By controlling the aluminum nitrogen ratio a complete conversion can be achieved and with proper control of the quenching rate, single phase hexagonal AlN can be obtained. A computer simulation of this reaction has been performed in parallel with the experimental work.

Since the TTPR allows injection of powder into the hot core of converging plasma jets, plasma spraying of ceramic materials has been explored.

Zirconium hydroxide doped with yttrium hydroxide equivalent to 9 mole % yittria produced by a sol-gel reaction has been used for making coatings of zirconia on mild steel substrates.

An anode assembly for transferred arc operation has been designed and manufactured in order to study this mode of operation in the TTPR. A micron size powder feeding system is under investigation to improve particulate feeding and resolve the problem encountered during the AlN synthesis.

National Institute Of Standards And Technology*

Thermophysics Division **$85,000**
Boulder, CO 80303 **06-A**
87-2

71. Neutron Scattering From a Sheared Liquid: a Proposal to Construct the Shearing Apparatus
H.J.M. Hanley

The project is to develop equipment to measure the microstructure of liquids out of equilibrium. The objective of the research is to investigate, via neutron scattering, liquids subject to a shear. The work will focus on the examination of the variation of the structure with respect to a universal parameter, the relaxation time. The relaxation time is the key to characterizing the complexity of the fluid (i.e., complex versus simple) and how it will behave out of equilibrium.

To a first approximation, the relaxation time is proportional to the viscosity. The relaxation time, and hence the viscosity, varies over many orders of magnitude. We, therefore, decided to construct two shearing cells for use in the neutron beam, one to accommodate a liquid with a low to moderate viscosity, the other to handle very viscous liquids.

We have constructed and tested a couette-type concentric cylinder apparatus to investigate liquids with viscosities of the order of 10 MPa or less at equilibrium and under shear. The apparatus is intended to be available to SANS users as a general purpose tool. Design features include: a) versatility and a rugged construction, b) a wide range of shear rates and operating temperatures, and c) fully automated computer controlled and programmable functions. Test results have shown shear-induced changes in the microstructure of polystyrene colloidal suspensions.

The preliminary shearing cell for liquids of high viscosity has been completed and preliminary neutron scattering data from supercooled (viscosity = 108 Pa.s) D-glycerol taken. The cell will be modified to investigate temperature gradients and viscous heating in the sample. Neutron scattering data will be remeasured. The structure of the liquid will be inferred from the intensity patterns when the fluid is at rest and when it is

* Formerly the National Bureau of Standards

sheared. Of particular interest is the possible structure that may extend over several molecular diameters.

National Institute Of Standards And Technology

Chemical Engineering Science Division — **$ 0**
Center for Chemical Engineering — **01-C**
Boulder, CO 80303-3328 — **87-2**

72. Residence Time Distribution Approach to the Study of Free Convection in Porous Media
M.C. Jones, J.D. Wolfe

The structure and dynamics of the global flow patterns of free-convective flows in confined porous media is an important area of study for many engineering applications. In this project, a new experimental approach is being developed based on the principles of residence time distributions. Earlier work has shown these to be a sensitive indicator of such flow patterns.

On the experimental side, a new laser fluorescence fiberoptic probe of superior sensitivity has been successfully developed. Arrays of such probes are being used with fluorescent dyes to detect flow patterns in fluid-saturated containers filled with uniform glass spheres subject to free-convective flows under precisely controlled conditions. In order to interpret the experimental results, a computer code is under development in which the progress of a tracer can be followed in three dimensions for convecting patterns appropriate to a range of Rayleigh numbers and throughflow Pellet numbers. The role of non-linear drag and of non-isotropic dispersion for both heat and mass transport is being studied. Unsteady flows known to exist at high Rayleigh numbers are of particular interest.

National Institute Of Standards And Technology

Electromagnetic Technology Division — **$100,000**
Boulder, CO 80303 — **06-C**
89-3

73. 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 stable, low-resistivity, ohmic contacts between semiconductors and the high-T_c oxide superconductors.

A method for making low resistivity metal contacts to $Y_1Ba_2Cu_3O_x$ (YBCO) with contact surface resistivities (area-resistance product) in the 10ijn 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 allow 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.

National Institute Of Standards And Technology

Thermophysics Division — **$538,000**
Boulder, CO 80303 — **03-B**
87-3

74. Thermophysical Property Measurements in Fluid Mixtures
R. Kayser, J.M.H. 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 NBS 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), PVTx (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.

The City University Of New York
The City College

The Benjamin Levich Institute for Physico-Chemical Hydrodynamics **$129,000**
New York, New York 10031 **01-C**
87-3

75. 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 has been developed. 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.

City University Of New York
The City College

Department of Chemical Engineering **$82,000**
New York, New York 10031 **01-C**
87-3

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

The research to be undertaken in this project is concerned with understanding the hydrodynamics of the flows of immiscible liquid phases in narrow capillaries. The research has experimental and theoretical components. The aim of the experimental component is to measure the pressure drops which are developed in these flows, and the film thicknesses of the wetting layers deposited on the inside surface of the capillary. The aim of the theoretical component is to develop a numerical algorithms to solve for the hydrodynamic flow, and to undertake a hydrodynamic stability analysis to describe the stability of the wetting layer to the destabilizing effects of capillary and viscosity stratification.

The major applications of the research are to the technologies of enhanced oil recovery and lubricated pipelining. Each of these technologies involves the movement of immiscible phases. The results of our experimental and theoretical work should lead to the identification of operating conditions for which the multiphase flows are ordered.

City University Of New York
The City College

The Benjamin Levich Institute of Physico-Chemical Hydrodynamics — **$124,000**
New York, New York 10031 — **06-C** — **87-3**

77. 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-field intensity 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 — **$69,300**
Raleigh, NC 27695-7910 — **06-B** — **87-3**

78. Analysis of Transport Mechanisms in Dense Fuel Droplet Sprays
C. Kleinstreuer

Of interest are the effects of droplet interaction on the droplet vaporization and heat transfer in spray systems. The dense spray portion is conceptualized as two of three streamers of several closely spaced droplets in a non-isothermal environment. Two basic approaches are carried out to analyze and solve this problem: (1) a finite element solution of the complete transport equations for thermal axisymmetric flow past a linear array of solid spheres and vaporizing droplets at different spacings; and (2) a boundary-layer type solution at appropriately high Reynolds numbers of single spheres/droplets with mixed convection and wall mass transfer effects, and for several dynamically interacting, vaporizing droplets.

The direct integration of the coupled momentum, heat and mass transfer equations for several closely-spaced spheres or droplets has been completed. The validated results in terms of drag/interaction coefficients and near-wake heat transfer parameters are being used in the approximate analysis of a single streamer of several spheres/droplets. The boundary-layer study of mixed thermal convection past a sphere with wall mass transfer and other effects has been completed. Some of the newly derived transformations from this fundamental research study will be useful for the more elaborate investigation of several interacting spheres/droplets.

The fundamental analysis of multiple droplet systems is important for the physical understanding of dense spray processes and for the improved design of fuel droplet combustion as well as spray cooling, coating and absorption.

North Carolina State University

Department of Mechanical and Aerospace Engineering **$ 97,000**
06-A
Raleigh, NC 27695-7910 **89-4**

79. 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 of 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 **$85,450**
Evanston, IL 60208 **03-B**
89-3

80. 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 **$312,617**
01-B
Evanston, IL 60208 **89-3**

81. Thinning And Rupture of a Thin Liquid File 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, thermo-capillarity 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 andvan 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.

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.

Northwestern University

Department of Engineering Sciences and Applied Mathematics — **$51,750**
Evanston, Illinois 60208 — **01-C** — **88-3**

82. 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 — **$51,948**
Notre Dame, IN 46556 — **01-C** — **88-3**

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

The objectives of the work are to develop a quantitative understanding of interfacial waves which occur in separated gas-liquid flows. While these waves exert a significant influence on pressure drop, transport rates, rate of atomization and flow regime stability, their fundamental nature is not well characterized.

The primary focus in the past year has been conditions where waves have wavelengths much longer than the film thickness. Far above the point of natural stability, under conditions typical of annular flows, the wave field is dominated by traveling solitary waves which are spaced randomly. Techniques to measure the distributions of the amplitudes and time spacings of solitary waves have been developed. These measurements indicate that as the gas velocity increases, the number and speed of these waves increases while their average amplitude decreases. Experiments to determine the degree of steadiness in shape with distance are underway. The question about the mechanism of the initial formation of these waves has been tentatively answered by examination of the flow with high speed (500 FPS) video imaging --solitary waves are observed to form from continued growth of some of the existing periodic waves. Periodic waves arise from the linear instability. To interpret the observed behavior, geometric factors (e.g. wave height to substrate height) associated with solitary waves are being examined. The theoretical and experimental study of periodic waves is continuing with a goal of predicting theoretically, from numerical solution of wave equations, the evolution with distance of the initial linearly unstable disturbances.

Oak Ridge National Laboratory

Engineering Physics and Mathematics Division — **$1,115,000**
Oak Ridge, TN 37831 — **03-C** — **87-5**

84. Center for Engineering Systems Advanced Research (CESAR)
C.R. Weisbin

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 1988 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.

Ohio State University

Physics Department — **$67,300**
Columbus, OH 43210 — **03-B** — **88-3**

85. 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 — **$110,150**
Philadelphia, PA 19141 — **03-B** — **88-3**

86. 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 on the 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 **$157,000**
Torrance, CA 90505 **03-B**
89-3

87. 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-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 noncoherent and noncoherent electromagnetic sources.

Physical Sciences Inc.

20 New England Business Center **$125,000**
Andover, MA 01810 **06-A**
88-4

88. 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 binary nucleation and droplet growth, 2) to stringently test theories of binary 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 much higher binary nucleation rates than have been studied previously. The nozzle is designed to ensure that steady-state nucleation occurs and to give satisfactory spatial resolution of the temperature profile as determined by interferometry. Laser light scattering combined with empirical calculations of the latent heat released during condensation is used to detect the "onset" of nucleation and to monitor subsequent droplet growth. Construction of the flow and optical systems has been completed in previous years; data collection is now being performed routinely. A new thermodynamic theory of binary cluster composition has been developed. Calculations with this theory have established the feasibility of using bulk liquid mixture surface tensions to compute nucleation onset (for small rates) in aqueous alcohol and acetone mixtures, thus removing a severe deficiency of classical binary nucleation theory.

Princeton University

Department of Mechanical and Aerospace Engineering **$97,000**
06-B
Princeton, NJ **87-3**

89. Structure and Stabilization of Premixed and Diffusion Flames
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 dynamics of the partially-remixed counterflow system consisting of a fuel jet impinging onto a jet fuel/oxidizer mixture. Results show that if the premixed jet is only slightly reactive, then the resulting flame resembles a diffusion flame. However, if it is moderately or strongly reactive, then a binary flame configuration results, consisting of either a premixed-diffusion flame ensemble or a premixed-premixed flame ensemble. It is further demonstrated that in all situations extinction of the flame ensemble takes place in a single stage, with the flame still separated in the binary configuration. These theoretical predictions have be substantiated by experimentation.

A detailed asymptotic analysis has been performed for a flame stabilized over a flat-flame burner. Previous studies have shown that two flame speeds can result with the same heat loss rate, leading to the classical anomaly of dual flame speeds. The present study demonstrates that each of these flame speeds actually has a distinctively different flamefront standoff distance, implying that they actually correspond to two different physical states. The previous anomaly is therefore unfounded.

Extensive experimentation has also been performed on measuring the laminar flame speeds and theory burning intensities of methane/air flames, with particular emphasis on identifying the role of branching versus inhibition reactions on the flame response. By systematically varying the flame temperature and system pressure, the overall reaction orders (n) and activation energies (E_a) have been determined. Results show that n is always less than two, and actually is close to one for the stoichiometric mixture at 1 atm. Further, n decreases with increasing pressure and can even attain negative values for sufficiently high pressures. The overall activation energy also increases with pressure. These results indicate the importance of chain mechanism in the overall kinetic scheme.

Purdue University

School of Mechanical Engineering — **$92,217**
West Lafayette, IN 47907 — **01-C**
87-3

90. 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 Mechanical Engineering — **$115,000**
West Lafayette, IN 47907 — **01-B**
85-4

91. Heating and Evaporation of Turbulent Liquid Films
I. Mudawwar

This project aims at studying transport phenomena associated with turbulent liquid film flow. Experiments have been performed with films undergoing sensible heating or interfacial evaporation and correlations have been developed for a wide range of operating conditions. To better understand the effects of interfacial waves on film motion a new high resolution film thickness probe has been developed. Instantaneous measurements of film thickness have been obtained for adiabatic film flow, and a modified probe design is expected to provide film thickness measurements on an electrically heated test section. The remaining tasks of this project will involve obtaining simultaneous measurements of film thickness and liquid temperature to better understand the transient variation of the heat transfer coefficient associated with film waviness. Parallel to this study, simultaneous measurements of the instantaneous longitudinal and transverse velocity components and of film thickness will be used to correlate a time-averaged eddy diffusivity profile which accounts for interfacial wave activity.

Rensselaer Polytechnic Institute

Department of Mechanical Engineering, Aeronautical Engineering & Mechanics **$233,471**
Troy, NY 12180-3590 **01-B**
89-4

92. 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, 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

Department of Mechanical Engineering, Aeronautical Engineering & Mechanics **$129,400**
Troy, NY 12180-3590 **01-A**
88-3

93. 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 **$124,000**
Troy, NY 12180-3590 **01-C**
86-3

94. 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 the postulates of continuum mechanics.

To this end, an analytical basis for the identification of unacceptable interfacial transfer laws is being developed. In addition, closure laws are being developed such that two-fluid models can be used to investigate many important phenomena, such as the prediction of interfacial area density and flow regime transition. Linear and nonlinear void wave phenomena are also being investigated in order to thoroughly understand the effect of the closure conditions on the eigenvalues of the two-fluid model (i.e., well posedness).

It is felt that the results of this research should significantly advance the state-of-the-art in the two-fluid modeling of the two-phase flows such that in the future, two-fluids models can be used with confidence for problems of industrial interest.

Rensselaer Polytechnic Institute

Department of Chemical Engineering **$85,000**
Troy, NY 12180-3590 **01-C**
89-3

95. 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

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

96. 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 the "fully frustrated" two dimensional regular Josephson junction array. I-V characteristics were computed and reasonable agreement found with experiment. Behavior was explained within a simple physical model, in which correlations between vortices is crucial for producing the critical excitations leading to vortex flow resistance.

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 and generators.

The Rockefeller University

Department of Physics **$82,400**
1230 York Avenue **06-C**
New York, NY 10021 **88-3**

97. 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 automat with independent particles moving on a lattice occupied by randomly placed scatterers is carried out. Two goals: 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 Laboratories

Combustion Research Facility **$140,000**
Thermofluids Division **06-B**
Livermore, CA 94550 **87-3**

98. Spatial Random Processes in Combustion
A.R. Kerstein

The goal of this project is to develop stochastic models which capture the dynamics of evolving spatial structures observed experimentally in various combustion environments. Examples of such evolving structures are the surface morphology of a burning coal particle, the shape of a flame front traversing a turbulent fuel-air mixture, and the temperature field in a turbulent diffusion flame.

The turbulent combustion environments are modeled by adopting a stochastic rearrangement process to simulate convective stirring, in conjunction with a deterministic representation of molecular diffusion and chemical reactions. Restriction of the computational domain to one spatial dimension facilitates the inclusion of all relevant length scales in high-Reynolds-number flow simulations. This approach avoids the difficulties that arise when the fine-scale processes are modeled separately. Work to date has demonstrated that this approach reproduces salient features observed in several turbulent mixing experiments. Further development and application of the method to combustion problems is in progress.

Combustion of heterogeneous solids is treated by means of stochastic network-breakup models representing, on a macroscopic scale, the disintegration of a reacting particle into fragments, or on a microscopic scale, the thermochemical dissociation of a macromolecular fuel such as coal. Such models have been formulated in work to date, and they are presently being validated based on comparison to coal pyrolysis and oxidation measurements.

Sandia National Laboratories

Combustion Research Facility **$140,000**
Thermofluids Division **06-B**
Livermore, CA 94551-0969 **87-3**

99. 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 ligaments and 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.

Science Applications International Corporation

Applied Plasma Physics and Technology Division **$88,000**
10260 Campus Point Drive **06-C**
San Diego, CA 92121 **88-2**

100. Transport Properties of Multi-Components Fluids and of Suspensions
I. Oppenheim, J. McBride

The first part of the research is to derive the non-linear hydrodynamic equations for multi-component fluids together with the conditions under which they are valid using the statistical mechanics theory of mode-mode coupling. The second part of the research is to study the transport properties of suspensions using recently developed methods for eliminating fast variables in many-particle systems. A general non-equilibrium ensemble averaging has been used to generate macroscopic, nonlinear fluid-transport equations with corrections due to long-time tail effects (the formalism can be used to derive hydrodynamic equations beyond the Navier-Stokes equations). The exact equations are nonlocal in both space and time and can be simplified to yield local equations. The present theory which is restricted to one-component fluids is to be generalized to include the effects of multi-component fields. The aim is to obtain the nonlinear hydrodynamic equations together with the properties of the appropriate long-time tail phenomena. A new technique for the derivation of the Fokker-Planck equation governing the probability density for the position and momentum of a heavy (Brownian) particle in a fluid has been developed. This technique is based on a scheme for eliminating fast variables for phenomenological equations. The present research plan is to utilize this technique to obtain the Fokker-Planck equation for many particles suspended in a fluid and for the perturbation of the fluid properties due to the motion of these particles. Previous treatments of suspensions have either been phenomenological or have used molecular theories which do not have the advantages outlines above.

Stanford University

Department of Mechanical Engineering **$68,000**
Stanford, CA 94305-3030 **01-B**
89-3

101. 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. The long term goal is to extend the extensive practical and theoretical understanding of 2D boundary layers to more commonly encountered 3D boundary layers. Early work on this project examined distortions of a 2D boundary layer with embedded longitudinal vortices. Extensive data including 3-component mean velocity, all Reynolds stresses, the temperature field, and the heat transfer coefficient demonstrated that conventional two-dimensional similarity laws are violated by this important subclass of three-dimensional boundary layers.

The most recent experiment is a study of an initially 2D boundary layer which is skewed laterally by a pressure gradient resulting in storing three dimensionality but little flow normal to the wall. Two different cases were examined in which the ratio of the streamwise to spanwise pressure gradient was varied. The turbulence measurements showed that the ratio of the Reynolds shearing stress to the turbulent kinetic energy falls rapidly and the shear stress vector in the plane of the wall is not aligned with the strain rate. Both of these effects suggest rapid distortion of the turbulence structure. However, the heat transfer behavior is not as complicated. A vector enthalpy thickness was defined based on an integral analysis of the 3D boundary layer. Using the magnitude of the vector in the standard correlation of Stanton number versus enthalpy thickness Reynolds number collapses the data from both the measured data sets.

Stanford University

Department of Mechanical Engineering **$170,000**
Stanford, CA 94305-3030 **01-A**
86-4

102. 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 examine 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 Laboratories of Physics **$ 0**
Stanford, CA 94305-3030 **03-B**
87-3

103. Nondestructive Testing
G.S. Kino

The aim of this project is to arrive at techniques for contactless nondestructive testing and range sensing. Devices which can be rapidly scanned over a surface so as to detect flaws and measure their profiles are badly needed. The measurement of parameters such as surface roughness are also required. For this purpose, we are developing acoustic sensors operating in air and contactless photoacoustic techniques.

We have developed a new type of PZT ceramic acoustic transducer with a quarter wavelength matching layer of RTV rubber which operates in air in the frequency range of 18 MHz. The transducer itself has been used for range sensing and for photoacoustic measurements. As an example, it has enabled us to measure regions of high surface recombination rates on semiconductors by varying the number of injected carriers in a semiconductor, using a laser beam modulated at 2 MHz. We detect the rf term in the surface temperature due to recombination. Similar techniques have been used by us to measure film thicknesses and profiles.

We are now developing a new acoustic transducer operating in air which utilized a 1000 A thick pellicle of boron nitride as the detector of acoustic waves in the air. The deflection of the surface is measured by highly sensitive optical phase measurement of an optical beam reflected from the pellicle. The system is as sensitive as our previous acoustic transducer, but has the advantage that it can be operated over a bandwidth from a few Hz to several MHz.

Stanford University

Department of Civil Engineering **$121,000**
Environmental Fluid Mechanics Laboratory **01-B**
Stanford, CA 94305-4020 **87-3**

104. 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 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 allow 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

Department of Mechanical Engineering **$ 0**
Stanford, CA 94305 **03-B**
88-4

105. Diagnostics For Plasma Chemistry
C.H. Kruger, M.A. Cappelli

This research is directed to the development of optical diagnostics for plasma chemistry and plasma processing, with an emphasis on methods that assess and measure departures from local thermodynamic equilibrium which can result from finite chemical reaction rates, elevated electron temperatures and densities, and radiation loss effects. The research utilizes a newly implemented induction-plasma facility and existing high-power lasers in the High Temperature Gas Dynamics Laboratory. Optical methods are being developed for concentrations of chemical species in plasmas and plasma parameters including electron density and temperature. The research is intended to provide a more firm scientific basis for the understanding of plasma chemistry and its practical development by providing diagnostic techniques to monitor plasma parameters and in investigating the importance and effects of nonequilibrium on so-called thermal plasmas.

Results to date from spectroscopic measurements of the inductively coupled plasma show significant nonequilibrium at the exit of a specially constructed 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. These results have been interpreted in terms of nonequilibrium effects in the earlier experiments. Preliminary results with an auxilary nonequilibrium discharge suggest that plasma nonequilibrium can have a significant effect on chemical reaction rates, as predicted theoretically.

Stanford University

Department of Chemistry **$229,390**
Stanford, CA 94305 **06-C**
89-3

106. 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

Department of Mechanical Engineering **$84,708**
Design Division **03-A**
Stanford, CA 94305 **88-3**

107. Global Optimization of Non-Polynomial Design Models
D.J. Wilde

This theoretical and computational research intends to bring the theory and practice of Monotonicity Analysis and Geometric Programming to bear on variational and 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.

Monotonicity Analysis would rapidly identify active constraints, and Geometric Programming would produce models more accurately describing the functions involved. Since for existing methods each iteration requires a computationally intensive finite element analysis of the structure involving thousands of variables, these innovations are intended to reduce the number of iterations. A Geometric Programming approximation of a finite element model of a cantilever support has converged after only four finite element analyses.

Earlier related work on non-convex optimization applied to geometric modeling has produced a unique **convergent** convex decomposition of 3-dimensional polyhedra, an extension of the Alternating Sum of Volumes (ASV) method which does not always converge. This hierarchical volumetric procedure can be applied to such 3D geometric problems as point inclusion, robot path planning, feature recognition, equality checking and mass property computation.

Stevens Institute Of Technology

Department of Physics and Engineering $ 66,757
Hoboken, NJ 07030 06-C
87-4

108. 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, 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.

University Of Texas At Austin

Center for Studies in Statistical Mech. $100,000
Austin, TX 78712 06-C
88-3

109. 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 **$147,000**
Austin, TX 78712 **06-C**
87-5

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

Dynamical systems methods are being developed and used to characterized 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.

University Of Texas At Austin

Department of Mechanical Engineering **$138,700**
and Center for Energy Studies **01-B**
Austin, TX 78712 **87-3**

111. Self-Shielding of Surfaces Irradiated by Intense Energy Fluxes
P.L. Varghese, J.R. Howell

The objective of this work is to study the interactions between high-temperature, high velocity plasmas and solid surfaces. There are two main thrusts in the program: numerical modeling and experimental testing of model predictions. This calibrated modeling procedure will provide information for reliable predictions of plasma-surface interactions with extremely high energy fluxes. The work will be conducted in unique facilities at the University of Texas at Austin. Plasmas at high temperatures (greater than 10,000 K) and densities ($10^{15}/cm^3$) will be accelerated in capacitor or homopolar generator driven rail guns. These plasmas will be studied using high speed emission spectroscopy and laser induced fluorescence in order to determine the composition and temperature of the plasma, and to detect the development and influence of the vapor shield produced by the surface when it is heated rapidly. The experimental results will be used to modify and refine the numerical model so as to provide an accurate and reliable predictive tool. The model will characterize the basic physical processes that govern the interaction between a surface and a transient energy flux. Because it is fundamentally based, rather than empirical, the model will be more readily adaptable to a wide range of situations in which surfaces are irradiated by intense energy fluxes. The model developed during the course of this work will allow better design of devices such as high current density brushes and switch gear, arc welding apparatus, rail guns, and fusion reactors.

Tufts University

Department of Mechanical Engineering **$ 57,000**
Medford, MA 02155 **01-A**
88-3

112. 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, microcracking in composite materials under fatigue conditions may noticeably reduce the stiffness of the material and make it ansiotropic. 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 **$185,024**
East Hartford, CT 06108 **06-A**
89-3

113. 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 State University

Department of Mechanical Engineering **$70,000**
Pullman, WA 99164-2920 **01-B**
89-2

114. Particle Dispersion by Ordered Motion in Mixing Layers

T.R. Troutt

Recent experimental and numerical results have shown that organized vortex structures in plane mixing layers dominate the particle dispersion process. These previous results show that if the time scale of organized vortex motion is of the same order as the particle aerodynamic response time significantly enhanced particle dispersions rates will occur. Moreover, these previous studies have also shown that advanced computer models can be employed to accurately predict the dispersion patterns for various size particles injected into a plane mixing layer.

The present research extends the previous study to the more complex flows associated with plane wakes. These flows have organized vortex patterns with differing senses of vorticity in addition to having near wake recirculation regions. Both the particle/vortex time scale ratio and a spatial ratio created at the wake initiation involving the upstream boundary layer thickness and the trailing edge thickness and the trailing edge thickness of the wake generation body become important parameters affecting the particle dispersion patterns. The specific objectives of this research program are to determine the role of organized vortices in the particle dispersion process in plane wakes, to determine the influence of both the time and spatial ratio parameters in the particle dispersion process in plane wakes, and to determine the effect of controlled forcing on the particle dispersion process in plane wakes. These objectives are to be pursued using a combined approach involving both advanced experimental and numerical techniques. The potential outcome of these studies is to determine if previously successful techniques and concepts can be applied to a more complex flow with close connections to many technologically important situations. If this outcome is realized implementation of these new concepts for practical advantages in new designs is highly plausible.

* UTRC consultant, presently at University of Connecticut/Institute of Materials Science

University Of Wisconsin

Mechanical Engineering Department **$103,200**
Madison, WI 53201 **01-C**
87-3

115. Interfacial Area and Interfacial Transfer in Two-Phase Flow Systems

G. Kocamustafaogullari

The research program is a joint effort by the members of the University of Wisconsin-Milwaukee and Argonne National Laboratory. The objective of the research program is to develop instrumentation techniques, a data base and predictive methods for describing the interfacial structure of horizontal and vertical two-phase flow, such as flow pattern transitions, interfacial area concentration and interfacial wave structure. The special emphasis will be placed on developing local interfacial area concentration measurement techniques, and two-phase flow-pattern transition criteria. The latter include 1) scaling criteria in terms of systems size and fluid properties 2) entrance geometry and developing flow effects, and 3) rational procedure and design criteria for predicting these effects.

To achieve the objectives, the technical approach is divided into three parts. The first part deals with theoretical modeling of the interfacial area and flow-pattern transitions based on physical mechanisms. The second part is concerned with designing and performing horizontal and vertical two-phase flow experiments to generate benchmark data using flow visualization and objective measurements. Finally, the third part deals with incorporating the results of theoretical and experimental studies to examine and verify the validity of proposed flow-pattern transition mechanisms and interfacial area concentration modeling.

The results of this research program will provide information in horizontal and vertical two-phase flow fundamentals and information critical to the design of advanced two-phase flow systems.

University Of Wisconsin

Department of Chemical Engineering **$110,000**
Madison, WI 53706 **03-A**
89-3

116. 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

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

ER-15