DOE/ER-0401

Summaries of FY 1988 Engineering Research

1988

U.S. Department of Energy

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

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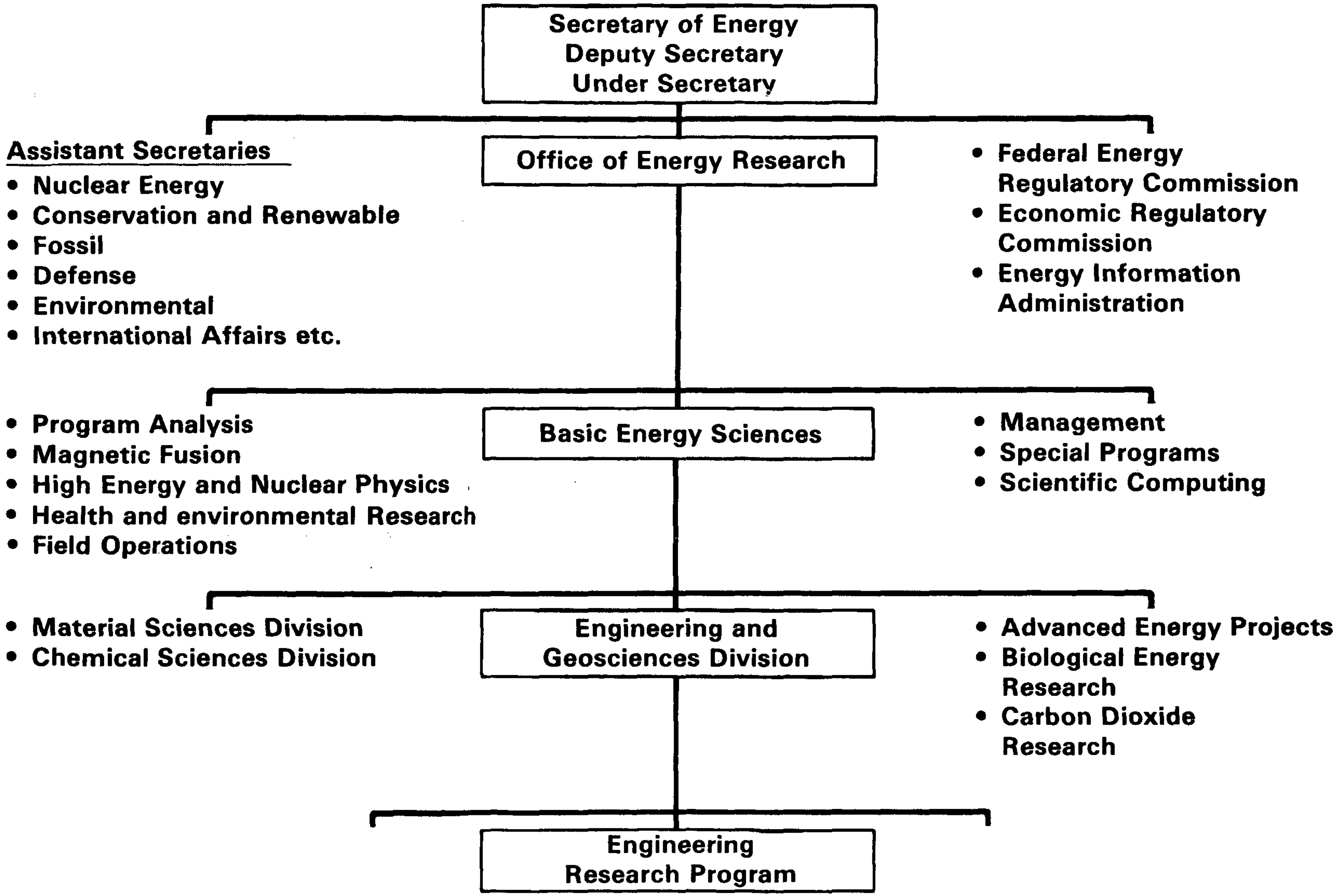
Washington, D.C. 20545

FOREWORD

This report documents the BES Engineering Research program for fiscal year 1988; 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 1988. The summaries received have been edited as 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 of the institutions at which projects were sponsored in fiscal year 1988.

The projects are numbered sequentially for individual identification in the indexes. Each project entry begins with a centered, institutional- departmental heading. The project number precedes the capitalized project title. The names of the investigators are listed immediately below the title. The funding level for fiscal year 1988 appears to the right of title; it is followed by the budget activity number (e.g., 01A). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The year in which the project began 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 on 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 on three carefully selected, high priority research areas; namely,

1) Mechanical Sciences including tribology (basic nature of friction reduction phenomena), 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 some growth in the program budget an important development has taken 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. It is expected that some resources will be available for coordinated, more narrowly focussed related, high quality research at universities and other research centers.

All such activities will be 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 has started a collaborative research effort between MIT and Idaho National Engineering Lab. At present, the collaboration is in four distinct areas: Plasma Process Engineering, Automated Welding, Fracture Mechanics, and Advanced Engineering Methods and Analysis.

Colateral, high quality research efforts at other institutions are supported by the Engineering Research program.

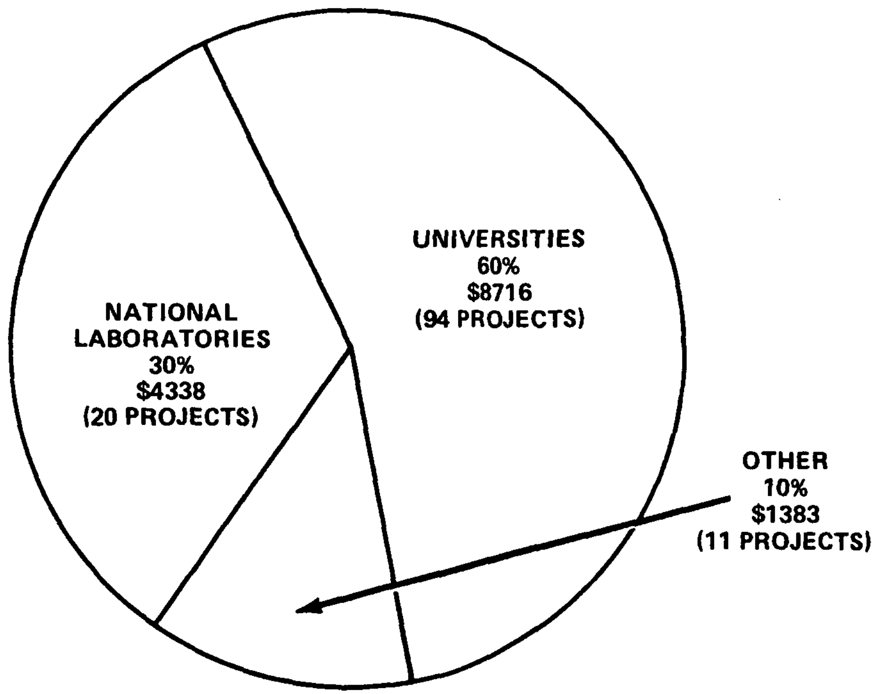
In the expectation of a future modest growth of this Program, two International Workshops on Two Phase Flow Fundamentals were held one in September 1985 and the other in March 1987. The meetings were used to identify basic research needs in the field of two phase flow and heat transfer; summary reports of the workshops are available from the Program Office. The full proceedings of the first workshop have been published as a volume in the series "Advances in Heat and Mass Transfer" (Hemisphere Publishing Company), while those of the second are in preparation for publication in the same series.

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 related wastes. Reports of both workshops are in preparation.

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 1988 the program operating funds available amounted to about $14.5 million. The distribution of these funds among various institutions and by topical areas 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 energyrelated 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 education 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 '88 BUDGET ($000's)
BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '88 BUDGET
BY TECHNICAL AREAS

	($000 s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	4283	30	46
SYSTEMS SCIENCES	4753	33	24
ENGINEERING ANALYSIS	5400	37	54

Table of Contents

AMES LABORATORY

Institute for Physical Research and Technology **$250,000**
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 and nondestructive measurements of material properties that are of importance in obtaining reliability and integrity in materials and structures. In order to achieve this goal, use is made of new and unique multiviewing instrumentation that was previously developed in this work and which uses quantitative inverse elastic wave scattering theories in the interpretation of results. Three major thrusts are being pursued:

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

2) Novel techniques are being explored that can be used to produce ultrasonic transducers with specialized features to significantly improve flaw and material property detection and characterization. One such technique is now in place for the development of practical Gaussian beam transducers. This transducer has many benefits including no sidelobes and no rapid fluctuations in the near field. The technique is being extended with the objective of discovering ways to fabricate other acoustic transducers that show essentially diffractionless features over a substantial propagation distance.

3) Studies have been initiated using broadband unipolar pulse techniques developed earlier on this project to characterize "fuzzy" boundaries in materials. This measurement depends largely upon being able to detect acoustic impedance changes over a small but finite spatial dimension, a condition that is nearly impossible to observe using conventional ultrasonics. The detection and characterization of "fuzzy" boundaries is of importance in the control of various materials processes and in the study of two-phase systems.

ARGONNE NATIONAL LABORATORY

Materials & Components Technology Div. **$125,000**
Argonne, IL 60439 **01-C**
86-3

2. 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 fluidelastic 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 **$125,000**
Argonne, IL 60439 **01-A**
84 - 3

3. Bounds on Dynamic Plastic Deformation
G.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 **$60,000**
Tempe, AZ 85287-6106 **06-B**
87-3

4. 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 for predicting the combustion and heat transfer characteristics in planar porous media as a function of the relevant factors is being developed. The model includes finite-rate reaction kinetics and the equation of transfer for describing radiative heat transfer in porous media. A heat transfer analysis has been performed indicating the influence of the optical and thermal properties of the porous media and the location of the heat generation zone of the radiant output. The effect of radiative heat transfer on flame structure and burning velocity have been revealed in some preliminary calculations using a single-step reaction model.

Experimental measurements are being conducted to validate the theoretical model. A laboratory-scale burner is being used to obtain flame speed, product species concentration and temperature profiles, and energy output data under various operating conditions for comparison to theoretical predictions. In addition, the limits for free-flame, stable interstitial combustion, and flashback are being determined.

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 for the industrial sector. 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 **$68,000**
Boston, MA 02215 **06-C**
86-3

5. Diffusion, Fluid Flow, and Sound Propagation in Disordered Media
T. Keyes

The goal of this project is a unified theoretical attack on transport processes-prime examples being those mentioned in the project title-in highly disordered, or inhomogeneous, materials. We are especially interested in materials with percolation thresholds, at which the disorder is so large that transport is blocked altogether, and in those with aspects of fractal structure. Another topic is the dynamics of the formation of disordered materials via phase separation. Since the theoretical methods needed to treat one problem can usually be applied to others, the presence of large disorder is more important than the particular process to be studied. In the past year, we have obtained results in several areas.

Porous materials may be modeled, with considerable flexibility, by appropriately placed, specularly reflecting spheres. For the case of randomly placed spheres which are allowed to overlap, free space is partitioned into islands above a critical density and transport must cease. In attempt to study gas flow in porous materials, we have considered the motion of a tagged point particle in this model solid with the "repeated ring" kinetic equation and found a critical density and, in general, good agreement with computer simulations. When the spheres are given some nontrivial structure, e.g., are forbidden from overlapping, the equation becomes very difficult to solve. In the past year, we have developed the method of "stochastic simulation" as a new tool for solving the equation. We deduce from the kinetic equations the rules for a simulation that solves the equation exactly. We have also augmented variational methods previously derived with a new approximation for the "boundary layer" around the tagged particle in a theory that should work for partially overlapping spheres.

On another front, we developed the method of "initial stage renormalization" to allow renormalization studies of unstable states. This was applied to the formation of two-phase systems via spinodal decomposition. The theory should allow a study of how the spatial structure of the initial state affects the phase separation.

Finally, we have continued our work on light scattering from disordered materials. We showed how, with very high angular resolution, it is possible to observe the statistics, not just the mean, of the scattered intensity. We identified a "critical angle" dividing two statistical regimes. From measurement of the critical angel, it is possible to measure the density of inhomogenieties in the sample; this is a completely new type of measurement. The method is now being applied to characterization of glass ceramics.

In related work, we gave a version of fractal geometry which allows the discussion of differences between fractal structures with identical fractal dimensions, and we used the scheme to calculate light scattering intensities from disordered materials modeled as fractals.

BROWN UNIVERSITY

Division of Engineering **$120,000**
Providence, RI 02912 **06-C**
84-3

6. 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 — **$65,000**
Berkeley, CA 94720 — **01-B**
87-3

7. 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 Mechanical Engineering — **$ 0**
Berkeley, CA 94720 — **06-C**
86-2

8. Investigation of Secondary Motions and Transition to Turbulence in Buoyancy-Driven Enclosure Flows with Streamline Curvature
J.A.C. Humphrey

A study is underway to clarify the role of secondary motions and transition to turbulence in buoyancy driven enclosure flows. The primary flow of interest is determined by the boundary conditions imposed along the side walls of the enclosure. The conditions induce the unsteady collision of two buoyancy driven, opposed, vertical boundary layers.

Experiments are underway with the objective to map 2 - and 3-D unsteady flow structures as a function of the Rayleigh number. The measurements consist of simultaneous determinations of temperature at two points as a function of the distance between them and time. Autocorrelations, power spectra, length and time scales are being derived from the time histories. These observations are being interpreted with corresponding flow visualization images. The results show that when the temperature difference of the plates is 2oC, corresponding to a Rayleigh number of ~ 109, the persisting 3-D vortices align themselves in the spanwise direction. The cross correlation of temperature measurements shows that there are wave propagations in the spanwise direction.

The results of this work are expected to contribute directly to the basic understanding of transition to turbulence and turbulent flow, and the ability to model these flows mathematically. In this regard, a direct numerical simulation has been performed that models a simplified aspect of the experimental flow configuration with shear super imposed. The calculations confirm the experimental evidence pointing to a dependence of the 3-D instability wavelength on the Richardson number.

UNIVERSITY OF CALIFORNIA, BERKELEY

Department of Electrical Engineering and Computer Sciences **$97,000**
Berkeley, CA 94720 **06-C**
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, BERKELEY

Department of Mechanical Engineering **$81,000**
Berkeley, CA 94720 **01-B**
87-3

10. Radiation in Particulate Systems
C.L. Tien

This study investigates, through a combined analytical and experimental program, inter-particle interactions in the radiative scattering absorption processes in densely packed systems. These inter-particle or dependents effects may be important in particle solar collectors, packed and fluidized beds combustors, deposited soot layers, soot conglomerates and microsphere insulation.

Particle sizes that range from very small, in the Rayleigh scattering regime, to the very large, in the geometric scattering regime, are considered. Analytical predictions of inter-particle effects in scattering and absorption are derived using electromagnetic theory. Experiments to verify these predictions are being conducted.

The dependent theory is developed to predict radiative characteristics of agglomerates of small particles such as those encountered in flames and combustion systems. The radiative characteristics of soot conglomerates are expressed in terms of effective diameters, which will be convenient in the optical diagnosis of particulates in combustion systems. Analytical predictions for soot conglomerates of different morphologies (straight chains, random clusters, and fractal clusters) are obtained and compared with experimental data.

UNIVERSITY OF CALIFORNIA, DAVIS

Department of Mechanical Engineering **$94,000**
Davis, CA 95616 **06-B**
87-3

11. Structure and Stabilization of Premixed and Diffusion Flames
C.K. Law

The program aims to gain fundamental understanding on the structure and stabilization of premixed and diffusion flames. The program involves both theoretical and experimental phases, and consists of three components, namely (1) Studies of the stabilization mechanisms of both premixed and diffusion flames in mixing-layer-type flows, with emphasis on the basically elliptic structure of the leading edge of the flame which controls flame holding and propagation; (2) Studies of the dynamics of stretched flames due to flame curvature and flow nonuniformity, with emphases on the extinction behavior and on synthesizing existing experimental and theoretical results from a unified viewpoint; and (3) Studies of the properties of thermal-diffusional flamefront instabilities, with emphases on the spinning and secondary bifurcation of polyhedral flames.

During the reporting period we have performed a nonlinear analysis of the dynamics of premixed flames subjected to heat loss and aerodynamic stretching. Specific cases studied include the adiabatic stretched flame, the nonadiabatic unstretched flame with distributed conductive and radiative heat losses, and stretched flames with conductive heat loss; these cases encompass and extend practically all previous theoretical models on this class of nonlinear premixed flame phenomena. Explicit expressions are obtained for the extinction states.

We have also experimentally determined the laminar flame speeds of methane/air mixtures as functions of stoichiometry, pressure, and flame temperature. The experimental data are then compared with calculated values using an accurate flame code and by assuming different kinetic schemes. This comparison allows the partial validation of two specific schemes.

Extensive theoretical work has also been performed on the flame behavior with branching-termination chain mechanisms. Results show that extinction can occur through either heat loss or chain termination. The predicted behavior agree well with our experimental data.

UNIVERSITY OF CALIFORNIA, LOS ANGELES

Mechanical, Aerospace and Nuclear Engineering Dept. **$80,000**
School of Engineering and Applied Science **01-C**
Los Angeles, CA 90024-1597 **82-6**

12. 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. Numerical predictions along with corroborative experimental evidence demonstrated that dispersion enhances the net heat transport through the layer, while inertia diminishes it! If the packed bed is very shallow (low layer thickness to bed diameter ratio), both effects decrease the Nusselt number. Dispersion dominates inertia unless the porous Prandtl number is order 0.001 or less.

Steam injection in a porous channel is being studied experimentally and theoretically. In the experimental studies the qualitative behavior of a steam-water interface in a porous channel will be analyzed through high speed movies of the two phase flow and interface movement. The principal parameters of interest include the frequency of the interface movement, the shape of two phase region and flow patterns. The pressure and temperature distributions will be measured along with flow rates of steam and water. The physical mechanisms causing the observed rapid oscillation of the interface between the two phase region and the subcooled water are being delineated. A stability analysis will be carried out. Numerical modeling will include mechanisms that are important.

UNIVERSITY OF CALIFORNIA, LOS ANGELES

Department of Mechanical, Aerospace, and Nuclear Engineering **$65,000**
School of Engineering and Applied Sciences **06-B**
Los Angeles, CA 90024-1597 **88-2**

13. 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 deformation, mass loss, breakup, and burning in liquid 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 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, and breakup of the liquid transverse jet in both subsonic and supersonic crossflow, in the absence of a chemical reaction. 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. The TVD method of Harten is employed for moderate subsonic crossflow (0.3.7) and the methods of Godunov is used at high subsonic and supersonic crossflows (M0.7). 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. Mass and momentum balances performed along the jet, with and without the inclusion of mass loss due to droplet shedding, are then incorporated so that liquid jet trajectories, bow shock penetration, and approximate breakup location may be calculated. 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 evaporation, ignition, and burning in the liquid jet, and on axisymmetric modeling of the liquid droplet in a convective environment.

UNIVERSITY OF CALIFORNIA, LOS ANGELES

Department of Physics	**$ 75,000**
Los Angeles, CA 90024	**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 distribution function for the higher order correlations. Particular aims are to describe the build-up of cross-correlations between different modes, and to generate a workable description of the role of mechanical noise in activation processes. Recent research also indicates that the wave turbulent state possesses structure in that it can support new propagating modes. This elasticity of turbulence is a classical analogue of second sound. Currently this effect is being calculated for wind waves in a stormy sea.

In one and two dimensional systems high amplitude wave motion can self-focus into long lived structures. These soliton-like properties are being studied as regards possible applications to flexing plates and shells. Of special interest are the thermal properties of the solitons, the role of damping in the formation of the solitary wave, and possible consequences for metal fatigue as regards the recently discovered non-propagating soliton.

UNIVERSITY OF CALIFORNIA, SAN DIEGO

Scripps Institution of Oceanograph	**$ 0**
La Jolla, CA 92093	**06-C**
	86-2

15. Nonlinear Dynamics in Dissipative Systems
H.D.I. Abarbanel

This work is directed toward the understanding of the dynamics and nonlinear stability of multi-phase flows from a Hamiltonian point of view. The Hamiltonian formulation of multiphase flow problems will be the first part of the research. As a second part the conservation laws, in addition to energy, for these flows will be investigated usingmethods originated by Sophus Lie and further developed in the past decade by these flows in hand, the nonlinear stability of particular flows can be investigated using the liapunov method of Arnol'd and others. The result of this work will be a set of critera for the stability of free boundary flows--material surfaces separating phases--under finite perturbations. Several examples of gravity drive flows will be studied.

The dissipative or viscous versions of these flows will build on the dynamical description of these results. A variational principle arising from the consideration of the evolution of the energy plus all conserved quantities will be used to provide ranges for the absolute stability of viscous multiphase flows. This extends the older energy methods often employed in this kind of analysis. The addition of other conserved quantities allows the exploration of a larger part of the allowed phase space for the deviations from a chosen flow whose stability one wishes to investigate.

UNIVERSITY OF CALIFORNIA, SAN DIEGO

Department of Applied Mechanics and Engineering Sciences — **$120,000**
La Jolla, CA 92093 — **06-B**
87-3

16. Fuel Droplets Subject to Straining Flow
P.A. Libby, K. Seshadri, F.A. Williams

This research is concerned with the behavior of single fuel droplets in a well defined, nonuniform flow field. At present our effort is primarily experimental but in due course will include complementary theoretical studies. The experiments involve determining photographically the trajectories of individual droplets and in the case of evaporating and/or combusting droplets the history of droplet diameter. Experiments have been completed on heptane droplets in a counterflowing, nonpremixed flame and in counterflowing streams of isothermal nitrogen. This second flow was taken up because its relative simplicity facilitates data interpretation. The equations of motion are used to determine the forces acting on the droplet along its trajectory. The results from both experiments indicate that the nonuniformity of the flow results in significant lift on the droplets. The available theory suggests that this lift can be due to inertia and/or spin. Unfortunately the relevant theories apply to Reynolds numbers small compared to unity whereas our droplets encounter numbers from one to ten. Attempts to correlate our force data by rational extensions of theoretical predictions are underway and are to present partially successful. The results from the flame experiments are especially interesting in that the droplets not only experience lift but drag forces considerably larger than predicted by current engineering correlations when approaching the reaction zone. The implication is that aspherical mass loss occurs.

UNIVERSITY OF CALIFORNIA, SAN DIEGO

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

17. Parameterization of Intermittent Turbulence and the Vorton Method
E.A. Novikov

This reseach 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, SAN DIEGO

Institute for Nonlinear Science, R-002 — **$ 88,000**
La Jolla, CA 92093 — **06-C**
86-3

18. The Stochastic Trajectory Analysis Technique (STAT) Applied to Chemical, Mechanical and Quantum Systems
B.J. West, K. Lindenberg

A number of important physical problems are described by dynamical equations containing fluctuating parameters. In dealing with such systems one has until recently been forced to assume that the fluctuations are delta-correlated, i.e. that their spectrum is white, 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 applications involving chemical reactions in fluids in which the rate coefficients fluctuate due to spatial inhomogeneities and thermal effects, dynamical processes in solid materials in which fluctuations arise due to spatial disorder and thermal effects, and wave propagation in random media in a geophysical context.

A number of methods to deal with the problem of correlated fluctuations have been developed under this program. One of these involves an explicit construction of trajectories (STAT). This procedure is particularly useful when the noise has simple statistics and can be used to deal with highly correlated noise. The approach has been applied to linear systems driven by dichotomous noise, multivalued noise, and shot noise. Another class of methods relies on perturbative approximations around the white noise limit. These methods can be applied most fruitfully to systems driven by weak Gaussian slightly colored noise, and have been used to calculate rates of transitions in bistable systems driven by colored noise.

UNIVERSITY OF CALIFORNIA, SANTA BARBARA

Department of Physics	**$124,000**
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 on 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 Nuclear Engineering	**$94,000**
	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

This project is a continuation of an ongoing project aimed at studying turbulence structure in liquid 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 LDA system provides detailed three-dimensional velocity measurements while the oxygen-bubble technique gives flow visualization as well as some velocity measurements. These experimental methods are complemented by a numerical approach in which the full Navier-Stokes equations are being solved by a pseudospectral method to provide quantities which are difficult to obtain by flow visualization and single-point velocity measurement. Both the experimental and computational techniques have been fully developed and tested.

The initial study focusing on phenomena in the absence of shear at the interface has been completed and the results indicate that turbulent "bursts" generated near the wall give rise to the dominant phenomenon in such a flow. At present, turbulence characteristics in the liquid when the free surface is under various shear rates imposed by co-current and countercurrent air flows are being studied. It is found that the low-speed streaks and bursts characteristic of wall-bounded shear flow also occur near a free surface when the shear on it exceeds a critical value.

CARNEGIE MELLON UNIVERSITY

Chemical Engineering Department and Graduate School of Industrial Administration **$150,000**
Pittsburgh, PA 15213 **03-A** **85-4**

21. Strategies for Optimal Redesign In a Changing Environment
L.T. Biegler, I.E. Grossmann, G.L. Thompson, A.W. Westerberg

As the chemical industry matures it is important to consider the redesign of existing processes. Redesign problems are harder to solve that "grassroots" problems because constraints dealing with the existing process need to be considered and determination of optimal modifications in an existing plant generally will be quite different from optimal solutions for a new plant. This project addresses the optimal redesign problem through the following areas:

1) Flowsheet optimization for process design. Recent work has led to the combination of rigorous simulation models for rating process equipment with sophisticated methods for mixed integer flowsheet optimization. For flowsheets with fixed topologies we have also demonstrated the potential for performing process retrofits optimally and automatically.

2) Primal/dual linear (LP) and quadratic programming (QP) algorithms. These new algorithms for solving LP and QP problems were developed during the first two years of this project. Computational tests showed that codes based on these algorithms were at least 10 times as fast as currently available codes, and they were especially effective for problems having more constraints than variables.

3) Redesign of energy management systems. A screening and optimization approach is being developed for the redesign of heat exchanger networks. The screening is based on parametric solutions for energy cost, area and structural modifications. The optimization is performed on a novel superstructure representation for redesigns, and is modelled as a mixedinteger nonlinear programming problem.

4) Redesign for flexibility and controllability. New mathematical models have been developed for optimizing flexibility in existing chemical processes, and to characterize controllability through speed of response of a process.

5) Redesign of multicomponent separation sequences - an existing flowsheet and a separation task different from the original flowsheet are given. The objective is to modify the flowsheet so as to accomplish the new separation task at minimum cost.

CARNEGIE MELLON UNIVERSITY

Mechanical Engineering Department **$100,000**
Pittsburgh, PA 15213 **01-C** **86-3**

22. Experimental And Theoretical Studies Of Vertical Annular Liquid Jets
N. Chigier, J.I. Ramos

The objective of this study is to determine the dynamics and convergence length of vertical annular jets as a function of the inlet inner radius inlet thickness, inlet velocity, inlet flow angle, surface tension, and turbulence. Another objective is to study the start-up and stability of annular liquid jets. The experimental part of the program is being performed with different liquid in order to determine the effects of the Froude, Reynolds, and Weber numbers and geometry on the convergence and stability of annular jets. The theoretical part of the research program deals with the development of an implicit finite-difference scheme for studying the dynamics and stability of annular liquid jets. The theoretical studies are based on the solution of the time-dependent axisymmetric form of the Navier-Stokes equations and account is taken of surface tension and the adverse axial pressure gradient which occurs near the annular liquid jet convergence. The results of these models are being compared with experimental data obtained at Carnegie Mellon University and at the Westinghouse R&D Center.

Experiments have been carried out on annular liquid curtains with an initial radius of 50 my and initial sheet thicknesses of 0.5 and 1.0 mm. Three Froude numbers have been studied: 1.27, 4.27, and 8.87 by variations of the liquid flow rate. Pressure within the curtains was varied progressively from 0 to 3 Pa. Several flow regimes were found: a) non-pressurized, b) pressurized, c) oscillating, and d) punctured. Curtain shape and convergence length were determined by photography. Velocity in the liquid curtain was measured by Laser Doppler Anemometry. The variation of liquid film thickness with axial distance was determined. Good agreement was found between predictions and experiments.

UNIVERSITY OF CHICAGO

Department of Chemistry **$78,000**
Chicago, IL 60637 **06-C**
86-3

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 anaylyses, such as emerged from the introduction of a suitable metric in the space of thermodyanmic 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 reemission 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 propogation 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, J.J. O'Gallagher

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 **$58,000**
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.

COLORADO SCHOOL OF MINES

Department of Chemical Engineering and Petroleum Refining **$49,000**
03-B
Golden, CO 80401 **87-2**

26. An Automated Flow Calorimeter for Heat Capacity and Enthalpy Measurements at Elevated Temperatures and Pressures

V.F. Yesavage

The need for thermal property data at process condition has been well documented in applications such as development of atmospherically inert refrigerants and design of petrochemical and synfuel plants. As such, the primary objective of this work is to construct an automated flow calorimeter to measure isobaric heat capacities and enthalpies of vaporization over the range 0-30MPa and 300-700K with an anticipated accuracy of 0.1%. The method of measurement is an adiabatic electrical power input technique with a unique calorimeter design utilizing a concentric coil/radiation shield structure which minimizes heat loss errors and simplifies the replacement of plugged components. Flow generation is accomplished with a precision Ruska pump eliminating the need for online flow rate measurement. In addition, the proposed instrument will be fully automated minimizing the need for high skilled operators which had previously been a severe limitation with this type of instrument.

Assembly of all hardware and implementation of the necessary software was completed within the past year. In addition, water was used as a heat capacity standard to evaluate overall system performance. Preliminary indications are that the apparatus is operating near expectations (+/- 0.2%) although some additional hardware refinements may be necessary achieve the design goals of +/- 0.1%. Plans for the remainder of the contract period include completion of the evaluation studies with water followed by additional evaluations with methanol or an initiation of studies on alternative refrigerants.

UNIVERSITY OF CONNECTICUT

Department of Mechanical Engineering **$65,000**
Storrs, CT 06268 **01-A**
88-3

27. 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 will be 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 will be used to verify the model. Single crystal properties used for input to the model will be determined experimentally for Hastelloy-x. Using these properties, the behavior of polycrystal Hastelloy-x will be predicted and then compared with experiments. 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.

The work will be done with the cooperation of Engineering Science Software, Inc. working under a related contract. Manufacture of single crystal specimens will be done by Pratt and Whitney, Inc.

CORNELL UNIVERSITY

Sibley School of Mechanical and Aerospace Engineering
Ithaca, NY 14853

$100,000
01-C
88-3

28. 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
Hanover, NH 03755

$ 0
01-C
86-3

29. Subcooled Sprays in a Vapor Environment-Tests of the Two-Fluid Model for Two-Phase Flow
G.B. Wallis, H.J. Richter

The "separated" or "two-fluid" model for two-phase flow is being used to describe the behavior of a subcooled spray in a vapor environment. Detailed measurements will be used to determine viable forms of the "interaction" terms describing mass, energy and momentum transfer between the phases. The overall purpose is to advance the stateof-the-art of basic analytical and computational tools for describing two-phase multidimensional flow.

In the two-fluid model each phase satisfies the usual set of equations of conservations of mass, momentum and energy with the influence of one phase on the other appearing as "interaction terms" that couple the two sets. While much effort has been devoted to writing down various forms of equations and discussing how they can be obtained by averaging the basic conservation laws for each phase, few workers have actually applied them to specific situations. It is likely that useful and reasonable simple expressions can be devised to represent coupling effects when the flow pattern is clearly defined: for instance, a dispersion of one phase in the other. Previously, physically-based formulations have been applied to a one-dimensonal representation of fluidized beds, sedimentation, and "mist-lift" processes or the two- and three-dimensional modeling of sprays in gases and particles interacting with a fluid.

This project concerns a dispersed flow regime in which heat and mass transfer play leading roles: the condensation of vapor on a subcooled spray of droplets. Analysis of this regime requires the inclusion of significant interaction terms in all of the conservation laws, thus providing a comprehensive test of the theory. Complementary analytical and experimental work are planned. The experiments are intended to build up to realistic complexity (e.g., a drop size spectrum in the spray, variations in spray flux as a function of angle) while keeping the flow pattern sufficiently well-defined to be amenable to theoretical representation.

ENGINEERING SCIENCE SOFTWARE, INC.

Smithfield, RI 02917 — $ 47,000 — 01-A — 88-3

30. 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.

G. A. TECHNOLOGIES, INC.

P. O. Box 85608 — $ 0
San Diego, CA 92138-5608 — 06-C — 85-3

31. Higher Dimensional Nonlinear Dynamics
J.M. Greene, J. Kim

The goal of this project is to explore how the methods of nonlinear dynamics can be applied to ever more complex systems.

The modern theory of nonlinear dynamics is, to a large extent, the understanding of the way in which computational results can be used to gain insight into the nature of chaotic and turbulent systems. A property of such systems is that two different orbits that are crudely indistinguishable are generally quite different in their detailed behavior. Thus, a single orbit, or realization, contains a confusing mixture of uninteresting detailed information, and usefully generalizable information. The most easily obtained, additional, exact information that computers can provide comes from the solution of equations linearized around a given orbit. The objective of this program is a thorough understanding of the information available through linearization.

This information mostly falls under the key words of Lyapunov exponents and directions. That is, this study emphasizes the information available in the rates and directions of separation of nearby orbits, or realizations. The methods are being developed and tested using the Lorenz model. The knowledge gained this way is being applied to the Kuramoto-Sivashinsky equation, a simple partial differential equation with chaotic solutions. The object is to develop representations in which these solutions can be most simply expressed.

UNIVERSITY OF HOUSTON

Department of Mechanical Engineering — $125,000
Houston, TX 77204-4792 — 01-C — 87-3

32. Comparative Study of the Vorticity Field in Turbulent Flows: Theory, Experiments, Computations
A.K.M. Hussain

Fluid turbulence affects many energy systems. On the negative side it contributes to noise generation and vibrations of key system components, while on the positive side it serves to enhance mixing and heat transfer. These are essentially empirically established facts. On the theoretical side over the years relatively slow progress has been made toward a better understanding of such flows on the fundamental level. A barrier to progress has been the difficult nature of the equations governing the behavior of fluids. It has been recognized for a long time that the mathematical difficulties could be mitigated to some extent if one had a prior knowledge of the vorticity field accompanying the velocity field. The present proposal will take advantage of progress in instrumentation developed under other auspices aimed at measuring vorticity directly.

A newly constructed nine-wire probe is expected to measure the components of vorticity with a resolution of about one to two millimeters. The direct measurement of vorticity simultaneously with velocity will permit the evaluation of the merits of a recent hypothesis that the observed large-scale coherence in turbulent flows is induced by a spontaneous, symmetry breaking onset of helicity. While helicity, that is the scalar product of vorticity and velocity vanishes in the mean, its mean square value need not vanish. How fluctuations would give rise to an observable helicity, and how given its onset it would affect the large-scale coherence of turbulent flows is a controversial theoretical issue. At this point, ultimately only a recourse to an experiment can resolve the controversy.

UNIVERSITY OF HOUSTON

Department of Mechanical Engineering	**$78,000**
Houston, TX 77204-4792	**01-B**
	88-3

33. 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	**$133,000**
Idaho Falls, ID 83415	**06-A**
	85-3

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

Knowledge of in-flight particle temperature is fundamental to understanding particle/plasma interactions in the physical and/or chemical processing of fine powders. The measurement of in-flight particle temperature is based on a two wavelength pyrometry technique. In addition, simultaneous particle size is obtained by a light scattering technique. The requirement of coincidence between sizing and pyrometry signals insures that only particles for which temperature data are available will be sized. The technique has been demonstrated on laboratory scale plasma torches. The influence of particle size, injection rate, torch power, etc., are currently being examined in detail. In addition methods of simultaneously obtaining particle size, velocity and temperature are under development.

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 **$183,000**
Idaho Falls, ID 83415 **03-B**
83-5

35. Nondestructive Characterization of Fracture Dynamics and Crack Growth

J.A. Johnson, B.A. Barna, R.T. Allemeir

The purpose of this research is to develop instrumentation and models to measure and predict the emission and interaction of ultrasound from growing cracks in engineering materials and to investigate methods of sensing the properties of growing cracks. 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. In addition, numerical methods are being used to model the interaction of acoustic emission stress waves with real crack geometries.

The AE detection system is being developed and is capable of detecting and digitizing AE signals with a larger bandwidth and with less dead time than in conventional systems. This will allow improved resolution in detecting the locations of the sources of emissions and in discriminating between types of sources. Automatic analysis methods are being developed for source location and source identification for each of the large number of acoustic emission events received in a typical fracture mechanics experiment. Other work includes transducer design, transducer calibration, generalized ray theory analysis (Green's functions), source location algorithms, and inverse source identification algorithms.

Models of the ultrasonic field/crack interaction are based on a numerical (finite element) solutions to the partial differential equations (PDE) describing the system. In the finite element model, a source of acoustic emission is modeled 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 to the PDE with the boundary conditions of the system. These boundary conditions include the geometry of the macrocrack near the source of acoustic emission and thus calculate receiver signals which include effects that cannot be calculated using generalized ray theory.

IDAHO NATIONAL ENGINEERING LABORATORY

Energy and Systems Technology Group **$262,000**
Idaho Falls, ID 83415 **06-C**
87-1

36. Modeling of Thermal Plasma Processes

V.H. Ransom, J.D. Ramshaw

Optimization of thermal plasma processing techniques will require a better understanding of the space- and time-resolved flow and temperature distributions in the plasma plume and of the interaction between the plasma and a particulate phase. This research is directed toward the development of a comprehensive computational model of thermal plasma processes and plasma-particle interactions capable of providing such information. The KIVA computer code was adopted as a starting point for the model development since it already contains many of the necessary features, including implicit numerics for efficient computation of acoustic waves and diffusion, multicomponent gas flow with real gas effects, turbulence models, kinetic and equilibrium chemical reactions, and discrete particles coupled to the gas flow. Work is in progress to develop and incorporate the additional submodels necessary to permit complete quantitative plasma processing simulations. In particular, models are needed for convective and radiative heat losses and for a variety of plasma-particle interaction processes, including evaporation, condensation, nucleation, agglomerations, and coalescence. Modeling these latter processes will be the most challenging task from a physical point of view, and their representation will require major modifications to and extensions of the KIVA particle model.

This research is closely coordinated with other plasma processing programs both within the Department of Science and Technology of the Idaho National Engineering Laboratory and at the Massachusetts Institute of Technology.

IDAHO NATIONAL ENGINEERING LABORATORY

Materials Technology Group **$439,000**
Idaho Falls, ID 83415-2218 **01-A**
81-6

37. 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 materials (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. These results are used to make 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 size for comparison with analytical models. Other techniques including microphotography and the replicating of the crack tip region, for future metallographic examination, are being used to complement the above measurements 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.

IDAHO NATIONAL ENGINEERING LABORATORY

Materials Technology Group **$319,000**
Idaho Falls, ID 83415 **06-A**
85-3

38. 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 **$450,000**
Idaho Falls, ID 83415 **03-A**
85-3

39. Integrated Sensor Model Development for Automated Welding

H.B. Smartt, J.A. Johnson

The objectives of this research are (1) to develop models of the physical phenomena occurring in the gas metal arc welding process suitable for real-time process control, (2) to develop sensors and signal processing algorithms for arc welding processes including optical and ultrasonic techniques, and (3) to integrate the above models and sensing with advanced control methodologies. This project is part of a collaborative research program with the Massachusetts Institute of Technology.

A fundamental model of the gas metal arc welding process has been developed which considers wire melting and heat and mass transfer to the base metal. This model is being extended to account for droplet detachment modes and the dynamic aspects of heat and mass transfer through the arc.

Sensing of the weld pool solid/liquid interface location is being developed using noncontract transducers. Signal generation is by use of laser pulses directed on the weld pool. Signal analysis/pattern recognition techniques are being developed based on AI methods for automated measurements.

Independent control of heat and mass input to the weld has been demonstrated. Sensing algorithms to characterized droplet transfer mode by acoustic and electrical signals have been developed. Control of weld bead cooling rate during gas metal arc welding has been demonstrated wherein the cooling rate has been varied independently of the weld reinforcement. This has allowed near steady-state cooling rates to be achieved during weld start-up, an important factor in reducing weld defects.

UNIVERSITY OF ILLINOIS

Coordinated Science Laboratory **$120,000**
Urbana, IL 61801 **03-A**
88-3

40. 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. Our research plan is first 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 hierarchies and multiple decision layers, and (iv) control and coordination of large scale systems based on (probabilistic multimodeling. Following this, we will develop a new framework which will allow for distributed and interactive model building and control, where both structural and decision making hierarchies evolve over time. It 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 **$106,000**
Urbana, IL 61801 **01-C**
86-3

41. 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	**$ 74,000**
Chicago, IL 60680	**01-B**
	85-2

42. 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 ILLINOS AT CHICAGO

Department of Civil Engineering,	**$54,000**
Mechanics and Metallurgy	**01-A**
Chicago, IL 60680	**88-1**

43. 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 **$ 80,000**
Chicago, IL 60616 **03-A**
84-3

44. 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:

(i) 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.

(ii) 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.

(iii) 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 **$78,000**
Pasadena, CA 91109 **03-B**
86-3

45. 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 σ_A (ε) 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 behaior in which σ_A (ε) 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. Experimental results in F_2 (published), and theoretical calculations in $CFCl_3$ and CCl_4 (to be published) have shown significant discrepancies with calculation and other experiments as to energy dependence of the σ_A (ε), and temperature dependence of the rate constants. These properties have bearing on the plasma-assisted etching process, and on soot (and/or electron density) reduction in combustion plasmas. To this end, experimental work on attachment to Cl_2 will be initiated, calculations in $CFCl_3$ and CCl_4 completed, and attachment properties of about six other molecules, currently being tested elsewhere as electron "sinks" or soot reducers in combustion plasmas, will be studied.

LAWRENCE BERKELEY LABORATORY

Accelerator and Fusion Research Division $120,000
University of California 06-C
Berkeley, CA 94720 87-3

46. 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

47. Controlled Combustion
A.K. Oppenheim

The principal objective of this study is to provide scientific background for the development of controlled combustion systems, i.e. prime movers whose combustors are not only sources of power, as they are today, but operate also as modern, high-tech chemical reactors, so that the evolution of exothermic energy is carried out under proper fluid mechanical and thermo-chemical conditions to eliminate all sorts of combustion instabilities and minimize the formation of pollutants. For automobile engines this offers the prospect of efficient and clean combustion associated with relatively low exhaust temperature, devoid of the problems of knock and cycle-to-cycle variation, leading thus to the annihilation of major technological constraints imposed upon the automotive industry: the octane standard and the catalytic converter. Means to accomplish this involve the exploitation of active radicals obtainable from plasma and flame jets as well as from recirculated products. Major laboratory apparatus for our studies consists of a shock tube and molecular beam mass spectrometer, associated with an assortment of laser-powered optical instuments, including apparatus for megacycle-frequency schlieren cinematography and laser induced fluorescence imagery. The experimental program is associated with a significant effort in numerical modeling of the fluid mechanical, thermodynamic, and chemical kinetic processes influencing the control of ignition and combustion in engineers.

LOS ALAMOS NATIONAL LABORATORY

Theoretical Division **$90,000**
Los Alamos, NM 87545 **01-C**
87-3

48. Lattice Gas Hydrodynamics: Theory and Simulations
B. Hasslacher, U. Frish, Y. Pomeau

Lattice gases, operating as cellular automata and amendable to massive parallelishm, which simulate the Navier-Stokes equation in two and three dimensions, were introduced in 1985 by the prinicpal 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 withother 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 MARYLAND

Department of Mechanical Engineering **$78,000**
College Park, MD 20742 **01-C**
87-2

49. 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 stero pairs, a number of methods have been developed to establish correspondence. These methods are time consuming and difficult to implement at the edges of ojects 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 experimetns for rigidly attached, parallel camera-pari configurations have shown that this relation is promising as a guid for establishing correspondence: potential matches can be tested by sustituting the measured positions and velocities of the features into the equation. In the present study, the binocular flow equation is being exp.ored 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 **$68,000**
College Park, MD 20742 **06-C**
83-4

50. Study of Magnetostatic Problems in Nonlinear Media with Hysteresis
I.C. Mayergoyz

This project has two main research objectives: (1) to develop boundary Galerkin's approach and its quasifiniteelement realization in order to circumvent the difficulties which are related to the unbounded regions of field distribution, and (2) to investigate mathematical models of hysteresis and develop the methods for the calculation of magnetostatic problems in media with hysteresis.

As far as the first objective is concerned, the calculation of magnetic fields in unbounded regions will be reduced to coupled boundary/volume Galerkin's forms and a new quasifiniteelement projection technique will be developed on this basis. The problems concerning convergence of the quasifiniteelement methods, existence and uniqueness of the solution of simultaneous nonlinear quasi- finiteelement equations and global iterative methods of the calculation of the solution of these equations will be the focus of this research.

For the second objective, mathematical models of hysteresis as continuous superposition of rectangular hysteresis nonlinearities will be investigated. Special attention will be paid to the solution of identification problems and to the generalization of these models for the case of vector hysteresis. The application of continuation methods to the calculation of magnetostatic fields in media with hysteresis will be studied.

UNIVERSITY OF MARYLAND

Department of Mechanical Engineering and Systems Research Center
College Park, MD 20742

$88,000
03-A
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 creation of mechanisms. The objective of this work is to develop a methodology for the creation of multi-DOF (Degree-Of-Freedom) epicyclic-gear-trains and to apply these gear trains for the design of robotic devices. In order to ensure all the potential epicyclic-gear-trains be systematically identified, it will be necessary to develop computational algorithms, based on graph theory and combinatorial analysis, for the enumeration of such mechanisms. The creation of multi-DOF mechanisms will not only provide an atlas for practicing engineering but also lead to more efficient design of these mechanisms with multiple actuating requirements.

The structural characteristics associated with the design of wrist mechanism has been investigated. We have found that most of the robot wrists are made up of a true two-DOF epicyclic-gear-train in series with the base link. We believe a class of new and novel robotic wrists can be synthesized in a similar manner. Further, we are also interested in the synthesis of wrist mechanisms with a redundant DOF. Clearly, wrist with redundant degrees of freedom can be used to avoid the singularity problem and to increase the dexterity of a robot.

For the reason of simplicity, most of the robot arms have been designed in an open-loop configuration which requires the actuators to be mounted on the moving links. Robot arms using gear trains for power transmission, can be configured with most of its actuators ground-connected which has the advantage of reduced inertia. We believe this is a new concept in robot design. We will be exploring the design of such robot arms from kinematic, dynamic and control points of view.

UNIVERSITY OF MARYLAND

Department of Mechanical Engineering
College Park, MD 20742

$125,000
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 sensing the instantaneous velocity and vorticity vector fields in turbulent flows will be further developed. Point measurements will be made in a variety of high quality flows (grid flow, jets, mixing layers, wakes, boundary layers) in order to obtain properties of the vorticity and helicity fields. From this data set, flow gradient quantities (helicity, enstrophy, vorticity, strain-rate) associated with coherent structures in these flows will be educted. This experimental part of the project is being carried out by the Universities of Maryland and Houston in a cooperative effort.

UNIVERSITY OF MASSACHUSETTS

Chemical Engineering Department **$ 91,000**
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 sub-tasks.

The above view of flowsheet synthesis can be radically altered when the reactions occur in the liquid phase. In such circumstances, it is often possible to combine the reaction and separation tasks by using reactive separators. Fundamental studies on the phase behavior, design and synthesis of this class of problems are proposed. It is expected that this will lead to a systematic technique for inventing improved technology and that this will be of lasting value to the profession.

UNIVERSITY OF MASSACHUSETTS

Chemical Engineering Department **$120,000**
Goessmann Laboratory **03-A**
Amherst, MA 01003-0011 **83-6**

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 a process is about 75% complete. 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 distrubances, 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 dynamic models of complete processes in order to 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 **$55,000**
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 **$135,000**
Cambridge, MA 02139 **06-B**
86-3

56. Turbulent Premixed Flame Study
W. Cheng, J. Keck, S. Pope
(Cornell University)

This program is a combined experimental and theoretical study of premixed turbulent flames. The primary aim of the experiment is to study the growth behavior and some detailed properties of statistically spherical flames. The theoretical part of the program centers on the description of the flame behavior using the pdf formulation. Techniques using a thin sheet laser light to illuminate the flame ball have been developed to look at the relationship between the flame structure and the burn rate. The illuminated flow will be recorded on high speed movies and the image will be digitized. Then the topology and dynamics of the flame structures will be analyzed statistically. Experiments to examine the effect of pressure gradient on the flame propagation characteristics is planned. The development of a pdf description of the turbulent flame behavior follows the experiment closely. The approach is to model the topology of the flame surface by studying their kinematics and dynamics. Initially the reaction zone will be modelled as a simple regular propagating surface which propagates at the laminar flame speed. Then the effects of curvature and stretching on the flame speed will be added and local breakdown on the regular surface due to self-intersection and the formation of cusps will be examined. The experimental and theoretical efforts will lead to a comprehensive description of the turbulent premixed flames.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

The Energy Laboratory **$127,000**
Cambridge, MA 02139 **03-B**
85-3

57. 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 **$125,000**
Cambridge, MA 02139 **06-A**
88-3

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

The purpose of the research is to examine the physicochemical behavior of individual organic particles for conditions simulating those to which particles are exposed during thermal plasma processing methods. 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 one or two milliseconds. Equipment is being installed for optical imaging of the particle during processing.

Study is in progress of melting and solidification of metal and oxide particles at high rates of heating and cooling. Measurements have been made of the evaporation of oxide particles while they are heated and cooled. Investigation of the ignition and combustion of metal particles is in progress also. Means have been developed for capturing individual particles and examining them by optical and electron microscopic methods.

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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Department of Materials Science and Engineering **$71,000**
06-A
Cambridge, MA 02139 **85-4**

59. Plasma Reduction of Metallic Oxides
J.F. Elliot, J. Szekely

The objective of this research is the characterization of reactions in composite carbon-metal oxide particles and the possible reduction of metal oxide particles injected into the tail flame of a thermal arc plasma. The experimental program consists of injecting particles in the size range of 5 to 50 microns into the plasma flame, and then extracting these particles with a quenching tool at various positions down stream from the injection point. The collected particles are examined by optical and electron microscopy to obtain information on the changes such as melting, evaporation, reduction, etc., that occur during the transit of the particles in the flame. Samples of powders with a very small size range will be employed in studies of evaporation and melting.

The temperature and velocity fields of the plasma flame are being calculated with a computer program that has been developed for that purpose. The rate of heat transfer from the flame to the particles will be determined in experiments in which particles with different, but always well characterized, thermo-physical properties are employed. By sectioning and analyzing these particles, it is possible to determine the extent of melting, and of vaporization that has occurred. The results will be compared with predictions by use of the computer model.

The work is closely coordinated with plasma modelling and gas-particle studies at MIT, and with measurements of particle trajectories and temperatures of plasma flames that are in progress at the Idaho National Engineering Laboratory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Energy Laboratory **$103,000**
Cambridge, MA 02139 **03-A**
88-3

60. 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

Energy Laboratory **$175,000**
Cambridge, MA 02139 **06-C**
88-3

61. A Parity Simulator for Nuclear Power Plant Dymanics
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 difficulat 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 componens 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 — **$156,000**
Cambridge, Massachusetts 02139 — **03-B** — **88-3**

62. 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 — **$68,000**
Cambridge, MA 02139 — **01-D** — **87-2**

63. 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 knowlege will contribute to a more reliable operation of superconducting magnets.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Department of Ocean Engineering — **$41,000**
Cambridge, MA 02139 — **03-A** — **85-4**

64. In-Process Control of Residual Stresses and Distortion in Automatic Welding
K. Masubuchi

The objective of this research is to develop the technology of in-process control of residual stresses and distortion in automatic welding. The program consists of the following phases:

Phase 1: In-process control of residual stresses and distortion in some weldments.

Phase 2: Development of technologies for minimizing and eliminating, if possible, tack welds.

Phase 2-1: Analytical and experimental studies of thermal stresses during welding and forces acting on tack welds.

Phase 2-2: GMAW process control to minimize interference from tack welds.

Phase 3: Plans for further development of the technology of in-process control of residual stresses and distortion.

Phase 2-2 has been added since July 1986. The research efforts thus far covered all phases but Phase 3, which will be done at the end of the program.

The major effort under Phase 1 has been to study means for reducing distortions and residual stresses in girth-welded pipes. It has been found that an application of internal pressures during welding is an effective means of reducing radial distortion.

The major effort under Phase 2-1 has been to study transient thermal stresses and metal movement during butt welding of steel and aluminum plates. It has been found through experiments that forces acting on tack welds can be significantly reduced by additional heating by oxyacetylene torches placed alongside the welding arc. Through an analytical study it has been found that the most effective way is to heat wide areas to relatively low temperatures so that (a) the counter metal movement produced by the additional heating is significant, but (b) the supplementary heating does not produce additional residual stresses.

Under Phase 2-2, basic research has been conducted on possible ways for minimizing interference of tack welds by increasing penetration of the main root-pass welding.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Department of Mechanical Engineering **$192,000**
Cambridge, MA 02139 **01-A**
88-3

65. 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 normal 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.

Finally, detailed three-dimensional studies of through-cracks in "thin" sheets has 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.

MASSACUSETTS INSTITUTE OF TECHNOLOGY

The Energy Laboratory **$130,000**
Cambridge, MA 02139 **01-A**
88-3

66. Energetics of Comminution
C. Peterson

This program is central to a broader program of comminution research that includes basic studies on the behavior of single particles, particulate beds, and the design and testing of a novel coal crushing concept.

Single particle work has progressed the furthest. A very rigid miniature compression testing device has been fabricated and data generation has just begun. Behavior of the device is satisfactory and computer data acquisition is being installed to permit routine testing of a statistically significant number of particles. This device will provide information on force and energy requirements for particle fracture as a function of particle size and material properties. A new theory of comminution has been proposed which seems to explain the shift in energies required for failure as size decreases for uniform materials. More complex materials such as particles with voids and composite materials will be examined next. The increased difficulty to fracture a particle of smaller size has a practical significance in the crushing behavior of particulate beds.

Particulated bed work will include both analytical and experimental studies, seeking the combination of bed stress and strain required to cause individual particle fracture within some zones of the bed. These studies will ultimately tie back to the individual particle failure studies when computer simulations are used to predict particle movements and forces acting on the particles.

A novel comminution mill has been designed which uses particle-to-particle shear to cause particle failure.

MASSACUSETTS INSTITUTE OF TECHNOLOGY

Department of Materials Science and Engineering	**$ 95,000**
Cambridge, MA 02139	**06-A**
	88-3

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

The purpose of this investigation is to develop a comprehensive mathematical representation of the velocity field and of the temperature field in thermal plasma systems and to compare the theoretical predictions with experimental measurements.

The problem has been formulated through the statement of the axi-symmetric Navier-Stokes equations and the associated differential thermal energy and mass conservation relationships. The theoretical predictions for the gas temperature profiles were found to be in excellent agreement with the experimental measurements obtained by Dr. C. Shaw and Dr. J. Batdorf of the Idaho National Engineering Laboratory. The work is continuing with the objective of modelling gas mixing and representing the interaction between the plasma gas and solid particles.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY[1]

Department of Chemical Engineering	**$54,000**
Cambridge, MA 02139	**06-C**
	88-3

LOS ALAMOS NATIONAL LABORATORY[2]

Design Engineering Division	**$25,000**
Los Alamos, NM 87545	**06-C**
	88-3

SANDIA NATIONAL LABORATORIES[3]

Fluid and Thermal Sciences Department	**$25,000**
Albuquerque, NM 87185	**06-C**
	88-3

68. 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 for predicting 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. Currently empirical design procedures in these technologies are deficient in understanding how overall system behavior is related to the system's micromechanics.

Our 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 balls as they settle through suspensions of neutrally-buoyant particles. Measurements of the average and higher moments of the position and velocity distributions of the falling ball will provide boundary conditions for computer simulations of the flow fields in the continuous phase surrounding individual particles. This statistical knowledge of the microscale mechanical response will enable 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 balls settling in quiescent suspensions have been made, varying the relative sizes of the ball and suspended spheres. A theory has been developed to relate the average ball velocity to the macroscopic suspension viscosity. Finally, various test problems have been performed to establish the appropriate boundary conditions for both finite-element and boundary-element models of suspensions.

UNIVERSITY OF MINNESOTA

Department of Mechanical Engineering **$116,000**
Minneapolis, MN 55455 **01-B**
87-4

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

In many real flow systems separation occurs either intentionally or unintentially. 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 and Mechanics **$ 70,000**
Minneapolis, MN 55455 **01-C**
87-3

70. 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 **$361,000**
Minneapolis, MN 55455 **06-C**
88-3

71. Thermal Plasma Processing of Materials
E. Pfender

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

For the experimental work, a new Triple Torch Plasma Reactor with three identical DC torches has been developed for plasma processing of materials. This new reactor offers enhanced flexibility in terms of torch orientation and increased power levels.

Fine ceramic powders have been successfully synthesized in a previously developed DC plasma jet reactor using a novel liquid injection method.

Aqueous solutions of inorganic metal salts have been used as the precursors to synthesize single phase or composite oxides such as the high T_c superconducting oxide. In the synthesis of single phase carbides such as SiC, non-aqueous organometallic solutions of a single metal component are used as precursors.

Vortex or swirl gas flows are frequently employed in plasma systems such as DC plasma torches for arc stabilization. A two-dimensional model for turbulent plasma jets with superimposed vortex flow has been developed, incorporating multiple time scales for velocity and temperature fluctuations, and a density-weighted averaging for the density fluctuation effect. Comparisons of theoretical predictions based on the present model with available experimental data are, in general, in reasonable agreement.

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY*

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

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

The project aims at the development of equipment to measure the microstructure of liquids out of equilibrium. The objective of the research is to investigate, via neutron scattering, liquids subjected 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.

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

* Formerly the National Bureau of Standards

A shearing cell for less viscous and aqueous solutions is under construction and scattering data will be taken in the near future. Candidate solutions are suspensions and solutions of biological interest.

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

Chemical Engineering Science Division	**$109,000**
Center for Chemical Engineering	**01-C**
Boulder, CO 80303-3328	**87-2**

73. Residence Time Distribution Approach to the Study of Free Convection in Porous Media
M. Jones, R. Perkins, J. Wolfe

The structure and dynamics of the global flow patterns of free-convective flows in confined porous media is an important area of study form 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 Peclet numbers. The role of non-linear drag and of non-isotropic dispersion for both heat and mass tranport is being studied. Unsteady flows known to exist at high Rayleigh numbers are of particular interest.

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

Thermophysics Division **$120,000**
Boulder, CO 80303 **03-B**
87-3

74. Thermophysical Property Measurements in Fluid Mixtures
N.A. Olien, 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 **$125,000**
for Physico-Chemical Hydrodynamics **01-C**
New York, New York 10031 **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	**$80,000**
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 inthese flows, and the film thicnesses 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 hydrodynaic 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 lubicated 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	**$120,000**
of Physico-Chemical Hydrodynamics	**06-C**
New York, New York 10031	**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 **$67,000**
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 **$ 94,000**
Raleigh, NC 27695-7910 **06-A**
86-3

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

This research program is concerned with the quantitative relationship between certain transport properties of a disordered porous medium that arise in various energy-related problems (e.g., thermal or electrical conductivity 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, phase conductivity, 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).

A theoretical formalism has been developed to represent a general n-point distribution function from which one may compute any of the various types of correlation functions that have arisen in the literature. An efficient computer-simulation technique has also been developed to obtain these statistical quantities. Employing such lower-order n-point distribution functions, sharp bounds on the conductivity, elastic moduli, and permeability of models of porous media have been computed. The rigorous bound on the permeability for random beds of spheres is relatively close to the well-known Kozeny-Carman empirical formula. Finally, the study of percolation of phenomena in continuum random-media models has recently begun.

NORTHWESTERN UNIVERSITY

Department of Civil Engineering **$68,000**
Evanston, IL 60208 **03-B**
86-3

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 paper, crack closure has the most significant effect on far-field scattering.

NORTHWESTERN UNIVERSITY

Department of Engineering Sciences	**$111,000**
and Applied Mathematics	**01-B**
Evanston, IL 60208	**86-3**

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, thermocapillarity and long-range molecular (van der Waals) forces in a nonlinear stability theory for the film.

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

In the latter case we examine experimentally the dimpling of an oil film and compare quantitatively the interface profiles measured and predicted, given the temperature profiles sensed with thermocouples.

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.

NORTHWESTERN UNIVERSITY

Department of Engineering Sciences	**$50,000**
and Applied Mathematics	**01-C**
Evanston, Illinois 60208	**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 **$70,000**
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 an understanding of and a quantitative method for describing the waves which occur at the interface of separated gas-liquid flows. These waves exert a significant influence on the character of flows in the stratified and annular flow regimes, however their fundamental nature is not well-understood.

Both theoretical and experimental techniques are being used. For very thin films, (e.g. annular flow conditions) waves are relatively uniform and noninteracting and can consequently be described through the use of solutions which predict the behavior for individual waveforms. Observations of waves when the fluid is moderately viscous (15 cP) indicate that transitions between wave types occur with increases in gas Reynolds number and exhibit a relative insensitivity to liquid flow rate. Theoretical predictions using a linear theory agree well with measurements of wavelengths and wave speeds near the point of wave inception but begin to deviate as the gas velocity is increased. Current work includes a comparison of experiments with solutions to a nonlinear wave equation. For thicker films, (e.g. in stratified flows) waves are random, exhibit a high degree of interaction and can be treated in terms of their energy spectra. Experiments have shown that the most important wave interactions are those between a wave and its first overtone and that film depth and gas shear significantly affect the rate at which these interactions occur. An equation for the wave spectrum, which has been derived based on the total wave energy, clearly demonstrates the importance of energy transfer, energy input and dissipation in determining the shape of the spectrum.

OAK RIDGE NATIONAL LABORATORY

Engineering Physics and **$1,075,000**
Mathematics Division **03-C**
Oak Ridge, TN 37831 **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; robotic systems for identification, navigation, and manipulation in unstructured environments: and multi-purpose plant management and maintenance.

Specific FY 1988 research initiatives resulting in archival publications have included: (1) Autonomous Navigation, Exploration and Recognition, (2) Stability. Storage Capacity and Design of Nonlinear Continuous Neural Networks, (3) Learning by an Autonomous Robot at a Process Control Panel, (4) Treatment of Systematic Errors in the Processing of Wide Angle, Sonar Sensor Data, (5) Simulated Annealing Using the Mean Field Approximation, (6) Foundations of O-Theory: Measurements and Relation to Fuzzy Set Theory, and (7) Real-Time Implementation of a Kinematic Gradient Projection Optimization Scheme for a Seven-Degree-of-Freedom Redundant Robot with Spherical Wrists.

In addition, design of the HERMIES-III robot was completed and fabrication begun.

PHYSICAL SCIENCES INC.

Dascomb Research Park **$121,000**
P. O. Box 3100 **06-A**
Andover, MA 01810 **88-4**

85. 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 adequeous alcohol and acetone mixtures, thus removing a severe deficiency of classical binary nucleation theory.

PURDUE UNIVERSITY

School of Mechanical Engineering — $ 85,000
West Lafayette, IN 47907 — 01-C
87-3

86. 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

87. 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,	**$125,000**
Aeronautical Engineering & Mechanics	**01-A**
Troy, NY 12180-3590	**88-3**

88. 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.

The previously developed viscoplasticity theory based on overstress (VBO) which uses neither a yield surface nor loading and unloading conditions will be augmented to include the effects of recovery and aging. This constitutive equation will be combined with an incremental damage accumulation law. It exists in uniaxial form and will be reviewed and extended to multiaxial, isotropic conditions. The theory will be checked against companion experiments.

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 will be used for the first time in this study of biaxial deformation and failure behavior. The biaxial test facility was checked out and is ready for testing.

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. Strain aging was further investigated by relaxation and strain-rate-jump tests at high temperature. A finite deformation theory of viscoplasticity based on overstress is being developed and is being implemented into a finite element computer program.

RENSSELAER POLYTECHNIC INSTITUTE

Department of Nuclear Engineering	$120,000
and Science	01-C
Troy, NY 12180-3590	86-3

89. An Analysis of the Closure Conditions for Two Fluid Models of Two-Phase Flow
R.T. Lahey, Jr., D.A. Drew

The objective of the analytical study being conducted is to investigate the constraints imposed on the closure conditions of two fluid models of two-phase flow by:

(1) The postulate of continuum mechanics.

(2) The second law of thermodynamics.

(3) Mathematical well-posedness.

(4) Stability considerations.

In particular, we plan to develop an analytical basis on which unacceptable interfacial transfer laws and parameters can be filtered out. We have now begun work on investigating some of the existing closure laws which are commonly used in two fluid models. Formulation for the virtual mass force and the Reynolds stress are now being investigated. In addition, numerically-based algebraic manipulations are being employed to investigate the eigenvalues of currentgeneration two-fluid models. It is felt that the results of this research should significantly advance the state-of-the-art in the two fluid modeling of two-phase flows such that, in the future, well-posed models can be developed which only exhibit instabilities of physical origin.

THE ROCKEFELLER UNIVERSITY

Department of Physics **$80,000**
1230 York Avenue **06-C**
New York, NY 10021 **88-3**

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

The project is concerned with the following objectives: 1) The prediction of the transport coefficients for mixtures of real fluids, using a new form of the modified Enskog theory; 2) To develop a kinetic theory that allows a computation of the transport properties of polydisperse fluid mixtures, based on procedures developed for the thermodynamic properties of such mixtures as well as on an extension of the Enskog theory for hard sphere mixtures; 3) To study the eigenmodes in binary hard sphere fluid mixtures in thermal equilibrium, for all mass ratios and densities. The study will be based on the generalized Enskog theory. The results will be compared with laboratory and computer experiments; 4) A systematic investigation of binary mixtures in the gaseous state--such as the noble gas mixtures--will be made to study the occurrence of a new type of sound, fast sound, in these mixtures. This fast sound mode has recently been predicted to exist in He-Xe mixtures; 5) A critical study of cellular automata fluids is undertaken that comprises not only their applicability to describe the flow properties of real fluids but also the diffusion properties of particles moving on lattices in the presence of randomly distributed stationary obstacles. In view of the many unrealistic features of these automata fluids as compared to real fluids, attempts will be made to incorporate into the existing models more realistic features.

SANDIA NATIONAL LABORATORIES

Combustion Research Facility **$135,000**
Thermofluids Division **06-B**
Livermore, CA 94550 **87-3**

91. 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 **$135,000**
Thermofluids Division **06-B**
Livermore, CA 94551-0098 **87-3**

92. 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. Two single droplet experiments are also nearing completion, one utilizing a flat flame burner and one using a levitator with laser ignition capabilities. These four experiments will provided needed deformation, breakup, and transport data for liquid ligaments and large droplets.

SCIENCE APPLICATIONS INTERNATIONAL CORPORATION

Applied Plasma Physics and Technology Division	**$85,000**
10260 Campus Point Drive	**06-C**
San Diego, CA 92121	**88-2**

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

The first part of the research is to derive the nonlinear 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.

SOLAR ENERGY RESEARCH INSTITUTE

Thermal Sciences Research Branch	**$ 50,000**
1617 Cole Blvd.	**01-C**
Golden, CO 80401	**85-4**

94. Shear-Induced Instabilities in a Double-Diffusive Partially Stratified Fluid
F. Zangrando

This basic experimental study concentrates on mixing mechanisms in a double-diffusive, stratified fluid subjected to the combined effects of bottom heating and horizontal flow. The fluid contains two components (in this case, heat and salt) that contribute in an opposing manner to the fluid density and have significantly different diffusivities (ratio of order 100). The tasks proposed emphasize qualitative and quantitative observation of the behavior of the interfacial layer between a double-diffusive stratification and an initially well mixed region, both of arbitrary thickness, in the presence of buoyancy driven convection due to bottom heating and of shear flow imposed on the mixed region. The effect of each destabilizing component, including line jet discharge and flow into a sink, will be first studied separately and compared with results obtained with single-component stratifications. The combined effect of buoyancy driven convection with a superposed lateral flow (recirculation) will then be studied in order to compare the various mixing mechanisms under similar experimental conditions and to determine the entrainment at the interfacial boundary layer.

STANFORD UNIVERSITY

Department of Mechanical Engineering **$66,000**
Stanford, CA 94305-3030 **01-B**
86-3

95. Heat Transfer in Three-Dimensional Turbulent Boundary Layers

J. Eaton

Most boundary layers in practical systems are three-dimensional while most basic research on convective heat transfer has focused on two-dimensional flows. The objectives of this work are to determine the effects of three-dimensionality on the heat transfer behavior and how these effects may be modeled. A series of simple flows with successively stronger three-dimensionality are being examined.

The first two experiments examined two-dimensional boundary layers with large-scale embedded longitudinal vortices. Detailed data including all components of the mean velocity vector and Reynolds stress tensor, spatially resolved heat transfer, temperature profiles, and skin friction have been obtained. Pairs of moderate strength vortices cause significant deviations from two-dimensional boundary layer behavior in regions where the cross-flow is strong. Both the momentum and thermal laws of the wall are violated showing that any models based on two-dimensional similarity laws will fail. The turbulent Prandtl number decreases strongly under the vortex. These effects are all tied to a reduction of the boundary layer turbulence length scale. Conventional two-equation turbulence models fail to predict the distorted Reynolds stress field. An improved model was proposed but is not itself entirely satisfactory.

The third experiment is a study of an initially 2D boundary layer which is skewed laterally by a pressure gradient resulting in strong three dimensionality. Fluid mechanics measurements in the fully three-dimensional flow indicate that the important near-wall layers are strongly perturbed. The ration of the Reynolds shearing stresses 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. The system for measuring heat transfer in this flow is being fabricated. Significant deviations from two-dimensional behavior are expected.

STANFORD UNIVERSITY

Department of Mechanical Engineering **$165,000**
Stanford, CA 94305-3030 **01-A**
86-4

96. 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.

An anisotropic elastic boundary integral method has been developed and used to predict the existence of stable void lattices in irradiated FCC and BCC metals; numerical results are in close agreement with experimental observations quoted in the literature. An apparent paradox in the dislocation literature has been resolved. Although it should be well-known that the energy of a (Volterra) dislocated solid is independent of the cut used to create it, virtually all such calculations in the literature are not cut-independent and are incorrect. Our resolution of this paradox has important implications for the appearance of misfit dislocations in epitaxial systems. A new investigation of energy changes and forces associated with dislocations in anisotropic layered media is being undertaken, and the theory of interfacial waves in anisotropic elastic media is being extended to include piezoelectricity.

An integral equation method has been developed to study problems of interaction between holes and defects in elastostatics, including the calculation of energy release rates. An elementary theory of defective beams in bending and of bars in tension, compression, and torsion has been developed. Based on an extended circle theorem originally established in potential flow theory, the temperature distribution in an infinite region containing a circular cavity (defect) was determined in terms of the distribution existing in the same region without the cavity. The stress distribution induced by the presence of the defect was shown to be universal, i.e., it depends essentially only on the magnitude of the heat flux vector existing at the center of the defect before it was created.

STANFORD UNIVERSITY

W.W. Hansen Laboraotories of Physics **$250,000**
Stanford, CA 94305-3030 **03-B**
87-3

97. 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 **$137,000**
Environmental Fluid Mechanics Laboratory **01-B**
Stanford, CA 94305-4020 **87-3**

98. 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 **$410,000**
Stanford, CA 94305 **03-B**
88-4

99. 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 which can 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 Gasdynamics Laboratory. Optical methods will be 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 the formation and removal of chemical species, so as to facilitate the rational design of plasma processing facilities.

Results to date from spectroscopic measurements of the inductively coupled plasma show differences between Boltzmann excitation temperatures and those inferred 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. This difference has been interpreted in terms of nonequilibrium effects in the earlier experiments and an upper-bound limit with respect to the decay of radiation source strength with decreasing temperature.

STANFORD UNIVERSITY

Department of Chemistry **$109,000**
Stanford, CA 94305 **06-C**
86-3

100. 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. 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 by preliminary 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. Bother theoretical and experimental studies are planned on optimization of efficiency by choices of functional forms of external perturbations.

STANFORD UNIVERSITY

Department of Civil Engineering **$160,000**
Environmental Fluid Mechanics Laboratory **01-B**
Stanford, CA 94305-4020 **87-2**

101. Momentum And Heat Transfer In A Complex But Well-Defined Turbulent Flow
R.L. Street, J.R. Koseff

A basic study of a three-dimensional, recirculating flow with variable density effects is being conducted in a lid-driven cavity. The overall objectives of the research are (1) an improved understanding of the influence of longitudinal vortices on heat transfer in the cavity and of the interaction between forced and natural convection processes, (2) achievement of three-dimensional numerical simulation of recirculating, natural, and mixed-convection flows, and (3) understanding the effects of cavity geometry on momentum and heat transfer processes in such flows.

The present major focus is on extending the work on square cavities (depth equal to width) to cavities of variable depth. Physical experiments are being performed in a lid-driven cavity facility using water as the working fluid. Measurements include those obtained by laser-Doppler anemometry, microthermocouples, heat-flux meters, and liquid crystal and polystyrene bead flow visualization. Image processing is being used to extract quantitative information from the flow visualization photographs.

Numerical experiments are also being performed in support of specific physical experiments and on a side-wall-heated natural convection flow. These numerical experiments are being conducted using the SEAFLOS1 code. This time-accurate, explicit code features a revised QUICK formulation and the Incomplete Cholesky Conjugate Gradient (ICCG) Method or the multigrid technique for solving the pressure equation. These last-mentioned techniques are producing significant savings in simulation runtime.

STANFORD UNIVERSITY

Department of Mechanical Engineering **$86,000**
Design Division **03-A**
Stanford, CA 94305 **86-3**

102. Global Optimization of Non-Posynomial Design Models
D.J. Wilde

Geometric Programming optimization problems can be solved by maximizing a dual function subject to linear constraints. This dual, although convex, is only poorly approximated by a homogeneous quadratic form, but allowing axis rotation gives a remarkably good fit by the method of least squares. The resulting quadratic program has a closed form matrix solution to be used iteratively. Proof of convergence, convergence rate estimation, and computer testing on engineering design problems are in Shensheng Zhang's Ph.D. dissertation "Generalized Polynomial Optimization in an Augmented Primary Space using General Quadratic Approximation" and in two research papers based on it.

A different approach to global optimization is being studied by Ph.D. candidate Yong Se Kim. His research concerns expressing a non-convex set uniquely as a difference of convex sets. Although the problem is motivated by the three-dimensional problem of computer characterization of machine parts, it may be extendable to more dimensions. This would allow non-posynomial optimization problems to be decomposed into convex posynomial problems separately solvable by known efficient algorithms

STEVENS INSTITUTE OF TECHNOLOGY

Department of Physics and Engineering **$ 64,000**
Hoboken, NJ 07030 **06-C**
87-4

103. 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

104. 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. First, the methods of nonlinear dynamical systems will be applied to investigate the transition phenomena occurring in physico-chemical problems such as atmospheric dynamics, the Belusov-Zhabotinski reaction and the oxidation of hydrocarbons in the gaseous phase. Both perturbative and global techniques will be applied, since current experimental evidence suggests that some of these transitions involve chaotic dynamics and homoclinic orbits. Second, problems arising in connection with selection of nonequilibrium states will be analyzed. In particular, the effect of extremely small influences in the selection of symmetry-breaking states -- which are realized in chemical, electronic, and other systems -- will be studied, taking both additive and multiplicative fluctuations into consideration. The implication of the results for the origin of biomolecular chirality will be assessed. Collaborative experiments are planned to substantiate the theoretical developments. Third, special attention will be focused on the problem of combustion. A fundamental analysis of this phenomenon, from both the standpoint of the theory of dynamical systems and the standpoint of stochastic theory, is still lacking. In the proposed research, the effect of stochastic perturbations, of inhomogeneities and of internal fluctuations during the process of ignition, in which the system is expected to present a high sensitivity, will be analyzed using Semenov's model for combustion as well as more realistic models. A fundamental theory of nucleation of flame fronts is expected to be one of the outcomes of these developments.

UNIVERSITY OF TEXAS AT AUSTIN

Department of Physics **$142,000**
Austin, TX 78712 **06-C**
87-5

105. 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 **$134,000**
and Center for Energy Studies **01-B**
Austin, TX 78712 **87-3**

106. 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	**$ 55,000**
Medford, MA 02155	**01-A**
	86-2

107. 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	**$185,000**
East Hartford, CT 06108	**06-A**
	86-3

108. Laser Diagnostics Of PACVD Processes
W. C. Roman, J. H. Stufflebeam, 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. optical emission and absorption spectroscopy, 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. 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, density, 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 (ultimate 10-8 torr); 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 and 5) demonstrated CARS collibrator sensitivity PSCVD reactor of 10m Torr.

WASHINGTON STATE UNIVERSITY

Department of Mechanical Engineering	**$ 0**
Pullman, WA 99164-2920	**01-B**
	86-3

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

This research program is directed towards understanding the role of quasi deterministic large scale vortices in the dispersion of particles by turbulent mixing layers. The primary objective of this experimental study is to determine the influence and importance of these vortex structures on the particle dispersion process over a range of particle and flow parameters. It is hypothesized that if the time scale associated with the vortex motion and the particle

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

relaxation time are of the same order, significantly enhanced particle dispersion may occur.

The experiments employ both high speed photographic methods and laser velocimetry techniques. The experimental results demonstrate that large scale vortex structures dominate the particle dispersion process for intermediate size particles. The experimental dispersion patterns appear qualitatively similar to numerical results obtained using time dependent numerical simulation techniques. Current efforts involve quantifying the experimental results for more detailed comparisons with numerical predictions. Initial experimental results also demonstrate that substantial modifications of the particle dispersion process can be achieved using controlled forcing techniques.

The primary anticipated result of this study is a new physical model for interpreting and predicting particle dispersion in unbounded turbulent shear flows. New techniques for controlling or modifying the dispersion of particles in turbulent flows are a possible outcome of this research program.

WESTINGHOUSE R&D CENTER

Chemical & Process Development Dept. **$151,000**
1310 Beulah Road **01-C**
Pittsburgh, PA 15235 **86-3**

110. The Design of a Cylindrical Film Chemical Reactor
R.M. Roidt

This research is to investigate the basic characteristics of a cylindricall film chemical reactor; i.e., a falling annulus of liquid within which gases and sprays may be injected to react chemically. The program is primarily experimental and focuses primarily on film stability, internal gas entrainment rates, and geometric variations in the film configuration. Studies have been completed on 5, 10, and 30 cm diameter annuli with .5, 1, and 2 mm annular clearances. Ranges of stable film operation with various liquid flow rates and internal gas injection rates have been investigated. The primary focus at present is the determination of the conditions under which internal sprays may be entered into the reaction volume to enhance surface area reactions for such application areas as scrubbers. The induced internal gas flows caused by the sprays are quite disruptive of film operation and various injection techniques are being investigated to alleviate these interactions. This work is closely coordinated with the Carnegie-Mellon University Combustion Laboratory.

UNIVERSITY OF WISCONSIN

Mechanical Engineering Department **$100,000**
Madison, WI 53201 **01-C**
87-3

111. Interfacial Area and Interfacial Transfer in Two-Phase Flow Systems
G. Kocamustafaogullari, M. Ishii
(ANL)

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
Madison, WI 53706

$106,000
03-A
86-3

112. 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.

BUDGET NUMBER INDEX

Mechanical Sciences:

01-A Solid Mechanics: macroscopic aspects of elastic and plastic deformations, and crack propagation
01-B Heat Transfer
01-C Fluid Mechanics
01-D Tribology

Control Systems and Instrumentation:

03-A Control systems, large scale systems
03-B Instrumentation for hostile environment, and NDE
03-C Intelligent systems

Engineering Data and Analysis:

06-A Thermophysical properties and processes
06-B Combustion
06-C Non-linear dynamics and engineering analysis

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WASHINGTON, D.C. 20545

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