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ANNUAL REPORT ON
THE COLLABORATIVE PROGRAM OF RESEARCH IN ENGINEERING SCIENCE

September 1, 1989 to December 31, 1990

Energy Laboratory of the
Massachusetts Institute of Technology
in collaboration with the
Idaho National Engineering Laboratory

December 1990

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A Proposal for Continuation of a Collaboration Engineering Research
Program--The Idaho National Engineering Laboratory and the
Massachusetts Institute of Technology. Vol. 1 and Vol. II February 1990

SUMMARY OF PROGRAMS
AND
PUBLICATIONS

COLLABORATIVE PROGRAM OF RESEARCH IN ENGINEERING SCIENCES

Principal Investigator:

Prof. D. C. White, Energy Laboratory and Department of Electrical Engineering and Computer Science

Associated Faculty:

Prof. T. W. Eagar, Department of Materials Science and Engineering
Prof. J. F. Elliott, Department of Materials Science and Engineering
Prof. L. B. Evans, Department of Chemical Engineering
Prof. D. E. Hardt, Laboratory for Manufacturing and Productivity
Prof. J. H. Lang, Department of Electrical Engineering and Computer Science
Prof. F. A. McClintock, Department of Mechanical Engineering
Prof. D. M. Parks, Department of Mechanical Engineering
Prof. C. R. Peterson, Department of Mechanical Engineering
Prof. J. Szekely, Department of Materials Science and Engineering

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71603, 73142)

Dates:

January 1988 - December 1990

MIT and the Idaho National Engineering Laboratory (INEL) are continuing the program of collaborative research on energy-related engineering. The collaboration is in response to recent suggestions that national laboratories cooperate with universities in developing cooperative research programs that use the strength of each to enhance research productivity.

The MIT/INEL program involves research in the following areas, which are examined in more detail in individual project summary writeups in this section

Mathematical modeling of thermal plasma systems. We have developed a comprehensive mathematical model that describes the electromagnetic, heat transfer, and fluid flow phenomena in thermal plasma systems. The model is two-dimensional and axi-symmetric, with provision for swirl. Its theoretical predictions for argon-argon systems agree well with measurements obtained by the researchers at INEL and also in France.

High-temperature gas-particle reactions. To design better plasma processing systems, we need to know how small particles respond chemically and physically to conditions inside thermal plasma flames. Using a special containerless reactor, we have exposed single particles to high temperatures for fractions of a millisecond and have obtained accurate single- and two-color particle temperature measurements during the heating and cooling cycle.

Metal transfer in gas-metal arc welding (GMAW). Automating the GMAW process requires a model that can predict the electrode melting rate and the mode of metal transfer. Through experimental and theoretical studies, we quantified the forces controlling droplet detachment from the electrode and developed a modified static force balance that explains observed experimental trends. Our analysis, coupled with a model of energy distribution in the electrode, provides an improved understanding of both constant-current and pulsed-current GMAW.

Multivariable control of gas-metal arc welding. We have been working on a control strategy for GMAW that will enable us to regulate a variety of geometric and metallurgical attributes of the weld in real time. We have developed and experimentally

confirmed analytical and empirically based models indicating that system dynamics depends mainly on welding velocity and that steady-state characteristics are highly nonlinear. The strong coupling among geometric features (bead width, height, and depth) and the small range of acceptable modulation of the welding current greatly limit the controllability of the process. We developed and tested several multivariable control systems, and our experiments indicate that we may have to redesign the process to enhance controllability.

Fundamentals of elastic-plastic fracture. Using methods of finite element analysis, we have performed detailed studies of the types of cracks that can lead to catastrophic failure in engineering structures made of normally ductile materials. The studies are providing a deeper understanding of three-dimensional crack front stress and deformation fields. Our calculations aid in establishing parametric limits of applicability for dominant singularity and local approaches to fracture analysis in ductile structures. We have also developed models for analyzing cracked structures that are nearly as accurate as finite-element methods but far simpler and less expensive.

Comminution of energy materials. To devise more efficient comminution methods, we examined the behavior of particle beds and the fracture of particles within such beds. We developed a computer simulation of two-dimensional beds of spherical particles that predicts well the behavior observed in large-particle, relatively homogeneous experimental beds. Work on individual particles established appropriate particle-failure criteria for brittle particles subject to multiple point loads as experienced within a bed. Based on those studies, we have designed a novel crusher/material transport concept that will be the focus of further studies and design work.

Synthesis and optimization of integrated chemical processes. This research has focused on developing computer-based methods to help engineers synthesize a process with improved energy integration. The strategy has been to combine modern mathematical programming techniques, sophisticated rigorous models of the process utilities system and heat recovery network, and heuristic methods to develop an overall methodology that is more powerful than traditional approaches. The net result of the research has been an improved understanding of the nature of the problem of energy integration in process plants and the development of methods to help engineers solve realistic industrial problems. The research is now being redirected to address the synthesis and optimization needs of batch and semi-continuous manufacturing processes. These processes are of increasing importance for the manufacture of high-value performance products such as those produced by biotechnology. Yet, the development of systematic computer-based methodologies for batch process is only in its infancy.

A key objective of this collaborative program is to serve as a prototype for other university/laboratory collaborative programs. Another important goal is to enhance the transfer of new technology to the industrial sector. In order to help reach these goals, the program has created advisory groups from industry, academia, and other national laboratories to assist in program direction, evolution, and evaluation.

MATHEMATICAL MODELING OF TRANSPORT PHENOMENA IN PLASMA SYSTEMS

Principal Investigator:

Prof. J. Szekely, Department of Materials Science and Engineering

Research Staff:

Prof. A. H. Dilawari, Institute of Chemical Engineering and Technology, Punjab University, Pakistan

Dr. J. H. Zong, Department of Materials Science and Engineering

Graduate Students:

G. Trapaga Martinez, R. C. Westhoff

Undergraduate Student:

M. Jansen

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71605, 73144)

Dates:

January 1985 - December 1990

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

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

Publications:

Choo, R. T. C., J. Szekely and R. C. Westhoff. "Modelling of high current arcs in welding with emphasis on free surface phenomena in weld pool." *Welding Journal*, 1990.

Dilawari, A. H., J. Szekely, J. Batdorf and C. B. Shaw. "The temperature profiles in an argon plasma issuing into an argon atmosphere: a comparison of measurements and predictions." *Plasma Chem. Plasma Process.*, v. 10, no. 2, p. 317, 1990.

Dilawari, A. H., J. Szekely and R. Westhoff. "A comparison of experimental measurements and theoretical predictions regarding the behavior of a turbulent argon plasma jet discharging into air." *Plasma Chem. Plasma Process.* v. 10, no. 3, p. 501, 1990.

Dilawari, A. H., J. Szekely and R. Westhoff. "An assessment of heat and fluid flow phenomena inside plasma torches in non-transferred arc systems." *ISIJ International*, v. 30, no. 5, p. 381, 1990.

Dilawari, A. H., R. Westhoff, J. Szekely, C. B. Shaw, Jr. and B. A. Detering. "A comparison of the experimentally measured and theoretically predicted temperature profiles for an argon plasma jet discharging into a nitrogen environment." MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA, 1990.

Szekely, J. "Transport phenomena in welds with emphasis on free surface phenomena." Second International Conference on Trends in Welding Research, Gatlinburg, TN, 1989.

Trapaga, G., R. Westhoff, J. Szekely, J. Fincke and D. Swank. "Particle and temperature histories in a plasma plume: a comparison of measurements and predictions." MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA, 1990.

Westhoff, R. C. *A Mathematical Model for Current, Heat Flux, and Pressure in a Welding Arc*. SM thesis, MIT Department of Materials Science and Engineering, Cambridge, MA, 1989.

Westhoff, R., A. H. Dilawari and J. Szekely. "A mathematical representation of transport phenomena inside a plasma torch." MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA, 1990.

STUDY OF HIGH-TEMPERATURE GAS-PARTICLE REACTIONS

Principal Investigator:

Prof. J. F. Elliott, Department of Materials Science and Engineering

Research Staff:

Dr. P. Bolsaitis, Energy Laboratory

Mr. V. Dekermendjian, Energy Laboratory

Graduate Student:

M. Salas-Morales

Undergraduate Student:

C. D. Smith

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71604, 73143)

Dates:

January 1985 - December 1990

Research is continuing on the measurement of temperatures and kinetics of phase transformations and reactions of small particles (10 μm to 150 μm) and thin fibers that are exposed to heating cycles and atmospheres encountered in plasma processing and flash smelting of materials. The materials studied include refractory ceramics (alumina, silica, silicon carbide, tungsten carbide), metals and alloys (chromium, iron nickel), sulfides (chalcopyrite, lead sulfide, nickel sulfide), and various types of carbon. The experimental setup permits heating and quenching rates of the order of one million degrees per second.

The final structure of materials processed at high-temperatures depends principally on their thermal history, especially their cooling rates. It is of interest for the design of optimal processes that involve high-temperatures and small particles to understand how the thermal history of individual particles affects their final structure and properties. The measurement of rapidly changing temperature of a small particle has been one of the principle issues of the research in progress. The changes of particle emissivities with temperature and of cross-sectional area by vaporization, together with complex instrument response characteristics make accurate temperature determinations an interesting problem. The common non-contact temperature measurement methods (one- and two-color pyrometry) have been analyzed to establish calibration and data correction methods to obtain more accurate temperature measurements of small, rapidly heated and cooled particles.

A study of heat-pulsing of alumina particles under conditions where vaporization takes place has been completed. This study has confirmed the previously measured vaporization rate, the measurement of levels of undercooling of liquid alumina under conditions of rapid cooling, and has resulted in better methods for correction of the apparent temperatures measured under such conditions.

Publications:

Bolsaitis, P., R. E. Spjut and J. F. Elliott. "High-temperature pulses in small alumina particles." *High-Temperature-High Pressure*, v. 21, pp. 601-611, 1989.

Fincke, J. R., W. Swank, P. Bolsaitis and J. F. Elliott. "The measurement of single particle temperatures in plasma sprays." *Proceedings, Symposium on Energy Engineering Sciences*, Argonne National Laboratory, Argonne, IL, May 9-11, 1990.

METAL TRANSFER IN GAS-METAL ARC WELDING

Principal Investigators:

Prof. T. W. Eagar, Department of Materials Science and Engineering

Prof. J. H. Lang, Department of Electrical Engineering and Computer Science

Graduate Student:

L. A. Jones

Undergraduate Students:

A. H. Cheng, D. F. Mulso

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71606, 73145)

Dates:

January 1985 - December 1990

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

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

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

Publications:

Eagar, T. W. "An iconoclast's view of the physics of welding--rethinking old ideas." In *Recent Trends in Welding Science and Technology*, S. A. David and J. M. Vitek, eds., ASM, Materials Park, OH, p. 341, 1990.

Eagar, T. W. "The physics of welding processes." *Proceedings of the 5th International Symposium of the Japan Welding Society on Advanced Technology in Welding, Materials Processing and Evaluation*, Makuhari, Tokyo, Japan, April 17-19, 1990.

Karl, W. C., S. B. Leeb, L. A. Jones, J. L. Kirtley and G. C. Berghese. "Applications of a class of nonlinear filters to problems in power electronics." *PESC '90 Record (I)*, 21st Annual IEEE Power Electronics Specialists Conference, p. 35, June 1990.

Kim, Y. S. and T. W. Eagar. "Temperature distribution and energy balance in the electrode during GMAW." In *Recent Trends in Welding Science and Technology*, S. A. David and J. M. Vitek, eds., ASM, Materials Park, OH, p. 13, 1990.

MULTIVARIABLE CONTROL OF GAS-METAL ARC WELDING

Principal Investigator:

Prof. D. E. Hardt, Laboratory for Manufacturing and Productivity

Research Staff:

Mr. F. P. Cote, Laboratory for Manufacturing and Productivity

Dr. A. Sharon, Laboratory for Manufacturing and Productivity

Graduate Students:

T. Chuang, M. B. Hale, R. A. Masmoudi, T. Reeder, J. B. Seng

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71607, 73146)

Dates:

January 1985 - December 1990

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

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

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

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

Rapid convergence and development of a depth control system based on this estimator is now being processed.

Publication:

Hale, M. B. *Multivariable Control of a GMA Welding Process*. PhD thesis, MIT Department of Materials Science and Engineering, Cambridge, MA, September 1989.

MODELING AND ANALYSIS OF SURFACE CRACKS

Principal Investigators:

Prof. D. M. Parks, Department of Mechanical Engineering

Prof. F. A. McClintock, Department of Mechanical Engineering

Graduate Students:

Y. J. Kim, H. Y. Lee, Y. Y. Wang

Undergraduate Students:

A. T. Singer, K. Y. Tung

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71609, 73148)

Dates:

January 1985 - June 1990

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

Publications:

McClintock, F. A. "Asymmetry lowers ductility." *International Journal of Fracture*, v. 42, pp. 357-370, 1990.

Nakamura, T. and D. M. Parks. "Anti-symmetric three-dimensional stress field near the crack front of a thin elastic plate." *International Journal of Solids and Structures*, v. 25, pp. 1411-1426, 1989.

Nakamura, T. and D. M. Parks. "Three-dimensional crack front fields in a thin ductile plate." *The MIT Report*, August 1989.

Parks, D. M. "A surface crack review: elastic-plastic behavior." in *Surface-Crack Growth: Models, Experiments, and Structures*, ASTM STP 1060, W. G. Reuter, et al., eds., ASTM, Philadelphia, PA, pp. 9-33, 1990.

Parks, D. M. "Three-dimensional aspects of HRR-Dominance." *The MIT Report*, October 1989.

Wang, Y. Y., D. M. Parks, W. R. Lloyd, W. G. Reuter and J. Epstein. "Elastic-plastic deformation in surface-cracked plates: experiment and numerical analysis." *The MIT Report*, May 1990.

BASIC ENGINEERING SCIENCES OF SOLIDS COMMINUTION

Principal Investigator:

Prof. C. R. Peterson, Department of Mechanical Engineering

Associated Faculty:

Prof. F. A. McClintock, Department of Mechanical Engineering

Graduate Students:

K. J. Annis, J. R. Easter, C. K. Ghaddar, S. D. Misra

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71610, 73149)

Dates:

January 1985 - December 1990

This work is part of a broader study of the energy and force requirements for fine grinding of minerals and coal. Research is directed to the crushing behavior of individual particles, down to perhaps 50 microns, and the behavior of particle beds, including in particular the failure of individual particles within such beds.

Experimental work has been completed on the force and energy necessary to fracture small glass spheres and on the behavior of beds of glass spheres, including the fracture of individual spheres within beds subjected to overall compression. Studies on the fracture behavior of large (one inch) brittle and plastic spheres have been completed.

Analytical work has developed a detailed simulation of the overall and interior behavior of beds of spheres subjected to compression, including the fracture of individual spheres when sufficiently stressed. The simulation was limited to a two-dimensional array of three-dimensional spheres. Correlation of simulated and experimental behavior has been encouraging, but it became clear that an appropriate failure criterion for spherical particles subjected to multiple point loads from neighboring particles was necessary. Four assumed criteria yielded significantly differing bed behavior.

Analytical and experimental work on fracture of individual spheres established an appropriate failure criterion, at least for brittle spheres (which happens to be the simplest of the four assumed criteria). The criterion is also appropriate for plastic spheres subjected to moderate secondary loads, but this is not the case when secondary loads are comparable to the major point load.

With the confirmation of an appropriate particle fracture criterion, at least for most particles, the bed simulation is now deemed suitable for use as a design tool.

Continuing studies have expanded to consider the combined actions of crushing and solids transport with particle beds, with particular attention to the size-dependent relative motion of particles to permit effective removal of fine material as it is formed. A novel comminution device has been conceived to provide the desired crushing and separation, and this concept serves to guide continuing research. Experimental determination of crushing efficiency within beds has shown a maximum efficiency at about 20% bed compaction, followed by rapidly declining efficiency at greater compaction as remaining void space approaches zero. Contrary to expectations, thin beds (about 3 particles deep) are not as efficient as thick beds (greater than 15 particles deep). Preliminary experiments to separate small and large particles with an upward fluid flow have been very successful.

SYNTHESIS AND OPTIMIZATION OF INTEGRATED CHEMICAL PROCESSES

Principal Investigator:

Prof. L. B. Evans, Department of Chemical Engineering

Research Staff:

Dr. A. G. Helget, Department of Chemical Engineering

Graduate Students:

M. D. Barrera, S. Sundaram, H. J. Yoon

Sponsor:

U.S. Department of Energy, Basic Energy Sciences (71608, 73147)

Dates:

January 1985 - December 1990

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

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

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

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

Publications:

Barrera, M. D. *Performance Modeling in the Design and Optimization of Batch Chemical Processing Systems*. PhD thesis, MIT Department of Chemical Engineering, Cambridge, MA, March 1990.

Barrera, M. D. and L. B. Evans. "Optimal design and operation of batch processes."
Chem. Eng. Comm., v. 82, pp. 45-66, 1990.

Yoon, H. J. *Heat and Work Integration in the Synthesis of Chemical Plants*. PhD thesis,
MIT Department of Chemical Engineering, Cambridge, MA, January 1990.

General Introduction

It is widely recognized that, if the United States is to maintain its leadership role among industrial nations, there are two key issues to which particular attention must be paid. These are (1) economical and environmentally safe production, transmission, and utilization of energy and (2) strengthening the nation's scientific knowledge base with attendant improvement in its ability to translate scientific knowledge into new products and processes. If these issues are to be dealt with adequately, engineering research, which may be defined as the adaptation and extension of fundamental science and technology to create and improve engineering applications, must be performed.

This document discusses the MIT portion of a collaborative engineering research program performed by the Idaho National Engineering laboratory (INEL) and the Massachusetts Institute of Technology (MIT). This program, which began in 1985, is motivated in part by the need to address the issues listed above. There are other motivations which make this program unique. The program is responsive to the "Packard Report," produced by the White House Science Council on Federal Laboratories, in which it is recommended that closer interaction occur between national laboratories and universities. The program is intended to become a prototype for such collaborative efforts. In addition, a significant motivation is the transfer to industry of technology developed in the course of the program. Both MIT and the INEL have close associations with industry that hold the promise of facilitating such technology transfer.

Management of the program rests with a program manager from each of the two institutions. The INEL Program Manager is responsible to a program monitor at the Idaho Operations Office of the Department of Energy for ensuring adherence to cost, scope, and schedule for the INEL program. The INEL and MIT Program Managers interact with each other and with a program monitor in the Division of Engineering and Geosciences, Office of Basic Energy Sciences, Department of Energy.

Because the program entails objectives which go beyond the research results normally expected in such an effort, a committee system is in place to ensure that all objectives are met. Technical Advisory Committees, consisting of experts in the various fields of research, attend an annual, overall review of the program. (Reviews are held on alternate years at MIT and the INEL.) These Committees have played a key role in assessing technical progress of the program, as well as program direction and management. The Committees

provide both oral and written reports of their findings to the Program Managers. The written reports from the July 17-18, 1990 Technical Reviews are included with each section. The DOE program monitors also attend the oral presentations. The written reports are subsequently transmitted to the Principal Investigators. Views expressed by the Committees are taken very seriously and frequently serve as bases for changes in research techniques, new avenues of approach, and altered management procedures. Membership of these Committees, responsible for the July 17-18 reviews are given in Table 2. A Steering Committee, consisting of representatives selected from the Technical Advisory Committees, has the charter of reviewing research progress, program management, quality of interlaboratory collaboration, responsiveness to industry's long-term needs, and potential new research areas. In addition, technology obtained in the program is examined for appropriateness for transfer to industry. The Committee is intended to establish mechanisms and industry candidates for technology transfer and implement means whereby MIT and INEL Principal Investigators and industry representatives can interact directly to assist in achieving program goals. Steering Committee members are listed in Table 3.

TABLE 2. TECHNICAL ADVISORY COMMITTEES

July 17-18, 1990

Thermal Plasma Processing

Dr. C. W. Hirt
Flow Science, Inc.

Dr. Richard E. Palmer
Sandia National Laboratories

Professor Emil Pfender
University of Minnesota

Dr. Thomas Meyer
ALCOA

Dr. Diran Apelian
Drexel University

Mr. Merle L. Thorpe
TAFE, Inc.

Sensing and Control of Droplet- Based Thermal Systems

Dr. Hugh Casey
Los Alamos National Laboratory

Professor David Olsen
Colorado School of Mines

Dr. Paul W. Ramsey
Ramsey and Associates

Mr. Howard B. Carey
Hobart Brothers Company

Dr. George E. Cook
Vanderbilt University

Mr. Richard Morris
David Taylor Research Center

Fracture Mechanics/Comminution/NDE

Professor Robert McMeeking
University of California, Santa Barbara

Dr. Sam S. Palusamy
Westinghouse Electric Corporation

Dr. J. C. Newman, Jr.
NASA Langley Research Center

Dr. John Gudas
David Taylor Research Center

TABLE 3. STEERING COMMITTEE

July 17-18, 1990

Thermal Plasma Processing

Mr. Merle L. Thorpe
TAFA, Inc.

Sensing and Control of Droplet Based Thermal Systems

Dr. Hugh Casey
Los Alamos National Laboratory

Solid Mechanics/NDE/Comminution

Dr. Sam S. Palusamy
Westinghouse Electric Corporation

THERMAL PLASMA PROCESSING

Technical Advisory Committee--Thermal Plasmas

Based upon today's presentations on the subject of Thermal Plasma, the Thermal Plasma Processing Technical Advisory Committee offers the following comments and suggestions:

1. More graduate student participation should be included in future efforts.
2. Improved program integration/coordination between INEL and MIT could provide significant benefit. This will require an energetic and decisive leader to provide much technical leadership.
3. The effort by C. Shaw should be modified to obtain measurements in a "single shot" and avoid unacceptable time averaging difficulties. A concentrated effort to do this and obtain a set of good velocity measurements should provide the basis to consider further efforts in this area at the next review meeting. Alternatively, if the technique does not work, other velocity measurement approaches should be considered.
4. The non-equilibrium effort by T. Eddy must be coupled with model development efforts by J. Ramshaw. Through this interaction the relative importance of non-LTE terms can be appreciated. A tangible demonstration of non-LTE measurements and the appropriate model predictions should be a goal for the next review meeting.
5. The diagnostic work by J. Fincke to measure particle velocity and size is extremely important and has broad application. As in Elliott's work, do measurements suffer due to errors in emissivity?
6. The attractive scheme to assess kinetics of phase transformation and condensed phase reactions is now found unexpectedly difficult. This difficulty is due to problems associated with surface emissivities. Progress to date to establish kinetics has been limited. It is recommended that Elliott/Bolsaitis select a material reaction system of interest and demonstrate the effectiveness of the scheme in obtaining kinetics data by the upcoming review or discontinue this specific approach.

7. At first hand, there appears to be significant duplication of the modeling effort. Ramshaw's LAVA model offers greater potential to include non-equilibrium terms than would seem true for Fluent and Phoenix codes. Szekely and Westhoff could provide potential benefit to the industry by applying available models to attractive, new plasma system concepts now heavily pursued. These include shrouded DC plasma jets and new supersonic plasma deposition systems. To compliment and support the model development, some diagnostics in these more modern plasma systems will be required and must be initiated at INEL soon.
8. Although Ramshaw indicated potential problems with prediction of concentrations resulting from turbulent diffusion, no action plan to resolve this question was indicated.

It is clear from the presentations that significant efforts have been made. It is hoped that the above suggestions will accelerate the progress over the next six months.

Technical Advisory Committee
Thermal Plasma

Diran Apelian
T.N. Meyer
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Introduction

THERMAL PLASMA PROCESSING

J.F. Elliott

Massachusetts Institute of Technology

This task addresses the national need for innovations that can leapfrog an American industries, such as metal processing, ahead of competitors in world markets by radical reduction of costs. Plasma processing has potential for several applications, e.g. extracting metal from its ore and converting it to useful form and the safe destruction of hazardous wastes. In the past technological innovations have generally been pursued by expensive empirical means such as by building a new type of apparatus and fiddling to make it operate in a desirable way. Even when the result of such costly blind exploration seems encouraging, it seldom shows how to scale=up for full production, or what changes need to be made for even a slightly different product.

To serve the stated need, this task is advancing the highly promising technology of plasma processing. Specifically, the goal is a paradigm for the design of thermal plasma generators to give optimum performance in any specific application. Such a paradigm requires creation and exercise of computational models of the plasma processing operation, generation of a body of reliable experimental data from diagnostic measurements of the plasma processing system, and critical comparison and interpretation of predictions and measurements to validate the models.

To achieve this goal, researchers at the INEL and MIT are pursuing a quantitative description of heat, mass, and momentum transfer when particles are immersed in a thermal plasma. New methods are being developed to measure plasma properties near particles. Experimental results are being compared with the predictions of computer models of the plasma systems developed for this purpose. Interpretation of these comparisons comes through close collaboration between the INEL and MIT investigators, in which results obtained at each institution strongly influence the course of further research at the other. Unique to this task are methods to measure plasma velocity and true kinetic temperature, and to avoid the often unjustified assumption that the plasma is always in local thermodynamic equilibrium.

The specific objectives of the proposed program are: (1) to develop a fundamental understanding of the underlying physical and chemical

phenomena that are important in the use of thermal plasmas for processing materials, destruction and immobilization of hazardous and mixed wastes, and for applying metal, alloy, and ceramic coatings to various types of substrates; (b) with use of this information, to improve our understanding of existing thermal plasma processing methods and of the relationships between processing variables and chemical and physical changes undergone by materials passing through the plasma flame and subsequently being deposited on a substrate or collected otherwise; and (c) to provide a basis for development of advanced methods and equipment for thermal plasma processing of materials, waste destruction, and spray coating of objects.

The research is carried out in the Department of Materials Science and Engineering at MIT and the Idaho National Engineering Laboratory (INEL). The program is a cooperative effort between an educational institution, MIT, and a national laboratory, INEL, and is designed to capitalize on the scientific and technical expertise pertinent to thermal plasma processing of materials and hazardous wastes at MIT and at INEL, and also to utilize the extensive experimental capabilities, particularly in plasma diagnostic methods, in the INEL laboratories.

The research program has three primary areas of activity: (a) Development of advanced diagnostic methods to determine the nonequilibrium states of the plasma flame so that studies on the chaotic nature of the torch, the plasma properties, plasma-particle interaction, and of potential monitoring and control methods can be made at INEL and elsewhere. This work is being conducted at INEL. (b) Study of the chemical and physical behavior of particles of various materials and the changes that they undergo when exposed to thermal plasma flames. Research in this area is being carried out at INEL on plasma flames into which various types of particles are injected, and at MIT where study is in progress of the detailed physicochemical behavior of individual particles of various materials exposed to conditions simulating those in thermal plasma flames. (c) Modeling of the physical and chemical conditions of the plasma flame itself, of the thermal and chemical interactions between the plasma flame and particles of various materials in the flame, and of the behavior, i.e., velocities, temperatures, heating and cooling rates, etc., of particles that are injected into the flame at various locations. Of particular interest are the mixing of injected gases and particles with the plasma flame, particle-flame interactions, the influence of conditions within the torch on flame characteristics, and the trajectories through the flame followed by particles injected at various points.

It is essential that modeling and experimental researchers interact intimately and often to get strong feedback on mechanisms, results, and needs experiments or theoretical data. Idealized assumptions and simplistic diagnostic models lose their sanctity in the light of real data and complex situations. Too much research is done with a single hypothesis or particular

experimental measurement in mind. The present trend is toward integrated multidisciplinary research, as proposed here.

Cooperation among the participants in the program at INEL and MIT is necessary for the successful pursuit of the overall goals of the program. The results of the diagnostic work on plasma flames by Dr. Shaw and Dr. Eddy at INEL, and the measurements on plasma flames and particles passing through the flame by Dr. Fincke, provide information essential to the modeling work of Professor Szekely's group at MIT and of Dr. Ramshaw at INEL. Conversely, the results of the modeling studies assist in the assessment of the results of the experimental studies. The single-particle studies of the chemical and physical changes of particles when exposed to simulated plasma conditions, by Professor Elliott's group at MIT, are dependent on knowledge of conditions in plasma flames, obtained from the experimental measurements at INEL, and on the modeling results. The investigations by Prof. Elliott's group involve some of the same materials that Dr. Fincke has studied, and they have shared information on, e.g., optical properties of particles and problems of obtaining precise temperature measurements of particles.

DATA
from
Thermal Plasma Project Reviews

July 17-18, 1990

PLASMA-PARTICLE REACTIONS

SCHEDULE OF TASKS

MATERIALS STUDIES

EQUIPMENT ENHANCEMENT

SIMULATION AND MODELLING

PERSONNEL

J. F. ELLIOTT

P. BOLSAITIS

M. SALAS

C. SMITH

R. LAM

Y. MATSUDA

TASKS

I. MATERIALS STUDIES

Recalescence, Solidification, &
Vaporization

W, WC, Co and Plasmalloy

Al-Ni, Ni₃Al, Al, Ni

Carbides: Cr_xC_y, BC, etc.

Oxides: ZrO₂, Cr₂O₃, etc.

Low Melting Alloys

Emissivities

Current	1991	1992	1993

II. EQUIPMENT ENHANCEMENT

IR Sensors for Low
Temperatures

Revamped Data Acquisition
System

Dry Ice Cooling of PMTs

High Speed Optical Imaging

Multi-Wavelength Pyrometers

Current	1991	1992	1993

III. SIMULATION AND MODELLING

Rate Processes

Undercooling and
Recalescence

Solidification

Vaporization

Current	1991	1992	1993

PLASMA-PARTICLE REACTIONS

J.F. ELLIOTT and P. BOLSAITIS

(COPIES OF SLIDES: 07-17-1990)

OBJECTIVES:

1. To develop a method for the study of single particle reaction and phase transformation kinetics under conditions simulating plasma torches, flash smelters and other high temperature processes:

Particle size range: 10 – 100 μm
 Temperature range: 800 – 4000 K
 Reaction times: 1 ms – 1 s

2. Apply the system to determine for materials of interest:

Rates of vaporization
 Liquid undercooling at recalescence
 Kinetics of oxidation/reduction reactions

SCHEMATIC OF QUADRUPOLE BALANCE CIRCUITRY

SCHEMATIC OF OPTICAL SYSTEM

TABLE I:
SYSTEM FEATURES:

LEVITATION: AC/DC QUADRUPOLE:	0 - 240V DC 0 - 10,000V AC
HEATING: CO2 LASER	20W, 50W
TEMP. DETECTION:	In-Sb detectors 400 - 1000 C PMT's + N.B. Filters >800 C
POS. DETECTION:	He-Ne illumination + image intensifier + split fiber optic
TEMP. CONTROL:	P.I.D. controller
POS. CONTROL:	P.I.D. controller
OPTICAL IMAGING:	Microscope QUESTAR telescoping microscope
DATA ACQUISITION:	PDP-11/73 Acq. rate: 100KHz

TECHNICAL ISSUES OF INTEREST:

- * High temperature stability
- * Particle recovery
- * Single particle microanalysis
- * Emissivity and temperature measurement

TEMPERATURE MEASUREMENT BY RADIATION PYROMETRY – WIEN'S LAW:

$$\ln (i_s - i_b) = \ln \left(\frac{2A_0 F G C_1 \Delta \lambda}{\lambda_a^5} E_a \right) - \frac{C_2}{T \lambda_a}$$

- i_s, i_b = PMT signal and background
- A_0 = Projected x-sectional area of particle
- F = View factor
- $G = G(i_s, \lambda)$ = Instrumental gain factor
- C_1, C_2 = Planck's constants
- λ_a = Average signal wavelength
- $\Delta \lambda_a$ = Detector bandwidth
- $\epsilon = \epsilon(\lambda, T)$ = Spectral emissivity for λ_a
- T = Temperature

ONE-COLOR TEMPERATURE:

$$\text{SIGNAL}(\lambda_1) = \ln (i_s - i_b) = A_1 - \frac{B_1}{T}$$

$$A_1 = f (A_o, G(i_s), \epsilon(\lambda, T)) ; \quad B_1 = C_2 \lambda_1^{-1}$$

TWO-COLOR TEMPERATURE:

$$\text{SIGNAL}(\lambda_1) - \text{SIGNAL}(\lambda_2) = A_{12} - \frac{B_{12}}{T}$$

$$A_{12} = A_{12} \left(\frac{\epsilon_1(\lambda, T)}{\epsilon_2(\lambda, T)} \cdot \frac{G(i_{s,1}, \lambda_1)}{G(i_{s,2}, \lambda_2)} \right) ; \quad B_{12} = C_2 (\lambda_1^{-1} - \lambda_2^{-1})$$

A_o = X-sectional area = f(thermal expansion, melting, vaporization)

G = Gain = f(instrument calibration)

ϵ = Emissivity = f(material, phase structure, surface condition)

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(5)

Table I. Liquid cooling rate and supercooling data collected from six remelting experiments performed in nitrogen.

<u>Run</u>	<u>Supercooling (K)</u>	<u>Cooling Rate (K/s)</u>
1	329	1.1×10^5
2	286	1.4×10^5
3	306	1.8×10^5
4	276	1.5×10^5
5	312	1.2×10^5
6	277	2.2×10^5

Table II. Liquid cooling rate and supercooling data collected from seven remelting experiments performed in air.

<u>Run</u>	<u>Supercooling (K)</u>	<u>Cooling Rate (K/s)</u>
1	168	*
2	156	4.2×10^5
3	145	3.9×10^5
4	150	2.4×10^5
5	175	2.4×10^5
6	177	1.3×10^5
7	175	1.4×10^5

* Unable to estimate cooling rate because of droplet heating by laser just prior to nucleation.

Table III. Transport and Thermodynamic Parameters of Iron and Nickel in Air and Nitrogen.

<u>parameter</u>	<u>value</u>	<u>units</u>	<u>reference</u>
k_l (Fe 2000K)	0.426	W/cmK	38
k_g (N ₂ 313 K)	2.68E-04	W/cmK	39
k_g (O ₂ 313 K)	2.81E-04	W/cmK	39
C_p (Fe liquid)	0.835	J/gK	39
C_p (Ni liquid)	0.770	J/gK	40
ρ (Fe 2000 K)	6.85	g/cm ³	40

Al₂O₃ particle, D = 65μm
Al112001.DAT

40um Cobalt Particle
One-color temperatures:
Co01*.DAT ($\epsilon - \epsilon(\lambda, T)$)

Cobalt Particle D=40um
Two-Color Temp. ($\epsilon=\epsilon(\lambda,T)$)
Co01.DAT

CALCULATED EMISSIVITY RATIOS FOR $A''/A' = \text{const.}$
 DATA: C019*.DAT-C026*.DAT ($T = 1768 \text{ K}$)

Figure 4B Two-color temperatures from 450nm, 650nm and 850nm s.c.i.c.s of a 30 μ m tungsten particle using the gray-body approximation and apparent emissivity ratio values at the melting point.

Figure 3: Reflectance spectra of tungsten oxides (after Porter, White, and Roy (1972))

TWO-COLOR TEMPERATURE CALIBRATION
vs Pt-Pt13Rh THERMOCOUPLE

ONE-COLOR TEMPERATURES
(Pt-Pt13Rh THERMOCOUPLE)

MATHEMATICAL MODELLING OF PLASMA SYSTEMS

PARTICIPANTS
PROF. J. SZEKELY
PROF. A.H. DILAWARI
MR. R.C. WESTHOFF
MR. L.G. TRAPAGA

PURPOSE:

- TO GAIN A MORE COMPLETE UNDERSTANDING OF PLASMA SYSTEMS, BY DEVELOPING A MATHEMATICAL DESCRIPTION OF THE FOLLOWING:**
 - PLASMA VELOCITY, TEMPERATURE AND CONCENTRATION (MIXING WITH AN ENTRAINED GAS).**
 - OPERATING CHARACTERISTICS OF A NON-TRANSFERRED ARC PLASMA TORCH**
 - PARTICLE VELOCITIES, TEMPERATURES AND TRAJECTORIES IN PLASMA SPRAYING.**
 - PLASMA SYNTHESIS OF MATERIALS.**

THE PURPOSE OF MODELLING

- IDEALLY THE MODEL IS HELPFUL IN PLANNING AND INTERPRETING EXPERIMENTAL RESULTS WHILE THE EXPERIMENTAL WORK IS CRUCIAL IN TESTING THE MODEL.**
- THE MODEL IS OF LITTLE USE UNLESS IT IS SUPPORTED AND VERIFIED BY A SUITABLE EXPERIMENT.**
- THE EXPERIMENT MAY ALSO BE OF LITTLE USE WITHOUT A FUNDAMENTAL UNDERSTANDING OF THE PROCESSES INVOLVED.**

MAJOR ACCOMPLISHMENTS

1. DEVELOPMENT OF A REALISTIC MODEL OF THE PLASMA PLUME RECOGNIZING THE IMPORTANT ISSUES OF

- SWIRL,**
- INTERMIXING,**
- REALISTIC PROPERTY VALUES,**
- REALISTIC BOUNDARY CONDITIONS,**
- LAMINAR AND TURBULENT FLOW, AND**
- SATISFYING HEAT AND MASS BALANCES.**

2. DEVELOPMENT OF A MODEL FOR PARTICLES IN THE PLASMA PLUME RECOGNIZING IMPORTANT ISSUES:

- PARTICLE DYNAMICS,**
- HEAT TRANSFER (MELTING AND SOLIDIFICATION),**
- PARTICLE VAPORIZATION**
- INTRA-PARTICLE CONDUCTION**
- NON-CONTINUUM EFFECTS.**

MAJOR ACCOMPLISHMENTS

3. DEVELOPMENT OF A MODEL FOR A TRANSFERRED ARC WHICH MAY BE EXTENDED TO WORK INSIDE THE PLASMA TORCH.
4. DEVELOPMENT OF A SIMPLIFIED MODEL OF THE PLASMA TORCH WHICH GIVES VALUABLE INSIGHTS INTO TORCH BEHAVIOR.
5. A TOTAL OF FIFTEEN PAPERS HAVE BEEN PUBLISHED OR SUBMITTED WITH SEVERAL MORE IN PREPARATION.

INTERACTIONS WITH INEL

- EXCELLENT TWO-WAY INTERACTIONS HAVE BEEN DEVELOPED WITH INEL.
- THESE INTERACTIONS HELP IN THE PLANNING OF EXPERIMENTS AND THE VERIFICATION OF RESULTS
- THREE JOINT PAPERS HAVE BEEN PUBLISHED IN THE LAST PROPOSAL PERIOD

PUBLICATIONS RESULTING FROM THIS RESEARCH

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3. Dilawari, A.H. and J. Szekely, Fluid flow and heat transfer in plasma reactors, Part I: Calculation of velocities, temperatures and mixing, Int. J. Heat and Mass Transfer, 30, No.11, p.2357, (1987).
4. Dilawari, A.H. and J. Szekely, J.F. Coudert, and P. Fauchais, Fluid flow and heat transfer in plasma reactors, Part II: A critical comparison of experimentally measured and theoretically predicted temperature profiles in plasma jets in the absence and presence of side stream injection, Int. J. Heat and Mass Transfer, 32, No. 1, p.35, (1989).
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6. Dilawari, A.H. and J. Szekely, The mathematical modelling of transport phenomena in non-transferred plasma systems: Accomplishments and unresolved problems, Proc. MRS Symposium on Materials Processing in Plasma Systems, 98, p. 3, (1987).
7. Westhoff, R.C., A Mathematical Model For Current, Heat Flux, and Pressure in a Welding Arc, S.M. Thesis, (1989).
8. J. Szekely, Transport phenomena in welds with emphasis on free surface phenomena, 2nd International Conference on Trends in Welding Research, Gatlinburg, TN., (1989).
9. A.H. Dilawari, J. Szekely and R. Westhoff, A comparison of Experimental Measurements and Theoretical Predictions Regarding the Behavior of a Turbulent Argon Plasma Jet Discharging into Air, Plasma Chem. Plasma Process. 10, (3), 501, (1990).
10. A.H. Dilawari, J. Szekely and R. Westhoff, "An Assessment of Heat and Fluid Flow Phenomena inside Plasma Torches in Non-transferred Arc Systems," *ISIJ International*, 30, (5), 381, (1990).

11. R.T.C. Choo, J. Szekely and R.C. Westhoff, "Modelling of high current arcs in welding with emphasis on free surface phenomena in weld pool," Accepted for publication, *Welding Journal*, (1990).
12. R. Westhoff, A.H. Dilawari and J. Szekely, "A Mathematical Representation of Transport Phenomena inside a Plasma Torch," MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA. (1990).

JOINT PUBLICATIONS WITH INEL

13. Dilawari, A.H. J. Szekely, J. Batdorf, and C.B. Shaw, "The temperature profiles in an argon plasma issuing into an argon atmosphere: A comparison of measurements and predictions", *Plasma Chem. Plasma Process.* 10, (2), 317 (1990).
- o 14. G. Trapaga, R. Westhoff, J. Szekely, J. Fincke and D. Swank, "Particle and Temperature Histories in a Plasma Plume: A Comparison of Measurements and Predictions," MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA. (1990).
15. A.H. Dilawari, R. Westhoff, J. Szekely, C.B. Shaw, Jr. and B. A. Detering, "A Comparison of the Experimentally Measured and Theoretically Predicted Temperature Profiles for an Argon Plasma Jet Discharging into a Nitrogen Environment," MRS Symp. on Plasma Processing and Synthesis of Materials, San Francisco, CA. (1990).

CURRENT WORK

1. SIMPLIFIED INSIDE TORCH MODEL, APPLICATION TO
 - PFENDER TORCH,
 - MILLER TORCH,
 - METCO TORCH, AND
 - THERMAL DYNAMICS TORCH.
2. MODEL OF PLASMA-PARTICLE INTERACTIONS
 - VERIFICATION: COMPARISON WITH PARTICLES INJECTED INTO A ROOM-TEMPERATURE AIR JET.
 - MODELLING OF ALUMINA PARTICLES INJECTED FROM INSIDE THE MILLER TORCH.
 - PAPER PRESENTED AT THE MRS PLASMA CONFERENCE
3. COMPARISON WITH THE CARS DATA FOR TEMPERATURE AND COMPOSITION TAKEN BY INEL

CURRENT WORK

- 4. MODEL OF NON-TRANSFERRED PLASMA TORCH (ELECTRIC POTENTIAL MODEL)**
- 5. USE OF A COMMERCIAL CODE FOR EXTENSION TO THREE-DIMENSIONS (VERIFICATION STAGE):**
 - REPRODUCTION OF RESULTS FROM THE PLUME MODEL**
 - REPRODUCTION OF RESULTS FOR COLD FLOW:**
 - AWAITING THE NEW VERSION WHICH ALLOWS USER DEFINED SUBROUTINES (DUE IN WEEKS).**
- 6. MODELLING OF LAMINAR-TURBULENT TRANSITION IN THE JET.**
- 4. INVESTIGATION OF NON-EQUILIBRIUM PLASMA PROPERTIES AND BEHAVIOR.**

SIMPLIFIED MODEL OF INSIDE TORCH

STATUS:

-THIS MODEL HAS BEEN APPLIED TO SEVERAL TORCHES WITH SOME SUCCESS.

- PFENDER TORCH**
- MILLER TORCH**
- METCO TORCH**
- THERMAL DYNAMICS TORCH**

-IN ESSENCE, THIS MODEL SPECIFIES A HEAT GENERATION PATTERN INSIDE THE TORCH AND SOLVES THE GOVERNING EQUATIONS BASED ON THIS.

GOVERNING EQUATIONS:

- Mass conservation or continuity

$$\frac{\partial(\rho u)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r v)}{\partial r} = 0 \quad [1]$$

- Conservation of axial momentum

$$\frac{\partial(\rho u^2)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r u v)}{\partial r} = -\frac{\partial P}{\partial z} + 2 \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right) \right] + j_r B_\theta \quad [2]$$

- Conservation of radial momentum

$$\frac{\partial(\rho u v)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r v^2)}{\partial r} = -\frac{\partial P}{\partial r} + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial u}{\partial r} \right) \right] + \frac{2}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial v}{\partial r} \right) \right] - \mu \frac{2v}{r^2} - j_i B_\theta \quad [3]$$

- Conservation of thermal energy

$$\frac{\partial(\rho u h)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r v h)}{\partial r} = \frac{\partial}{\partial z} \left(\frac{k}{C_p} \frac{\partial h}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r k}{C_p} \frac{\partial h}{\partial r} \right) + S_I - S_R \quad [4]$$

- Conservation of angular momentum

$$\frac{\partial(\rho r w)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r^2 v w)}{\partial r} = \frac{\partial}{\partial z} \left(\mu \frac{\partial(rw)}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left[\mu r \left(\frac{\partial(rw)}{\partial r} \right) \right] - \frac{2}{r} \frac{\partial(\mu r w)}{\partial r} \quad [5]$$

- Conservation of turbulent kinetic energy

$$\frac{\partial(\rho u K)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r v K)}{\partial r} = \frac{\partial}{\partial z} \left(\frac{\mu_t}{\sigma_K} \frac{\partial K}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_t}{\sigma_K} \frac{\partial K}{\partial r} \right) + G - \rho \epsilon \quad [6]$$

- Turbulent energy dissipation

$$\frac{\partial(\rho u \epsilon)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r v \epsilon)}{\partial r} = \frac{\partial}{\partial z} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial r} \right) + \frac{\epsilon}{K} (C_1 G - C_2) \quad [7]$$

$$G = 2\mu_t \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial r} \right)^2 + \left(\frac{v}{r} \right)^2 + \frac{1}{2} \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right)^2 \right] \quad [8]$$

$$\mu_t = \frac{C_D \rho K^2}{\epsilon} \quad [9]$$

- Conservation of species

$$\frac{\partial(\rho r u m)}{\partial z} + \frac{1}{r} \frac{\partial(\rho r^2 v m)}{\partial r} = \frac{\partial}{\partial z} \left(\frac{\mu}{\sigma_m} \frac{\partial(rm)}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left[\frac{\mu}{\sigma_m} r \left(\frac{\partial(rm)}{\partial r} \right) \right] \quad [10]$$

PFENDER TORCH

- EXPERIMENTS DONE AT INEL - BES RUNS**
- NATURE OF THE PLUME NEAR THE TORCH EXIT IS LAMINAR**
- CURRENT LEVELS 250, 500 AND 750 AMPS**
- ARGON - ARGON SYSTEM**

**Radial Temperature Profiles at Five
Axial Positions - B32**

MILLER TORCH

- EXPERIMENTS DONE AT INEL - PLASMA-PARTICLE CASE**
- NATURE OF THE PLUME NEAR THE TORCH EXIT IS FULLY TURBULENT**
- CURRENT LEVELS 900 AMPS**
- ARGON - HELIUM SYSTEM IN AIR ENVIRONMENT**

Figure 10- Comparison of measured and calculated axial temperature profiles in the turbulent plasma jet issuing from a plasma torch.

Figure 11- Comparison of measured and calculated radial temperature profiles in a turbulent plasma jet.

METCO TORCH

- EXPERIMENTS DONE BY BROSSA AND PFENDER AT THE UNIVERSITY OF MINNESOTA**
- NATURE OF THE PLUME NEAR THE TORCH EXIT IS IN THE RANGE OF LAMINAR-TURBULENT TRANSITION.**
- CURRENT LEVELS 450 AND 600 AMPS**
- ARGON SYSTEM IN AIR ENVIRONMENT**

Plasma temperature on the torch axis calculated by the inside torch model and the plume model compared to experimental measurements. Brossa and Pfender, 600 Amp case

THERMAL DYNAMICS TORCH

- EXPERIMENTS DONE BY LEWIS AND GAUVIN AT MCGILL UNIVERSITY.**
- NATURE OF THE PLUME NEAR THE TORCH EXIT IS LARGELY TURBULENT.**
- CURRENT LEVEL IS 650 AMPS**
- ARGON SYSTEM IN AIR ENVIRONMENT**

Axial temperature profile for the U-51 Thermal Dynamics torch
 operating at 650 A, Lewis and Gauvin

SUMMARY OF SIMPLIFIED TORCH MODEL

- THE MODEL SHOWS THAT SWIRL IS DIFFICULT TO GENERATE IN THE PLUME**
- THE MODEL REPRESENTS THE TEMPERATURES IN LAMINAR SYSTEMS QUITE WELL (BES RUNS).**
- THE REPRESENTATION OF FULLY TURBULENT SYSTEMS IS REASONABLE BUT LESS SATISFACTORY (MILLER, THERMAL DYNAMICS TORCHES).**
- FOR THE LAMINAR TO FULLY TURBULENT TRANSITION RANGE THE MODEL IS STILL LESS SATISFACTORY (METCO).**
- SIMPLIFICATIONS MADE MAY LEAD TO UNDESIED ERRORS IN THE VELOCITIES (JXB FORCES IMPORTANT).**

PARTICLE MODELLING AND COMPARISON WITH INEL MEASUREMENTS

STATUS:

- PARTICLE MODEL WAS VERIFIED USING EXPERIMENTAL DATA FOR A SIMPLE CASE OF ALUMINA PARTICLES INJECTED INTO A ROOM TEMPERATURE AIR JET.**
- PREVIOUS MODEL UPDATED, COMPARISON WITH MEASUREMENTS IS QUITE REASONABLE (PAPER IN MRS CONFERENCE).**

Particle velocity and trajectory

Basset-Boussinesq-Ossen equation:

(axial)

$$\frac{dU_p}{dt} = \underbrace{-\frac{3}{4} \frac{\rho}{\rho_p} \frac{C_d}{D_p} (U_p - U) |U_p - U|}_{\text{(drag force)}} - \underbrace{\frac{9}{\rho_p D_p} \sqrt{\frac{\mu \rho}{\pi}} \int \frac{d}{dt'} (U_p - U) \frac{dt'}{\sqrt{t - t'}}}_{\text{(history term)}} + \underbrace{\sum F_i}_{\text{(gravity)}}$$

(radial)

$$\frac{dV_p}{dt} = -\frac{3}{4} \frac{\rho}{\rho_p} \frac{C_D}{D_p} (V_p - V) |V_p - V| + \sum F_r$$

(P- particle; U,V- velocity components)

$$C_D = \frac{24}{Re} + \frac{6}{1 + Re^{1/2}} + 0.4 \quad (\text{continuum})$$

$$Re = \frac{\rho U_r D_p}{\mu}$$

$$U_r = \sqrt{(U - U_p)^2 + (V - V_p)^2}$$

Particle heat and mass transfer

Thermal energy balance:

$$\frac{\partial H}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(k_r r^2 \frac{\partial T}{\partial r} \right)$$

Solution $\left\{ \begin{array}{l} - \text{Lumped Parameter method} \\ - \text{Enthalpy method} \end{array} \right.$

Boundary conditions:

- Convection (Ranz-Marshall correlation for Nusselt Number)
- Radiation
- Vaporization
- Evaporation
- Melting and Solidification
- Particle change of size

Temperature properties dependence: (mean integrated values)

$$\bar{\Phi}_r = \frac{1}{(T_f - T_i)} \int_{T_i}^{T_f} \Phi dT \quad (\Phi \rightarrow \rho, \mu, k)$$

The above integral also defines the conduction potential when $\Phi = k$

VAPORIZATION

Rate of mass loss:

$$\dot{m} = K_{MX}(C_s^* - C_\infty) \approx K_{MX}C_s^*$$

$$C_s^* = \frac{MP_s}{RT_s} = \text{concentration of evaporating specie at the particle surface}$$

$$K_{MX} = \left(\frac{1}{h_m} + \frac{1}{h_s} \right)^{-1} = \text{overall transfer coefficient}$$

$$h_s = \alpha \sqrt{\frac{RT}{2\pi M}} \quad (\text{Langmuir evaporation rate coefficient})$$

α - sticking coefficient
 T - temperature (K)
 R - gas constant
 M - molecular weight

$$h_m = \frac{\mathcal{D}}{D_p} (2.0 + 0.6 \text{Re}^{1/2} \text{Sc}^{1/3}) \quad (\text{mass transfer coefficient})$$

$\text{Sc} = \text{Schmit number } (\nu / \mathcal{D})$
 $\mathcal{D} = \text{Diffusion coefficient}$
 (Chapman - Enskog theory)
 $\nu = \text{kinematic viscosity}$

Rate of heat loss by vaporization:

$$Q_{\dot{m}} = \dot{m} \left\{ L_v + (H_{v(T_s)} - H_{v(T_\infty)}) + (H_{l(T_s)} - H_{l(T_\infty)}) \right\}$$

(H - Enthalpy)

NON-CONTINUUM EFFECTS

(based on Chen and Pfender's analysis)

$$(C_D)_{NC} = (\alpha_{KN})^{0.45} C_D \quad (\text{on the drag coefficient})$$

$$(Nu)_{NC} = \alpha_{KN} Nu \quad (\text{on the Nusselt number})$$

where, NC denotes non continuum, and

$$\alpha_{KN} = \frac{1}{1 + (z^*/r_p)} \quad (\text{Knudsen effect correction factor})$$

$$z^* = \left(\frac{2-a}{a} \right) \left(\frac{\gamma}{1+\gamma} \right) \left(\frac{4\bar{k}}{\rho_s v_s \bar{c}_p} \right) \quad (\text{temperature jump distance})$$

a – thermal accomodation coefficient

γ – c_p / c_v

ρ_s – gas density at particle surface temperature

v_s – average molecular speed at the particle surface temperature

$\bar{c}_p$ – heat capacity (integrated average value between particle and jump temperatures)

$\bar{k}$ – Thermal conductivity (integrated average value)

T_j – Jump temperature (calculated by iteration based on the pure conduction model by Chen and Pfender)

$$Q_c = 4\pi r_p \alpha_{KN} (S_\infty - S_s) \rightarrow \left. \frac{dS}{dr} \right|_s = \frac{Q_c}{4\pi r_p^2} \rightarrow S_\infty - S_s = z^* \left(\frac{dS}{dr} \right)_s$$

Q_c – non - continuum heat input due to conduction

S – heat conduction potential

COLD FLOW CASE

- DONE FOR VERIFICATION:**
- COMPARISON WITH PARTICLES INJECTED INTO A ROOM-TEMPERATURE AIR JET (100 M/S CHARACTERISTIC VELOCITY).**
- 97 MICRON AND 13.7 MICRON PARTICLES OF ALUMINA.**

Figure 5 - Comparison of the measured mean particle velocities (shown by the solid lines) with those calculated with the particle model (discrete points) for particles with a mean diameter of $97 \mu m$.

Figure 6 - Comparison of the measured mean particle velocities (shown by the solid lines) with those calculated with the particle model (discrete points) for particles with a mean diameter of $13.7 \mu m$.

PLASMA-PARTICLE INTERACTIONS

- SIMULTANEOUS MEASUREMENTS OF PARTICLE SIZE, VELOCITY AND TEMPERATURE DONE AT INEL**
- ALUMINA PARTICLES INJECTED INSIDE THE MILLER TORCH.**

Figure 12- Comparison of measured (at the center line) and calculated particle velocities (a), and particle surface temperatures (b), for two different particle sizes and for an injection velocity of 13 m/s.

SUMMARY OF PARTICLE MODELLING

- SOME UNCERTAINTIES ARE PRESENT ABOUT THE MODELLING OF SMALL PARTICLES IN AN AIR JET.
- THREE DIMENSIONAL EFFECTS IN THE JET FLOW AND PLASMA PLUME MAY BE SIGNIFICANT.
- UNCERTAINTIES IN THE PLASMA: TURBULENT FLOW, MIXING , AND POSSIBLE DEPARTURES FROM EQUILIBRIUM.
- THE NON-CONTINUUM EFFECTS ARE SIGNIFICANT IN THIS SYSTEM (ARGON-HELIUM WORKING GAS).
- VAPORIZATION WILL AFFECT THE HEATING RATE OF SMALL PARTICLES .
- LARGE TEMPERATURE GRADIENTS EXIST IN THE PARTICLES.
- PARTICLE VELOCITIES WERE OVERESTIMATED BY ABOUT 37%
- PARTICLE TEMPERATURES WERE OVERESTIMATED BY ABOUT 20%

COMPARISON OF CARS TEMPERATURE AND CONCENTRATION DATA WITH CALCULATIONS

STATUS:

- NEW DATA: COMPARED WITH THE PLUME MODEL FOR
PFENDER TORCH DISCHARGING INTO AIR**
- TEMPERATURE AND CONCENTRATION DATA AT LOW
TEMPERATURES.**

RADIAL TEMP. PROFILE-BES25A (LAMINAR)

(a)

AXIAL TEMPERATURE PROFILE-BES25A

RADIAL TEMP. PROFILE-BES25A (TURBULENT)

(a)

AXIAL TEMPERATURE PROFILE-BES25A

SUMMARY OF CARS COMPARISON

- AT PRESENT THE MODELLING AND MEASUREMENTS SHOW SOME SIGNIFICANT DISCREPANCIES:
 - TEMPERATURE DATA AGREE BETTER WITH TURBULENT MODEL.
 - CONCENTRATION DATA AGREE BETTER WITH LAMINAR MODEL.
- IT APPEARS THAT THE EXPERIMENTAL PROFILES MAY NOT SATISFY A SPECIES BALANCE.
- THE NATURE OF THE EXPERIMENT MAY HAVE BEEN TIME DEPENDENT AND HENCE ARGON ACCUMULATES AT THE DOWNSTREAM OF THE PLUME.

USE OF COMMERCIAL CODE FOR EXTENSION TO THREE DIMENSIONS

STATUS:

- VERIFICATION STAGE WITH FLUENT**
- APPLICATION TO ROOM TEMPERATURE AIR JET WITH
INJECTED ALUMINA PARTICLES**
- REPRODUCTION OF PREVIOUS PLUME MODEL CASE**
- INVESTIGATION INTO FLEXIBILITY ALLOWED BY USER DEFINED
SUBROUTINES**

ISSUES:

- SUITABILITY OF THE CODE FOR THIS APPLICATION
(COMPARED WITH OTHERS)**

COLD FLOW USING FLUENT

- DONE FOR VERIFICATION:**
- COMPARISON WITH PARTICLES INJECTED INTO A ROOM-TEMPERATURE AIR JET (100 M/S CHARACTERISTIC VELOCITY).**
- 97 MICRON AND 13.7 MICRON PARTICLES OF ALUMINA.**

Axial velocity of 97 micron (a) and 13.7 micron alumina particles at four axial positions (solid lines represent measurements and discrete points denote calculations using FLUENT)

PLASMA PLUME USING FLUENT 2

- DONE FOR VERIFICATION:**
- REPEAT OF RUN BES23 USING FLUENT (AT PRESENT NO ALLOWANCE IS MADE FOR RADIATION).**
- FIRST IS FLUENT, SECOND IS PREVIOUS PLUME MODEL.**

AXIAL TEMP. PROFILE-BES23 (FLUENT)

RADIAL TEMP. PROFILE-BES23 (FLUENT)

MODELLING OF THE NON-TRANSFERRED ARC

PLASMA TORCH

STATUS:

- NEW AREA; PRELIMINARY MODEL COMPLETED.**
- MODEL WILL BE FURTHER TESTED AS TO ITS ABILITY TO ACCURATELY DESCRIBE THE BEHAVIOR OF A NUMBER OF PLASMA TORCHES**

ISSUES:

- THE MODEL PROVIDES CURRENT DENSITIES, JOULE HEATING TEMPERATURES AND VELOCITIES IN THE ARC AND OUTSIDE THE TORCH.**

1	1000
2	3000
3	5000
4	7000
5	9000
6	11000
7	13000
8	15000
9	17000
10	19000
11	21000
12	23000
13	25000
14	27000
15	29000
16	31000
17	33000

Contours of Temperature

MODELLING OF LAMINAR-TURBULENT TRANSITION IN THE JET

- USING A MODIFIED K-E TRANSITIONAL MODEL AS A PRELIMINARY STEP
- INVESTIGATING THE USE OF LARGE EDDY SIMULATION AND DIRECT SIMULATION MODELS OF TURBULENCE.
- NEGOTIATIONS IN PROGRESS WITH NIPPON STEEL ON USE OF NSMAC CODE FOR DIRECT SIMULATION OF TURBULENCE.
- CONTINUED INTERACTIONS WITH OTHER INVESTGATORS AT MIT, U.C. SANTA BARBARA AND AEA TECHNOLOGY (U.K.) ABOUT LARGE EDDY AND DIRECT SIMULATION OF TURBULENCE

Table.1 Experimental conditions

Mold size	200(T)*1200(W)*5000(L)
Casting speed	1.6 (-in)
Nozzle angle	15 °

Table.2 Comparison of time-averaged velocities between measurement and calculations

Point	Measured value [cm/s]	k-ε	Direct	Direct
		38*20*22	34*17*26	67*33*52
No. 1	9.4	8.5	6.3	8.7
No. 2	11.4	7.9	9.7	11.2
No. 3	14.6	9.5	10.5	11.1
No. 4	14.5	9.6	8.8	11.5
No. 5	12.0	9.3	6.9	10.4
No. 6	20.6	12.4	18.4	26.3

Fig.2 Schematic illustration of water model equipment

Fig.3 Locations where velocities were measured

WORK PROPOSED FOR THE NEXT YEAR PERIOD:

- (1) IMPROVE THE PRELIMINARY MODEL OF THE TRANSFERRED ARC PLASMA TORCH, MAKE COMPARISON WITH EXPERIMENTAL DATA FROM SEVERAL TORCHES.**
- (2) CONTINUE STUDY OF PLASMA PARTICLE INTERACTIONS: EXTENDED THE STUDY TO DIFFERENT SPRAY SYSTEMS (NICKEL-ALUMINUM SYSTEM, TUNGSTEN COBALT CARBIDE SYSTEM, AND OTHERS).**
- (3) EXAMINATION OF NON-EQUILIBRIUM EFFECTS.**
- (4) CONTINUE MODEL DEVELOPMENT TO REPRESENT THE LAMINAR-TURBULENT TRANSITION.**
- (5) CONTINUE WITH THE EXTENSION OF THE PLASMA AND PLASMA PARTICLE MODELS TO THREE DIMENSIONS.**

CONCLUSIONS

- (1) WE HAVE DEVELOPED A SIMPLIFIED MODEL OF THE NON-TRANSFERRED ARC PLASMA TORCH WHICH DESCRIBES SOME ASPECTS OF TORCH BEHAVIOR. IT HAS PROVIDED VALUABLE INSIGHT, BUT ITS DRAWBACKS POINT TO THE NEED FOR A MORE COMPLETE MODEL OF THE TORCH.
- (2) WE HAVE UPDATED THE PLASMA-PARTICLE INTERACTION MODEL TO INCLUDE VAPORIZATION, KNUDSEN EFFECTS AND CONDUCTION INSIDE THE PARTICLE. AGREEMENT WITH EXPERIMENTS IS REASONABLE.
- (3) WE HAVE MADE A COMPARISON WITH THE CARS DATA GENERATED AT INEL. THE DISCREPANCIES PRESENT PROVIDE ADDITIONAL IMPETUS FOR REFINEMENT OF THE MODEL AND/OR MEASUREMENTS.

CONCLUSIONS

- (4) WE HAVE DEVELOPED A PRELIMINARY MODEL FOR A NON-TRANSFERRED ARC PLASMA TORCH, WHICH WE EXPECT TO GIVE US A GREAT DEAL OF INSIGHT INTO TORCH BEHAVIOR.**
- (5) WE ARE INVESTIGATING THE USE OF COMMERCIAL CODES TO FACILITATE A QUICK EXTENSION OF OUR WORK TO THREE DIMENSIONS.**
- (6) WE ARE INVESTIGATING A MODEL WHICH WILL ACCOUNT FOR THE TRANSITIONAL NATURE OF THE PLASMA PLUME.**
- (7) WE ARE IN CONTACT WITH A NUMBER OF INVESTIGATORS WORKING IN LARGE EDDY AND DIRECT SIMULATION OF TURBULENCE.**

SENSING AND CONTROL
OF
DROPLET-BASED THERMAL SYSTEMS

VANDERBILT UNIVERSITY

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July 23, 1990

Technical Advisory Committee

Sensing & Control of Droplet-Based Thermal Systems

On behalf of the Technical Advisory Committee for the Sensing & Control of Droplet-Based Thermal Systems group, INEL/MIT Engineering Research Program, I am submitting the following comments relevant to the July 17-18, 1990 renewal proposal evaluation and annual review.

- As previously stated in our July '88 program review drafted by Hugh Casey (letter of August 10, 1989), we believe the program is well aligned with current national interests in manufacturing research and is addressing the appropriate components necessary to attempt development of fully automated droplet-based thermal systems with real-time process control.
- The work to date has identified some major voids in our understanding of droplet-based thermal systems and of our ability to control these processes. Specifically, the process models are not well developed, and means of decoupling heat and mass transfer are needed for stable multivariable control.
- There is a need for continued collaboration between the respective INEL and MIT teams.
- The initial work has shown that GMAW is an extremely complex process that requires more fundamental understanding of the droplet-based system and means of decoupling variables to realize multivariable process control. The emphasis should be on obtaining a better understanding of the process fundamentals. This in turn, may point the way to process modifications to make GMAW and other droplet-based thermal processes more predictable and suitable for process control.

July 23, 1990

- Finally, the sensor technology research has led to some very innovative results. The vision sensor has been commercialized and is well-received in the welding community and in other areas as well. The ultrasonic sensors will be used on David Taylor Research Center's automated GMAW welding system program. Even though these sensor-based technology transfer successes are perhaps the most outstanding examples that can be pointed to in the overall INEL/MIT program, we believe the sensor technology is still a long way from maturity, and continued innovation is required in this area to assure the future availability of nonintrusive sensors which provide the required real-time process control parameters and defect precursor signatures. We believe the proposed research on sensing microstructure is on target with future process control needs.

The Technical Advisory Committee members present at the July 17-18 meeting and who participated in the preparation of these comments were Paul Ramsey, Richard Morris and myself.

Sincerely yours,

George E. Cook

INTRODUCTION

SENSING AND CONTROL OF DROPLET-BASED THERMAL SYSTEMS

The Massachusetts Institute of Technology (MIT) and Idaho National Engineering Laboratory (INEL) are conducting a collaborative research program directed toward providing the fundamental basis for sensing and control of product geometry and structure for droplet-based thermophysical processes. The research specifically addresses fundamental process physics that is common to a family of processes involving droplet-based, multiphase systems. These processes include arc welding and plasma spraying, as well as spray casting.

The gas metal arc (GMA) and plasma arc welding processes are used as model systems for sensing and control of droplet-based thermal processes. Considerable fundamental information on GMA has been developed at the INEL and MIT during the past six years. Research is being conducted on an extension of the fundamental process physics, application of neural network-like controllers and signal processors, and development of sensing techniques. Tasks include physics of nonlinear aspects of droplet growth, transfer, and substrate interaction; understanding the relationship of neural network structure to model development and learning dynamics in neural networks; control methodologies and advanced sensing, including the propagation and interaction of ultrasound in metallic solid and liquid media.

PROJECT HISTORY

The first five years of research on this project concentrated on providing the fundamental basis for development of automated welding technology for the GMAW process. During this work it became obvious that to make significant advances required the development of intelligent control capability, including a dynamic model of the nonlinear aspects of the process. The dominant nonlinear phenomena pertain to the formation, growth, detachment, transfer, and substrate interaction of liquid metal droplets. These factors also govern other materials processes. Additional research needs were identified in the development of artificial intelligence techniques applicable to dynamic nonlinear systems and in sensing techniques.

The application of intelligent control to welding is structured as shown in Figure 1. In earlier years, it was determined that a set of sensors is required to sense the metal transfer mode; the cooling rate of the weld bead; the geometry of the weld groove, pool, and deposited weld bead; and to characterize defects in the fusion and heat affected zones. Information from these various sensors is to be passed to a logic function that will determine the desired heat and mass input to the weldment, based on an understanding of "good" welding practice and the physical limitations of the process. Finally, a model and control strategy was required to obtain the desired heat and mass input. This project conducted basic research in those areas.

Development of an effective process control model often requires a detailed understanding of the process physics. Unfortunately, such an understanding **does** not exist for many commercially important processes.

Figure 1. Schematic diagram of intelligent control for arc welding.

Part of the MIT effort began by developing prototypical models of GMAW, which gave insight into the crucial thermophysical processes controlling melting rate, droplet formation, droplet shape and droplet detachment. Some detailed simulations were developed in order to link experimental observations such as melting rate and droplet frequency to critical process quantities. This work was extended to pulsed current welding, to provide a method to predict values of the crucial process parameters.

The other work at MIT focussed on multivariable control modeling of the thermal and geometrical problems, again using GMAW as the model process. Several different new control schemes were demonstrated using this process. The results show that standard, temporally based modeling and control methods are inadequate for this process, and that considerable simplification may be achievable using spatial control methods. In addition, GMAW was shown to lack sufficient controllability and observability. Thus, a more fundamental look at droplet based processes is warranted.

DATA

from

Sensing & Control of Droplet-Based Thermal Systems

Project Reviews

July 17-18, 1990

MASSACHUSETTS
INSTITUTE OF
TECHNOLOGY

CONTROL OF DROPLET PROCESSES

Prof. T. W. Eagar
Mr. L. Jones
Prof. J.H. Lang

WELDING
L.A.B.O.R.A.T.O.R.Y

II 8

DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING
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PRIOR WORK

- Plasma Spectral Analysis
 - Weld Image Improvement
 - Arc monitor
- GMAW Droplet Formation
 - Anode spot behavior
 - Melting rate analysis
 - Thermal model
 - Pulse current control
 - Improved melting rate
 - Use of different shielding gases

Droplet Processes

- Metal refining
- Spray forming
- Plasma melting
- Plasma spraying
- Electroslag remelting
- Vacuum arc remelting
- Powder production
- Rapid solidification
- Plasma welding
- Hard facing
- Cladding
- etc.

Common Themes:

- Decouple Heat and Mass Transfer
- Sense and Control Drop Formation and Detachment

Presentation

- Partially Transferred Arc
- Decouple heating of drops and heating of substrate
- Filtering of voltage and current traces
- Use of external energy sources
 - Mechanical
 - Thermal

METHODS OF DECOUPLING HEAT TRANSFER TO DROPS FROM HEAT TRANSFER TO SUBSTRATE

Pulsed Current - previously studied

- External Energy Sources**
 - Mechanical vibration**
 - Laser heating**
- Partially Transferred Arc**

ML-7340

X400

PLASMA SPRAYED (AS-IS) SAMPLE AT INTERFACE

ML-7341

X400

PLASMA SPRAYED (AS-IS) SAMPLE AT CENTRE

(a)

II 15

Droplet Control in Arc Processes

Professor Jeffrey H. Lang

Larry Jones - grad. student -

Proposed Research

- I. Independent control of droplet processes
- II. Sensing the transfer mode
- III. Controlling metal transfer

Topic I

Independent Control of Droplet Processes

Processes are:

A. Electrode melting rate

B. Droplet size

C. Base-plate heating

Benefits of Independent Control

- Increase metal deposition for a given welding current
- Reduce spattering by reducing droplet size
- Decrease base-plate distortion by reducing base-plate heating
- Reduce metal vapor fumes by preventing excess heating of the drop

Partial Decoupling: Pulsed-Current

Important Observations

- Drop detachment determined by
gravity
magnetic
plasma drag
forces
- Pulsed current utilizes magnetic forces to help effect detachment
- Drop insulates the solid electrode from arc heat

Problem:

Only one energy input——welding current

Solution:

Add additional, independent energy sources

Proposed Solutions

Additional energy sources:

- Excess drop heat: Control with pulsing and mechanical vibration
- Non-transferred arc: separate arc for melting the electrode

Mechanical Vibration

Utilize excess heating of drops

Excess heat from drops used to vary the melting rate

Process efficiency and cleanliness improved

Force: $\sim 50 \text{ g's}$

Vibration frequency: $\sim 200 \text{ Hz}$

Amplitude: $< 1 \text{ mm}$

Ultrasonic Vibrations

Micro-drops ejected from liquid
surface of electrode

Maximum heat transfer to solid
electrode

External Heating

Use a small, nontransferred arc

Application of controlled-transfer plasma
welding research

Independent Control

Combination of:

- Current pulsing
- Mechanical vibrations
- Independent electrode heating

Topic II

Sensing Metal Transfer

Metal transfer modes:

- Globular
- Spray
- Streaming

Sensing Tasks

- Mode Transitions
- Droplet Sensing

Sensing Methods

- Visual
- Pool vibration
- Acoustic
- Voltage and current

Frequency-based filtering techniques not effective [Siewert]

Non-linear Filtering Techniques

Ranked-order Filtering

Morphological Filtering

Special Problems of Sensing with Pulsed Current

Arc

voltage
current
resistance

all have a square-wave component

Need to remove to detect drop signature

Ranked-order filters good for this

Median Filter

Filter Size = N

Window Size = $2N+1$

Delay = N

Example

After median filtering...

After linear filtering...

Reference:

*Applications of a Class of Nonlinear
Filters to Problems in
Power Electronics*

W. Clem Karl, et al
1990 Power Electronics Specialists Conference
San Antonio, Texas
DOE contract DE-FG02-85ER13331

Topic III

Controlling Metal Transfer

- Define control criterion
- Design and test control system

Example

Controller Structure

MIT-INEL Collaborative Research Program

Multivariable Geometry Control of Welding

**David Hardt
Michael Hale**

July 17, 1990

Figure 63. Schematic of a Two-Camera Bead Geometry Measurement System

Measured Bead Geometry Response for Two Successive Step in Feedrate.
Note that the abscissa is distance along the bead.

Model Form

$$(1) \begin{vmatrix} \delta W \\ \delta H \\ \delta D \end{vmatrix} = \begin{vmatrix} K_{Wf} & K_{Wv} \\ K_{Hf} & K_{Hv} \\ K_{Df} & K_{Dv} \end{vmatrix} \begin{vmatrix} f \\ v^{-1} \end{vmatrix}$$

$$K_{if} = \alpha_i + \beta_i \delta f \quad i = 1, 3 \quad (2)$$

where δf is the deviation from a nominal value for f

Steady-State Outputs as a Function of Inverse Velocity

Steady-State Outputs as a Function of Wirefeed

PROCESS DELAYS

$$\left| \begin{array}{c} \delta W \\ \delta H \end{array} \right| = \frac{(1 + B_1 + B_2) z}{z^2 + B_1 z + B_2} \left| \begin{array}{cc} K_{Wf} z^{-d_1} & K_{Wv} z^{-d_2} \\ K_{Hf} z^{-d_3} & K_{Hv} z^{-d_4} \end{array} \right| \left| \begin{array}{c} f \\ v^{-1} \end{array} \right|$$

DYNAMICS

Z-plane plot of Pole Locations for Transient Response for Both Inputs

$$\begin{vmatrix} \delta W \\ \delta H \\ \delta D \end{vmatrix} = \frac{(1 + B_1 + B_2) z}{z^2 + B_1 z + B_2} \begin{vmatrix} K_{Wf} & K_{Wv} \\ K_{Hf} & K_{Hv} \\ K_{Df} & K_{Dv} \end{vmatrix} \begin{vmatrix} f \\ v^{-1} \end{vmatrix}$$

Control Range

Fig. 9 Input-Output Map for GMAW

Fig. 10 Input-Output Mapping

The General Welding Control Problem

PROCESS MODEL

$$\begin{bmatrix} H \\ W \end{bmatrix} = \begin{bmatrix} G_{Hf} & G_{Hv} \\ G_{Wf} & G_{Wv} \end{bmatrix} \begin{bmatrix} f \\ v^{-1} \end{bmatrix}$$

Typical Width Response to a Step in Wirefeed

In discrete form, the resulting process model is given by:

$$\begin{vmatrix} \delta W \\ \delta H \end{vmatrix} = \frac{(1 + B_1 + B_2) z}{z^2 + B_1 z + B_2} \mathbf{K} \begin{vmatrix} f \\ v^{-1} \end{vmatrix}$$

$$\text{where } \mathbf{K} = \begin{vmatrix} K_{Wf} z^{-d_1} & K_{Wv} z^{-d_2} \\ K_{Hf} z^{-d_3} & K_{Hv} z^{-d_4} \end{vmatrix}$$

$$B_1 = 2e^{a\tau} \cos(b\tau)$$

$$\text{where } \tau \equiv 0.04 \text{ v}^{-1}$$

$$B_2 = (e^{b\tau})^2$$

Hardware for Control

Controller Design

Scheduled Gain Independent Loops

$$F(z) = \frac{z^2 + B_1 z + B_2}{z(z-1)} K_f E_f(z)$$

$$V^{-1}(z) = \frac{z^2 + B_1 z + B_2}{z(z-1)} K_v E_v(z)$$

Locus of Roots for Variable Gains with Zero Tracking Controller

a)

Perfect Cancellation

b)

Cancellation Error

RESULTS

Experimental and Simulated Step Responses for Zero Tracking Controller

Step Commands = $\delta W = 0.25$ in and $\delta H = 0.06$ in.

Effect of Nominal Condition Changes

a) Time Response with Velocity Nominal Condition Changed from $v^{-1} = 0.055$ to 0.15

b) Comparison of Spatial Response for Different Nominal Conditions

Effect of the Bi-Valued I/O Map

- a) Stable Equilibria on either side of the fold line for different gain values
 b) slow drift between two equilibrium solutions for an intermediate gain value.

Experimental and Simulated Response of Decoupled Control Schemes

Decoupled Control

$$\begin{bmatrix} \delta U_1 \\ \delta U_2 \end{bmatrix} = \mathbf{K}' \begin{bmatrix} f \\ v^{-1} \end{bmatrix}$$

$$\text{where } \mathbf{K}' = \begin{bmatrix} K_{Wf} & K_{Wv} \\ K_{Hf} & K_{Hv} \end{bmatrix},$$

$$- \begin{bmatrix} \delta W \\ \delta H \end{bmatrix} = \frac{(1 + B_1 + B_2) z}{z^2 + B_1 z + B_2} \mathbf{I} \begin{bmatrix} \delta U_1 \\ \delta U_2 \end{bmatrix}$$

Disturbances

Response to a Fill Volume Disturbance

Effect of Gains

Delay Compensation: Effect of Smith Predictor on Decoupling Controller Response

Simulation of Decoupling controller with Smith Predictor and Random Measurement Noise on the Height outputs of 0.0025 in. magnitude.

CONCLUSIONS

- Control Range for Existing GMAW Process is Very Limited
- Process is Bi-Valued and Non-linear
- Scheduled Gain Control is Possible, but Decoupling control is Sensitive to Non-Linearities and Delays
- System Response in the *Spatial Domain* is More Linear

Estimation of Weld Bead Depth for In-Process Control

Jae-Bok Song
David E. Hardt

Multivariable Control of Welding Processes: Depth Estimation

Problem Formulation

Typical Weld Cross Section for Gas Metal Arc Welding

Dual Gaussian Source Model and Subsequent Weld Bead Profile

Dual Heat Source Model

Single Gaussian Source

$$T(x, y, z, t) - T_0 = \eta \int_0^t \frac{Q}{\pi \rho c} \frac{(4\pi\alpha\tau)^{-1/2}}{2\alpha\tau + \sigma^2} \exp\left(-\frac{(x + v\tau)^2 + y^2}{4\alpha\tau + 2\sigma^2} - \frac{z^2}{4\alpha\tau}\right) d\tau$$

Dual Gaussian Sources

$$T(x, y, z, t) - T_0 = \sum_{k=-\infty}^{\infty} \left[\eta_1 \int_0^t \frac{Q}{\pi \rho c} \frac{(4\pi\alpha\tau)^{-1/2}}{2\alpha\tau + \sigma_1^2} \exp\left(-\frac{(x + v\tau)^2 + y^2}{4\alpha\tau + 2\sigma_1^2} - \frac{(z + 2kh)^2}{4\alpha\tau}\right) d\tau + \right. \\ \left. \eta_2 \int_0^t \frac{Q}{\pi \rho c} \frac{(4\pi\alpha\tau)^{-1/2}}{2\alpha\tau + \sigma_2^2} \exp\left(-\frac{(x + v\tau)^2 + (z - z_0 + 2kh)^2}{4\alpha\tau + 2\sigma_2^2} - \frac{y^2}{4\alpha\tau}\right) d\tau \right]$$

h is the thickness of the plate

z_0 is the displacement of the center of the lateral source

1. Using estimated values for (η_1, σ_1) and (η_2, σ_2) , T_i is computed from at specific top and bottom surface locations, (x_i, y_i, z_i) , at which actual temperatures (T_i^*) can be measured during welding.
2. The actual measured values are compared with the predictions, and the error is calculated.
3. The estimates of (η_1, σ_1) and (η_2, σ_2) are then adjusted until the error is minimized.
4. When acceptable error is reached, $T(x,y,z)$ is searched for the isotherm corresponding to the melting temperature of the material. This isotherm corresponds to the pool boundary, and can be interrogated to find the pool depth.

$$E = \sum_{i=1}^N (T_i - T_i^*)^2$$

$$\frac{\partial E}{\partial q_j} = 0, \quad j = 1, \dots, 4 \quad (5)$$

Experiments

Selection of Measurement Points

Backside temperature Distributions

Results

Backside Temperature Measurement Locations for Experiment

Experimental and Estimated Weld Bead Cross Section
 (Experimental condition : Mild steel, Arc voltage; 30V ,
 Wire feedrate ; 21.2 cm/sec, Travel speed ; 5.0 mm/sec,
 Shielding gas; Ar+2% O₂)

Isothermal Curves on the yz Plane from Estimated Heat Source Parameters

**SPATIAL -BASED CONTROL for
DROPLET BASED PROCESSES**

GENERAL PROCESS CONTROL PROBLEM

Properties and Geometry are Primary Outputs of *any* Process

Serial Processes: (Welding, Cutting, Machining ...)

- Global Geometry via Trajectory Control
- Complex Local Geometry decoupled from Global

Parallel Processes (Casting, Forming, Molding)

- Simultaneous Global Geometry Change
- No Decoupling of Local and Global

Time Based

Distance Based

Figure 1 Time Transients and the Spatial Equivalent for a Velocity Dependent Non-Linear system

MOTIVATION FOR SPACE-BASED CONTROL

- Final **Geometry** is Output of Concern
- Evidence that Spatial Base Simplifies the Control Problem

Welding

Forming

- Improved Trajectory Control for Serial Processes

Weld Disturbances

Plasma Spray

PROPOSED RESEARCH

Objectives:

- Develop a paradigm for spatial control of geometry-change processes
- Examine this paradigm in the context of droplet based processes
- ^{II 83} Begin the process of distilling these results into a distinct modeling methodology and control theory for this class of systems.

Model System:

- Droplet - Part Geometry Processes

Welding, Plasma Spray and Spray Forming

RESEARCH TASKS

Task 1:

Examine a simple time - space basis shift within existing control systems.

- Existing Welding Model and Controllers
- Dependent Variable Transformation: Distant for Time
- Effect of Variable Sampling times during Process
- Experiments using GMAW and Distance as “clock”

Task 2:

Develop a time-space basis shift at the model stage, and subsequently, a fully space-based controller design

- Existing Models, Transformed to Distance Basis
- Controller Design in Spatial Domain
- System Evaluation By Experiment

Task 3.

Development of a space-based system modeling method.

- Scaling of Simple Thermal Laws (e.g. diffusion) on a Spatial Basis
- Droplet - Interaction Modeling
- Development of *Spatial Elements* for network type modeling
- Use of Models with Spatial Controllers (Welding, Plasma Spray)

SOLID MECHANICS

Technical Advisory Comments* on Solid Mechanics Research

I.0 Summary

- o The research completed and proposed in both the areas of Fracture Mechanics and Communion of Energy Materials are of significant national interest.
- o The funding should be continued for both projects taking into consideration the comments provided below.
- o It should also be recognized that the Fracture Mechanics work is more complex and has the potential for a broader impact on the industry. Nevertheless, both projects should be continued.

2.0 Fracture Mechanics

2.1 Collaboration

MIT is focusing on the development of analytical methods whereas INEL is focusing on experimental work to shed light on key material behaviors to be modeled. We have seen the collaborative effort grow between the teams over the years. There is room for further growth and exploitation of benefits of team work. We recommend that MIT take a lead role in designing critical experiments to drive the analytical effort. We like to see definition and rationale for experiments from the viewpoint of how it is going to help the modeling effort. We like to see INEL spend more effort on the interpretation of data and less on generation of data. It is not clear the volume of data generated is necessary for the purpose of developing the analytical model. The project has produced break throughs in the area of modeling the behavior of stationary cracks and quantifying the crack front constraint which are keys to the next step of modelling crack growth and instability.

2.2 Goals and Objectives

Even in the context of basic research the goals and objectives noted in the proposal are at best vague and confusing. The goals and objectives statements are better focused in the MIT description. Improved goals and objectives definition is necessary. The discussion provided by MIT at the meeting is satisfactory and this should be incorporated in the write up. Further we like to see a single statement of goals and objectives for the project rather than one for MIT and one for

* These comments include material presented in the INEL-MIT Proposal Vol. I-II, dated February 1990.

INEL. We would go along with expanding the MIT statement to include objectives of INEL that may not have been included in the MIT discussion, for example; development of a standard testing procedure and discovering new material phenomena that is important for modelling. It should be emphasized that the present write up, particularly the one from the INEL side, promises much more than the funding can deliver. For example, there is very little in the scope to address the key issues of life extension. However, the description alludes that the research will solve life extension problems.

Although the proposed research in welds is important, both the description and presentation were vague. Significantly more effort should be spent on identifying critical issues and how the solution to these issues will lead to improved tools for the industry. Much work needs to be done in problem definition. INEL should visit industrial activities such as the EPRI NDE Center activities at Charlotte to understand the key issues that are important to the industry. Our recommendation is that there should be a period for problem definition and for designing critical experiments and modelling. Perhaps 3 months is appropriate. Thereafter, the effort on weld cracks should commence. Such a well planned and designed effort will have substantial impact on the emerging technology of using very high strength welded steels in the commercial and defense arena.

2.3 Funding Level

MIT's request is judged in proportion to the scope identified. We do not see the specifics of INEL scope description supports the level of funding requested.

2.4 Training of People and New Measurement Techniques

The project has helped support 5 undergraduates and graduates, in addition to providing support for three post-doctors (two of them full-time faculty). INEL has trained at least two people with its funding and has developed Moire and Microtopography measurement techniques.

2.5 Interaction with Industry

Interaction with the industry should continue with the emphasis on identifying the specific deficiencies in the currently used methodologies. For example, instead of saying this research will help leak-before-break, the researchers

should identify what are the deficiencies, how the solution sought in the research will help improve the methodology and whether the improvement is significant enough to justify the expenditure.

3.0 Communion of Energy Materials

3.1 Collaboration

Thus far the work was being conducted independently by MIT who has been concentrating on modelling and experiment. INEL is proposing to participate and contribute in two areas: use of Acoustic Emission techniques to identify fracture occurrences and study fracture behavior of practical materials. MIT's work thus far was focused on ideal materials (glass and plastic beads).

This collaboration should help the project. However, we like to see MIT take the lead role in identifying and directing the experiment. Emphasis should be on focused experiment rather than generating more data. On the INEL side, equal emphasis should be put from the beginning on the interpretation of test data. The INEL proposal should be revised to show task definition and how they integrate with the goals and objectives of the project.

3.2 Goals and Objectives

The MIT proposal is well written and focused on the goals and objectives. The relationship of the research to the real world problem is clearly defined. The work scope is broken up into clearly defined tasks. The integration of the tasks toward the final objectives is also well defined.

Success criteria is defined in terms of significantly improving the efficiency of communion devices. This criteria needs to be sharpened in the light of real world materials. Discussion and interface with users and designers of these devices would be useful.

3.3 Funding Level

MIT's request is judged to be in proportion to the scope identified. On the INEL side, breakdowns are not presented to make such a judgement. This program needs the requested financial commitment for 3 graduate students.

3.4 Training of People

MIT has produced at least 4 post-graduates. Two masters and one Ph.D. level students are on the project now. INEL does not show any plan for training new people in this area although one would expect that to happen.

3.5 Interaction with the Industry

Industry interaction should be continued to a point of involving either a user or a designer to commit to providing continued feedback and comment on the research.

DUCTILE FRACTURE ANALYSIS--EMPHASIS ON SURFACE FLAWS

INTRODUCTION

A federally funded study showed that the cost of fracture in the United States (primarily associated with the transportation and construction industries) is nearly \$119 billion annually (1982 dollars). This cost is based on the resources required for fracture prevention (overdesign, inspection, repairs, research, etc.) and the cost (safety and dollars) of fracture-related failures. Although fracture prevention is a very significant part of the cost, this expense is not necessarily associated with increased safety. In fact, the report notes that equally safe or safer structures could be produced, at lower cost, through improved predictions of structural performance. The report estimates that nearly a quarter of the annual cost for fracture prevention could be saved through fracture-related research. One of the major categories of research identified was structural research [e.g. to develop better fabrication techniques, improve lifetime prediction models, develop tests to increase structural reliability, establish meaningful requirements for nondestructive evaluation (NDE)]. A recent development in the transportation industry is the desire to establish criteria and allowable conditions for operating again aircraft; obviously this task is critical from both safety and cost standpoints. Fracture mechanics concepts are being applied as one of the techniques to solve the problem.

The high cost of fracture noted in the previous paragraph is not unique to the United States, but is also of concern to other countries. The European Group on fracture has initiated a study on "Economic Effect of Fracture in Europe. Several European countries (United Kingdom, France, Portugal, Federal Republic of Germany, Italy, and Switzerland) are participating to collect economic and technical data for the study. The Interim Report contains a preliminary list of research needed to reduce the economic effects of fracture.

It has been proposed that accurate prediction methods, as opposed to the use of empirically developed acceptance curves, are needed to predict the integrity and lifetime of structural components. These methods could provide major cost benefits by providing a basis for (1) optimizing downtime schedules for plant maintenance and repair, (2) optimizing plant operating conditions, (3) developing NDE strategies, (4) extending plant life, and (5) developing a model for ensuring plant safety. [Accurate experimentally verified methods have been used in the Advanced Test Reactor at the Idaho National Engineering Laboratory (INEL) to save considerable time and cost

without detracting from plant safety.] The European Group on Fracture is conducting fracture mechanics research to develop proven analytical/numerical techniques for predicting fracture of structural components.

The energy generation and chemical industries are attempting to extend the lifetime of structural components beyond that of the original design. The ability to do so (safely) would result in the saving of billions of dollars. Of the many technical issues being examined, three are related to fracture mechanics:

1. Changes in fracture toughness due to environmental effects such as time at temperature, irradiation, etc.
2. Use of leak-before-burst "safe" failure criteria under loading conditions ranging from thermal displacement control to hydrostatic to pneumatic. The U.S. Nuclear Regulatory Commission (USNRC) has been funding considerable research on this problem relative to the primary coolant systems in commercial nuclear reactors. The materials in the NRC study include 304 stainless steel (SS) which is in the fully plastic fracture regime in this application.
3. Are the capabilities of existing models adequate for predicting structural integrity when calculations of subcritical crack growth have grown a hypothetical crack and the structure then experiences a design condition peak stress or deformation?

Fracture mechanics must account for all combinations of brittle and ductile micromechanisms and brittle and ductile structures (i.e., structural response) that may occur, see Table 1. (The different acronyms used to describe varying degrees of structural plasticity are summarized in Table 2.) Considerable progress has been made in developing LEFM concepts for assessing integrity and predicting lifetime for brittle specimens and structures. LEFM accounts for many catastrophic fractures; it is now relatively well understood and many of these failures can be predicted. However, the accuracy and limits of such predictions have not been quantified for general crack geometries and loadings, especially for high stress gradients, e.g., due to thermal stresses. Weldments, with heterogeneous mechanical properties also present a problem.

TABLE 1. EXAMPLES OF BRITTLE-DUCTILE BEHAVIOR IN MICROMECHANISMS AND STRUCTURES

<u>Micromechanism</u>	<u>Structural Behavior</u>	
	<u>Brittle</u>	<u>Ductile</u>
Brittle	Lower shelf in ferritic steels	Transition zone cleavage in ferritic steels
Ductile	Hole growth in high strength aluminum alloys	Hole growth in low strength aluminum alloys

TABLE 2. DEFINITIONS OF ACRONYMS DESCRIBING STRUCTURAL PLASTICITY

<u>Acronym</u>	<u>Definition</u>
LEFM	Linear elastic fracture mechanics
EPFM	Elastic plastic fracture mechanics lies between LEFM and FPFM
FPFM	Fully plastic fracture mechanics
RPFM	Rigid plastic fracture mechanics, it is at extreme ductility of FPFM
NLEFM	A subdivision of EPFM, where J-integral is applicable

As with linear elastic fracture mechanics, NLEFM is only valid when the singular field found in some region between the scale of the micromechanism and the region of influence of the far field boundary condition satisfies the HRR (Hutchinson and Rice and Rosengren) conditions. The single fracture parameters such as stress intensity (K), J-integral (J), and crack tip opening displacement (δ) can be used in LEFM and J and δ can be used in NLEFM. Beyond NLEFM it appears as if two parameters consisting of J or δ plus a constraint term are necessary.

The objective of the research work is to develop improved analytical/numerical techniques for predicting integrity of cracked, ductile structures (those fabricated from low-strength materials, including weldments, containing partial-penetrating surface flaws, and subjected to essentially monotonic loading). Lifetime prediction and structural integrity assessments of such structures require the ability to predict crack growth initiation, stable crack growth, and instability. The primary concern of this research is the elastic-plastic and fully plastic regimes, but elastic conditions are included in the research to quantify the accuracy of predictions based on using K_{Ic} and applicable analytical solutions, and to identify the limits of their effectiveness.

The current research is being conducted jointly by the INEL and the Massachusetts Institute of Technology (MIT). The INEL is primarily responsible for the experimental efforts while MIT is primarily responsible for development of analytical/numerical models. This project is responsive to the needs of the Departments of Energy, Transportation, and Defense. Successful completion of the project will lead to decreased fabrication costs, establishing meaningful requirements for NDE, optimizing scheduled plant downtimes, decreased downtime attributed to defects discovered in operating components, elimination of needless and sometimes harmful repairs, improved methods for lifetime prediction and extension, improved structural designs, and optimization of plant operating conditions.

DATA

from

Project Reviews

Solid Mechanics: Ductile Fracture Analysis

July 17-18, 1990

Ductile Fracture Analysis — Emphasis on Surface Flaws

**D. M. Parks and F. A. McClintock
Department of Mechanical Engineering
Massachusetts Institute of Technology
Cambridge, MA 02319**

**Presented at
D.O.E. MIT/INEL Program Review
Cambridge, MA
July 17-18, 1990**

Outline of Presentation

- Major Accomplishments

- 3D Elastic-Plastic Studies of Surface Cracks

- p 5-7 * Documented deviation from one-parameter fields

- p 8-14 * Recent 2-D Studies on Two-Parameter Fields

- p 13-24 * Quantitative 2-Parameter Predictions for Surface Flaws

- p 25-31 * Enhanced Simplified Models: Line-Spring - ABACUS

- 3D Studies of Through-Cracked Plates

- * Elastic analysis in thin plates

- * Elastic-plastic analysis in thin plates

- Future Directions

- Ductile Surface Crack Penetration

- Extended (Constraint-Sensitive) Ductile Fracture Mechanics Methodology

- Ductile Fracture Phenomena in Heterogeneous Material: Welds and Bonds

- 3D "Statistical" Aspects of Crack Constraint and Cleavage

DOE MIT/INEL Fracture Research: Reviewed Publications

MCCLINTOCK	1989	<i>Int. J. Fract.</i>	"Asymmetry Lowers Ductility"
NAKAMURA & PARKS	1988	<i>J. Applied Mechanics</i>	"3D ... Thin Elastic Plate"
NAKAMURA & PARKS	1989	<i>Int. J. Solids & Structures</i>	"3D Antisymmetric ... Thin Elastic Plate"
NAKAMURA & PARKS	1990	<i>J. Mech. Phys. Solids</i> (in press)	"3D ... Thin Ductile Plate"
NAKAMURA & SHAWKI	1988	<i>Int. J. Fract.</i>	"Deep-Crack Power Law ..."
PARKS	1990	<i>ASTM STP # 1060</i>	"A Surface Crack Review ..."
PARKS & WANG	1988	in <i>ASME AMD-91</i> , Eds. Rosakis & Rajapakse	"HRR-Dominance ..."
SHAWKI, NAKAMURA, & PARKS	1989	<i>Int. J. Fract.</i>	"Power-law Line-Spring"
WANG, PARKS, LLOYD, KUTER, & EPSTEIN	1990	to appear, <i>J. Appl. Mech.</i>	"Elastic-Plastic ... Surface-Cracked Plate"
PARKS	1990	to appear, Proc. Eur. Symp. Fract.	"Three-Dimensional ... HRR-Dominance"
WANG & PARKS	1990	to be submitted to <i>Int. J. Fract.</i>	"T-Stress in Surface Cracks Using Line-Spring"

DOE MIT/INEL Fracture Research: Major Presentations

MCCLINTOCK	March, 1988	IUTAM Symposium on Nonlinear Fracture	(Pasadena)
PARKS	April, 1988	ASTM Symposium on Surface Cracks (Keynote Address)	(Reno)
PARKS	March, 1989	Southwest Mechanics Seminar Series	(Norman, Arlington, College Station, & San Antonio)
PARKS	October, 1989	European Conference on Fracture (Keynote Address)	(Freiburg)
WANG	November, 1989	ASTM	(Orlando)
PARKS	April, 1990	5th Int. Conf. Num. Meths. Fract. (Keynote Address)	(Freiburg)

Fig. 2

$$\sigma_{yy}(r; \theta=0; \phi) / \sigma_{ssy}(r/J(\phi))$$

HRR:

$$\delta_t = d_n \left(\frac{n}{2} \right) \frac{J}{\sigma_0}$$

Small-Scale Yielding

(Plane Strain
Boundary Layer Formulation)

- Mathematical Definition:

as $r \rightarrow \infty$,

$$\sigma_{\alpha\beta}(r, \theta) \rightarrow \frac{K_I}{\sqrt{2\pi r}} \bar{t}_{\alpha\beta}(\theta)$$

- Similarity Length Scale: $\left(\frac{K_I}{\sigma_0}\right)^2$ or $\frac{J}{\sigma_0}$, etc.

- Results:

$$\sigma_{ij}(r, \theta; n; K_I) = \sigma_0 \cdot \hat{\sigma}_{ij}\left(\frac{r}{(K_I/\sigma_0)^2}, \theta; n\right)$$

$$\equiv \sigma_{ij}^{SSY}$$

$$\epsilon_{ij}(r, \theta; n; K_I) = \alpha \epsilon_0 \cdot \hat{\epsilon}_{ij}\left(\frac{r}{(K_I/\sigma_0)^2}, \theta; n\right)$$

$$\equiv \epsilon_{ij}^{SSY}$$

- ASYMPTOTICS

$$\lim_{r \rightarrow 0} \sigma_{ij}^{SSY} = \sigma_{ij}^{HRR} \quad (\text{III } 18)$$

(Deformation Theory)

$$r / (d_n J / \sigma_0) \doteq r / \delta_t$$

$$\left\{ \begin{array}{l} \alpha \epsilon_0 = \frac{1}{300} \\ n = 10 \\ d_n = .53 \end{array} \right\}$$

Fig. 1a

Fig. 1b

Modified Boundary Layer (MBL) Formulation (Plane Strain)

• Mathematical Model

as $r \rightarrow \infty$,

$$\sigma_{\alpha\beta}(r, \theta) \rightarrow \frac{K_I}{\sqrt{2\pi r}} f_{\alpha\beta}(\theta) + T_{\alpha\beta}$$

$$[T_{\alpha\beta}] = \begin{bmatrix} T_{11} & 0 \\ 0 & 0 \end{bmatrix} \equiv \begin{bmatrix} T'' & 0 \\ 0 & 0 \end{bmatrix}$$

• History (Abbreviated)

73/74	-	Larsson & Carlsson	{	T-stress influences size & shape of plastic zone
	-	Rice		
* 86	-	Bilby, et al	{	T-stress influences σ_{ij} <u>deep inside</u> plastic zone
* 89	-	Betegón & Hancock		
89	-	Wang		
90	-	Du & Hancock		
90	-	Shih; Sharma & Aravas		

• Results

as $r \rightarrow 0$

$$\sigma_{\alpha\beta} \rightarrow \sigma_0 \cdot \left(\frac{J}{\alpha \epsilon_0 \sigma_0 I_n r} \right)^{\frac{1}{1+n}} \sigma_{\alpha\beta}^+ (\theta; n; \tau)$$

$$\equiv \sigma_{\alpha\beta}^{MBL};$$

$$(\tau \equiv T / \sigma_0)$$

$$\sigma_{\alpha\beta}^{MBL} \Big|_{\tau=0} \equiv \sigma_{\alpha\beta}^{SSY} \quad \left(\text{+ Analogous Result for } \epsilon_{\alpha\beta} \right)$$

(Wang, 1989)
(Deformation Theory)
Plane Strain

$r/(f^{\text{far}}/\sigma_0)$

MBL with $\tau = T_n/\sigma_0$
(Plane Strain)

Observation #1: One-parameter descriptions of Surface-crack-front constraint gradually, then abruptly, become inappropriate.

Observation #2: In plane strain, the T-stress correlates a family of crack tip fields of varying constraint.

Question: Can T-stress concepts be applied to explain loss of constraint in 3-D surface cracks?

Approach:

- T-stress correlation: $T(\phi) = \hat{t}(\phi, \dots) \cdot \sigma^\infty$
- Normalizations: $\left\{ \begin{array}{l} \tau(\phi) \equiv T(\phi) / \sigma_0 \\ \Sigma^\infty \equiv \sigma^\infty / \sigma_0 \end{array} \right\} \Rightarrow \tau = \hat{\tau} \cdot \hat{\Sigma}^\infty$
- Crack-opening Stress: $\sigma_{yy}^{MBL} = \sigma_{yy}^{SSY} + A_n \tau + B_n \tau^2$
(Betegón-Hancock)
- Re-arrange:

$$\frac{\sigma_{yy}^{MBL}}{\sigma_{yy}^{SSY}} = 1 + \frac{A_n (\hat{t} \hat{\Sigma}^\infty) + B_n (\hat{t} \hat{\Sigma}^\infty)^2}{\sigma_{yy}^{SSY}}$$

Numerical Evaluation of T-Stress

• Two-Dimensional Planar Configurations

1. Fine Mesh / "Brute Force" Method (Larsson, Carlsson)

$$r/a \ll 1:$$

$$\sigma_{\alpha\beta}(r, \theta) = \frac{K_I}{\sqrt{2\pi r}} f_{\alpha\beta}(\theta) + T \delta_{1\alpha} \delta_{1\beta}$$

$$\Rightarrow T = \frac{K_I}{\sqrt{2\pi r_i}} (f_{22}^{(i)} - f_{11}^{(i)}) - (\sigma_{22}^{FEH} - \sigma_{11}^{FEH})$$

2. Higher Order Weight Functions (Sham)

$$T = \int_A \rho \underline{\underline{f}} \cdot \underline{\underline{t}} dA + \int_{\partial A} (\underline{\underline{\sigma}} \underline{\underline{n}}) \cdot \underline{\underline{t}} ds$$

3. "Eshelby's Theorem" (Kfoury; Goldthorpe, Cardew, et al)

$$J^{(2)}(Q, t, t_0) = J^{(1)}(Q) + Tt/E'$$

Numerical Evaluation of T-Stress (cont.)

- Three-Dimensional Crack Fronts

1. Fine Mesh / "Brute Force" Method
(very expensive)

2. Part-Through Surface Cracks:
The Line-Spring (Wang & Parks)

plate +
shell

3. Domain Integral Versions of
Eshelby Interaction Integral

(currently underway with Prof. T. Nakamura
SUNY)

Fig. 1

(a)

(b)

$$\sigma_b = 6M/t^2$$

$$\sigma_t = N/t$$

Fig. 2

BASIC LINE-SPRING:

$$K_I(x) = N(x) \cdot k_N(\alpha(x)) + M(x) \cdot k_m(\alpha(x))$$

Extended Application:

(II 27)

$$T(x) = (?) N(x) \cdot t_N(\alpha(x)) + M(x) \cdot t_m(\alpha(x))$$

Fig. 3

(a)

(b)

Fig. 4

$$(a/c = 0.24)$$

φ
(a)

φ
(c)

φ
(b)

φ
(d)

- composite curve
- - - $t_m N(\phi) / (\sigma^- t)$
- $6 t_m M(\phi) / (\sigma^- t^2)$

Fig. 5

— 3-D FE solution
 — line-spring solution

Fig. 6

Fig. 7

Fig. 8

unexplained

Fig. 9

Normalized axial force vs. cracked displacement
for pure tension of plane strain SEN

Effective Crack Length Correction

$$a_e = a + \beta \left(\frac{Q \cdot k(a^c)}{\sigma_0} \right)^2$$

Normalized axial force vs. cracked displacement
for pure tension of plane strain SEN

Normalized J vs. cracked displacement
for pure tension of plane strain SEN

Normalized J vs. axial force
for pure tension of plane strain SEN

STRAIN HARDENING FACTOR : f

Elastic-Plastic Tangent Stiffness

$$\dot{Q}_i = S_{ij} \dot{q}_j$$

$$\dot{q}_j = \dot{q}_j^{(e)} + \dot{q}_j^{(p)}$$

normality, consistency and
plastic work rate
(Parks & White, 1982)

$$\dot{W}^{(p)} = Q_i \dot{q}_i^{(p)}$$

$$\begin{aligned} \dot{W}^{(p)} &= \int_{A^*} \bar{\sigma} \dot{\epsilon}^{(p)} dA \\ &= f \sigma_0 \dot{\epsilon}^{(p)} c^2 \end{aligned}$$

$$f = 0(1)$$

Parks/White : $f \approx 0.4$
(Crude)

Normalized J vs. axial force
for mid-ligament tension of plane strain SEN

Combined tension and bending yield surface
normalized with SEN thickness t

Combined tension and bending yield surface
normalized with SEN ligament c

Normalized axial force vs. cracked displacement
for pure tension of plane strain SEN

Energetics of Comminution

Data and Discussion

ENERGETICS OF COMMINUTION

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ABSTRACT

Continuing work on the processes of particle fracture within particle beds is presented. Experimental work on bed compression and fracture is qualitatively duplicated in computer simulations of two-dimensional beds of non-uniform spheres, including detailed behavior within the bed. The build-up and collapse of frictionally supported force structures within the bed are seen, and the distribution of energy in losses and storage is determined. Failure of multiply-loaded brittle spheres is dependent upon the maximum individual load only, but lateral loads can inhibit fracture of plastic spheres. A "bed efficiency" is defined and initial experimental investigations of efficiency as a function of compression parameters are presented. Means for transporting fine material from the active crushing zone are discussed and an initial experiment demonstrating very effective separation by size is presented.

INTRODUCTION

This work is a continuation of basic comminution research initially reported at a previous Symposium on Energy Engineering Sciences[1]. The purpose is to gain an understanding of individual particle fracture and transport within particle beds, as are present in devices used in practical crushing and grinding operations. These operations, which are believed to be extremely inefficient, are of increasing importance as finer grinding is necessary to provide better cleaning of coal, and as dwindling domestic reserves require lower cost processing of low grade ores.

Work to date has provided insights that have led to a new comminution concept that offers the potential for improved efficiency. However, continuing research work is still basic research, directed to the development of an understanding of physical phenomena that will permit effective design work in the future. Attention has expanded beyond a study of quasi-static particle fracture within beds to a combined study of fracture and material transport within beds.

COMPLETED WORK

Earlier work by Drlik[2] demonstrated the feasibility of a computer simulation of a two-dimensional particle bed. Pflueger[3] has since developed an advanced and more convenient simulation of a two-dimensional bed of spheres. His work shows good qualitative agreement with Laffey's experimental work[4], including such details as the rise and collapse of bed forces, and the tendency for fracture to begin near the upper surface for bed compression between two horizontal flat plates. Figs. 1a and 1b illustrate typical simulated behavior for a bed subjected to a descending upper

2

surface. Particle-to-particle and particle-to-boundary forces are shown by vectors, with the line thickness proportional to force magnitude. In Fig. 1a, the bed has been compressed by about 1.3 average particle diameters, three particles have been broken (each replaced by a group of six smaller particles), and a strong force structure extends through the bed just to the left of center. In Fig. 1b, after continued compression to about 1.4 particle diameters, several more particles have broken, and the force structure has essentially collapsed. This behavior is typical.

The simulation also computes energy stored and lost within the bed as compression progresses, as illustrated in Fig. 2. Energy is stored in the elastic deformation of spheres subject to both normal and shear contact forces. Energy is lost to friction as spheres slide against one another and the boundaries. "Energy lost to breakage" is elastically stored energy which disappears with the sudden loss of contact forces around a sphere which fractures. In reality, a small fraction of this is actually useful energy that goes into the fracture. This simulation makes no attempt to accurately model the fracture process in terms of the creation of new surface area; hence, this portion of the energy is not determined. The majority of this lost energy is converted to kinetic energy in very rapid local motions and ultimately lost in friction. The computation is not fast enough to follow the details of that local motion, but the representation as an ultimate loss is believed to be realistic.

It is also possible to independently compute total work input to the bed by integrating the normal force-displacement product on the moving upper boundary. Fig. 2 shows that these two energy calculations are in excellent agreement. A slight step error may be seen at about .028 meters displacement, in this case, where very rapid changes occur as several spheres fracture in a very short time, but outside that numerical error (which could be reduced by smaller integration steps), the simulation seems to be internally consistent.

The simulation model requires selection of a failure criterion to specify under what conditions of loading a sphere should be assumed to fracture. Four different criteria were assumed, and it was found that overall bed behavior differed significantly with this selection. The simplest, and ultimately the best failure criterion was a size-dependent critical load which, if exceeded by any of the contact forces on the sphere, caused failure. A second criterion specified failure if the maximum shear stress within the particle exceeded a critical value. Two other criteria attempted to account for a "hydrostatic" inhibition of fracture that might accompany a large number of compressive loads distributed over the surface of a sphere. Figs. 3a and 3b indicate a significant difference in overall bed behavior for the first two of these criteria. The maximum force criterion bed behavior is consistent with experimental observation of bed behavior, with fracture starting from the top of the bed and progressing downward, followed by fracture progression upward from the bottom. This criteria was also determined to be the best from work on individual brittle particles, as discussed below. Fig. 4 indicates that, among other phenomena, bed elastic energy storage versus displacement depends strongly on the choice of particle failure criterion for four otherwise identical beds.

The need to determine a meaningful particle failure model led to research by Kurfess [4] on the failure of brittle (glass) and plastic (acrylic) spheres subject to multiple point loads. Apart from the need for realistic input for the bed simulation, there was serious concern over possible fracture inhibition from multiple loads, however they might be modeled in the simulation. It is known that external loads can be "blunted", i.e., distributed on a large number of harmless smaller forces, by excessively fine material. This might be overcome by greater external loads, provided the crushing machine has sufficient capacity. However, if such loading also causes a "hydrostatic" stress within the particle, there may be no fracture, and this behavior could not be overcome by greater external loads. Kurfess worked with one-inch diameter spheres, subjected to opposing primary or axial loads between flat plates, and also subjected to such primary loads plus secondary lateral loads in the

"equatorial" plane of the sphere (i.e., normal to the axial load direction). Three or four secondary loads were applied, evenly spaced around the equator. For secondary loads up to about 25% of the axial failure load, Kurfess found that there was no inhibiting effect from the lateral loading. For brittle particles it appears that transition from stable to unstable fracture growth occurs very near the surface under the maximum load point. Easter [6] provided an approximate stress distribution within elastic spheres subjected to multiple loads which indicates that the state of stress beneath the primary load is essentially independent of loads at other locations, in keeping with the conclusion that transition to catastrophic failure is a very local phenomena beneath the maximum load point.

Misra, in work not yet reported, extended the work of Kurfess to lateral loads approaching the primary load in magnitude. He found that failure of brittle spheres was uninfluenced by lateral loads, even of that magnitude. Failure of plastic spheres, however, was significantly inhibited by lateral loads exceeding 50% of the nominal failure load. As might be expected, there appear to be rate-dependent effects and other complications. For example, intermediate lateral loads seem to be more effective in preventing failure than do lateral loads essentially equal to the primary loads. Failure of plastic particles will ultimately be of importance as finer crushing is demanded, since all materials behave in this fashion if in sufficiently small particles.

CURRENT WORK

Though the bed simulation work will be expanded to three-dimensional geometries, the present two-dimensional results provide an adequate qualitative understanding of quasi-static bed behavior. Consequently, the present work has shifted to that other important aspect of bed behavior--the transport of material within the bed. Particular attention is given to size-dependent relative motion within the bed, with the intent of developing systems to continuously sweep fine material from the active crushing zone. A specific arrangement has been conceived which, it is believed, will provide this behavior, using fluid transport to move the solid material, but the present research work centers on exploring the basic phenomena. The work has just gotten underway, by students Karen Annis, Chahid Ghaddar and Deb Misra, but some interesting progress can be reported.

To outline the important issues, consider a "continuity" equation which describes the flow of a single-size fraction within the walls of a comminution device as shown in Fig. 5. While the flow may be unsteady in detail, due to oscillating walls (like a jaw crusher) or pulsating fluid flow (see following), we shall limit this discussion to average conditions which are steady in time.

Consider the i^{th} size fraction, where the material is divided into size fractions ranging from 1, the smallest, to I, the largest. In steady flow the rate of change of the mass of that size material in a control volume between two sections 1 and 2, shown in Fig. 5, will be zero. The mass flow rate of that size material entering through section 1, $\dot{m}_{i1}$, is given by

$$\dot{m}_{i1} = n_{i1} m_i A_1 V_{i1}$$

where n_{i1} is the spacial density of particles expressed as number of particles per unit volume, m_i is the average mass per particle, A_1 is the flow area, and V_{i1} is the particle velocity of size i crossing section 1. Similarly, the mass flow rate of size i leaving at section 2 is

$$\dot{m}_{12} = n_{12} m_1 A_2 V_{12}$$

Due to crushing action, particles of size i will be generated within the control volume from larger particles, while some of size i will be destroyed. The net generation rate of size i , $\dot{m}_{ig}$ per unit volume is given by

$$\dot{m}_{ig} = \sum_{j=i+1}^I n_j m_j c_{ij} - n_i m_i c_i$$

where c_{ij} describes the local production of size i particles from larger size j particles, and c_i describes the local destruction of size i (and production of sizes i to $i-1$). It is assumed that the destruction rate of any size fraction is proportional to the total mass of that size present. The constants of proportionality, c_{ij} and c_i , will be functions of crushing variables such as frequency and amplitude of wall motion, width of the passage relative to particle size, and perhaps other variables having to do with the local size distribution within the moving bed. Combining equations, the overall continuity equation for size i is

$$m_i \left[n_{i1} A_1 V_{i1} - n_{i2} A_2 V_{i2} \right] + (\text{Vol}) \left[\sum_{j=i+1}^I n_j m_j c_{ij} - n_i m_i c_i \right] = 0$$

where (Vol) is the volume between sections 1 and 2. Much can be done to refine this equation (for example, it will be reduced to differential form), but for present purposes it serves to identify two separate experimental approaches which, for the present, allow us to avoid the complications of combined crushing and material transport behavior.

The coefficients c_{ij} are being investigated in experiments similar to those of Laffey, but in greater quantitative detail. For convenience, a "bed efficiency" η_{bi} has been defined to describe bed behavior as follows:

$$\eta_{bi} = \frac{\text{energy per particle crushed individually between flat plates}}{\text{energy per particle crushed in a particle bed}}$$

This definition anticipates that there are inherent, and apparently unavoidable, losses associated with the excessive elastic energy input to crush a single particle between flat plates*, and that there are additional, perhaps avoidable, losses which can be ascribed to bed action. An improved design will maximize bed efficiency, while it may not be realistic to expect that the inherent single particle losses can be reduced in practical devices. Initial experimental work has been limited to beds of limited initial size range (2.0 to 1.7 mm glass spheres, as used by Laffey). Crushing within the bed is treated entirely as the primary fracture of full-sized particles (i.e., useful subsequent fracturing of primary fragments is ignored). Experimentally, beds are compressed and primary fractures are determined by sieving the products to determine how many full-sized particles remain. The efficiency is then

$$\eta_{bi} = \frac{\text{energy per particle crushed individually (experimentally determined)}}{\text{measured bed energy input/number of primary fractures}}$$

*Except for very small particles as discussed by Peterson in Weiss et al [7].

5

The "sub 1" is intended to denote the "first order" nature of this efficiency, both in terms of a reasonably uniform initial size and the limitation to concern with only primary fracturing. It is obviously an experimental simplification, but one which provides an interesting beginning to an ultimately much more complex study. At the same time, this simple definition also represents the limiting case of very good material transport which manages to sweep all fine material from the crushing zone before the next compression stroke of the walls.

One would expect bed efficiency so defined to vary with bed thickness, expressed as a multiple of particle size, and % compression of the bed. Efficiency should be 100% for a single-particle bed depth since each particle would be crushed essentially individually. It should decrease monotonically as bed thickness increases. As a function of % compression, η_{b1} should be zero or very low for small compressions, as the bed is deformed and compacted with little fracturing. It should then increase with continuing compression as more crushing occurs, and it is expected to decrease at high compressions as the accumulation of fine material (and the diminishing population of full-sized particles) inhibit further primary fracturing. Fig. 6 seems to confirm this latter behavior for beds of one inch and one-half inch depth (12.7 and 6.4 particles, respectively).^{*} Fig. 7, a typical force-deflection curve, seems to show three distinct zones corresponding to this behavior: a rising force as the bed is initially rearranged and compacted without much breakage, a surprisingly long zone of essentially constant stress as the bed behaves macroscopically as a plastic material while substantial breakage occurs, and an abrupt rising stress and falling efficiency as breakage ceases. On the other hand, the expected variation of efficiency with bed depth is not observed: the one-inch bed is significantly more efficient than the one-half inch. There is no explanation for this behavior at this time.

The other current work is investigating the possibility of size-dependent relative motion within the bed in an attempt to flush fine material from the crushing zone. Specifically, we are examining the term V_1 in the foregoing equation with the expectation that fluid transport will preferentially move fine material relative to larger material. Fluid discharge of fine material is used in some ball ring mills [9], with subsequent classification and recycling of oversize, but the present work is directed to size-dependent relative motion within the crushing zone itself. Preliminary results are very encouraging.

Consider crushing between oscillating vertical walls, with material carried upwardly between the walls by an upward fluid flow--in effect, an upside down jaw crusher. It was reasoned that, if the solid material could be "fluidized" by the moving fluid, smaller particles should move upward relative to larger ones because the smaller particles will have a lower terminal velocity relative to the fluid. In addition, if oscillating walls periodically clamp the solids in place, smaller particles, having a higher drag-to-mass ratio, will accelerate more rapidly. Both of these arguments are simplifications because of the major particle-to-particle interactions in dense fluidized flow, but the tendency for relative upward motion of finer material is clearly evident.

A simple experiment has verified this reasoning and demonstrated a remarkably effective size separation. A mixture of two sizes of spherical glass particles was placed in a vertical tube and fluidized by an upward flow of air. Fig. 8a shows the initial, reasonably uniform mixture of nominal 2 mm spheres (1.680 - 2.360 mm) and nominal .8 mm spheres (.707 - 1.190 mm). The smaller size was selected as the largest size would just fit within the interstices between the larger spheres (see Ding [10]). After a short period of fluidization, the sharp separation seen in Fig. 8b was accomplished.

^{*}The single-particle fracture energy used in these computations was from Larson [8] for particles of 1.7 mm diameter, so the actual efficiencies may be a little lower.

Fluidization in this simple experiment was accompanied by somewhat violent "boiling" of the solids with plugs of solid material separated by large (several tube diameters), upwardly moving "bubbles" of air. The added void fraction, with total volume perhaps 25 - 50% greater than that of the stationary solids column, would be excessive in a comminution device, but it is probably not essential for effective separation. Experiments will be undertaken with a high frequency pulsed flow on top of a low steady flow to agitate the pile without large overall translations. Agitation and periodic clamping from oscillating walls will also be of importance.

SUMMARY

Computer simulations of two-dimensional quasi-static bed behavior have provided insight into comminution mechanisms within particle beds. Work has now progressed to a study of material transport behavior within the bed, with attention to the generation and relative motion of fine material in the crushing zone. Early experimental results suggest that combined crushing and flushing of fine material from the crushing zone may be possible.

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a. 1.3 diameters compression

b. 1.4 diameters compression

Figure 1. Build-up and collapse of frictional load structures.

Figure 2. Bed energy storage and losses.

a. Maximum force criterion

b. Maximum shear criterion

Figure 3. Bed behavior for different particle failure criterion.

Figure 4. Stored energy as a function of displacement for different particle failure criteria.

Figure 5. Control volume for material flow.

Figure 6. Bed efficiency as a function of compression.

Figure 7. Stress-strain curve for one-inch bed.

Figure 8. Mixed bed before and after fluidized separation.

SYNTHESIS AND OPTIMIZATION
OF
INTEGRATED CHEMICAL PROCESSES

REPORT - TECHNICAL ADVISORY COMMITTEE

INEL/MIT ENGINEERING RESEARCH PROGRAM

OTHER TOPICS

Irven H. Rinard

July 18, 1990

Synthesis and Optimization of Integrated Chemical Process
(Evans)

This work has been underway for six years. Up til now the primary focus has been on synthesizing the utility and power networks required by a chemical process so as to maximize energy efficiency. The primary target for these efforts are world-scale commodity chemical plants with production rates in the range of a billion pounds of product per year. Since most of these processes make extensive use of energy-intensive separations such as distillation, the potential for energy conservation is substantial.

The approach to these problems, namely the formulation in terms of a mathematical programming problem, is not unique. In particular the work of Ignacio Grossman at Carnegie-Mellon comes to mind. However, the work by Evans and his students is of high caliber and the results are definitely of use.

So far this effort has produced three PhD's but only a small number of journal publications. However, there are several other papers in preparation so that one feels that the effort so far has been reasonably productive.

Recently, a new class of problems have been studied as part of these effort. These involve the optimal design and scheduling of batch processing plants. There is no particular emphasis on energy efficiency. Even if there were, the scale of these plants (1000 to 10,000,000 pounds per year more or less) makes the overall potential for energy savings much less than for their world-scale commodity-chemical cousins.

Finally, there appears to be not collaboration with INEL in this area of endeavor.

SYNTHESIS AND OPTIMIZATION OF INTEGRATED CHEMICAL PROCESSES

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1. INTRODUCTION

In the past twenty years there has been enormous progress in the development of computer-based methods for synthesis and design of chemical processes. These process plants are generally large and complex. The flowsheet for a typical process is shown in Figure 1.

By developing more efficient manufacturing processes, the U.S. has maintained world leadership and the chemical industry, today, is one of the few segments of American industry with a large favorable balance of trade. The chemical industry is also one of the largest consumers of energy in the country. It is, therefore, important that the industry maintain its leadership position in developing new chemically-based manufacturing processes and in retrofitting existing plants.

Most of the computer-aided engineering methods have been developed for the synthesis and design of continuous plants. These plants are used for large-scale manufacture of commodity products, such as ethylene and ammonia. Today, no major commodity plant would be designed without first simulating it on the computer.

Figure 1. Example of a Petrochemical Process with Heat Integration.

The development of techniques for computer-aided chemical engineering fall into three areas: analysis, optimization, and synthesis. The role of these three tasks is shown in Figure 2.

The goal of computer-aided analysis is to predict the performance of a proposed or existing plant. The input to such an analysis is a description of the process flowsheet and values of all of the design and operating parameters. The performance of the plant is calculated using rigorous mathematical models to carry out the heat and material balances. Existing commercial computer programs such as ASPEN PLUS (Aspen Technology, Inc., 1988), DESIGN II (ChemShare Corporation, 1988), and PROCESS (Simulation Sciences, Inc., 1988) are now widely used in industry to perform this task of flowsheet simulation.

Optimization is at a higher level than analysis. In any proposed flowsheet, there are many degrees of freedom in the selection of design and operating parameters. There are tradeoffs in the proper choice of values for the parameters. Optimization, whether done manually by conducting a series of case studies or automatically using a mathematical programming algorithm, seeks to balance these competing forces to maximize an objective function such as profit.

Before optimization can be performed, it is necessary to know the structure of the flowsheet. The conception of the structure of the manufacturing process is a task in process synthesis. The field of process synthesis has received much attention in the past decade. Our work under this grant has dealt with an important class of problems in the field focussing on the effect of heat and work integration on the synthesis of process plants.

The philosophy underlying our work has been that the role of the university is to develop generic methodologies for solving problems of industrial importance. These methods can be demonstrated using prototype software on problems typical of those encountered in industry. The result is

Figure 2: Role of Process Synthesis, Optimization and Analysis

improved understanding and insight into the nature of the problem and the development of better algorithms for solving problems. The knowledge produced from this research, then establishes the technology base that industry can use to produce industrially useful software systems to solve problems in a production environment.

The vast majority of previous research in computer-aided chemical engineering has dealt with continuous processes. As much of the U.S. industry is turning its attention to the manufacture of higher value specialty products, it is important to begin developing computer methodologies for the synthesis of batch and semi-continuous processes used to manufacture these products.

RESULTS TO DATE

Our work, since the beginning of the Project in 1985, has focussed on developing improved methodologies for the synthesis of heat and work integration systems in process plants. A typical plant of the type shown in Figure 1, such as a petroleum refinery, a petrochemical plant, or a paper mill, requires energy in the form of heat to raise the temperature of process streams and in the form of work to drive pumps and compressors and meet other mechanical energy needs. The goal of heat and work integration is to reduce this external energy requirement through better process integration. For example, the heating requirement can be reduced by allowing hot streams that must be cooled to exchange heat with cold streams that must be heated. Also, the process itself can be used to generate mechanical energy by introducing heat engines.

The objective of this research has been to develop computer-based methods to help engineers synthesize a process with improved energy integration. The strategy has been to combine modern mathematical programming techniques, sophisticated rigorous models of the process utilities system and heat recovery network, and heuristic methods to develop an overall methodology that is more powerful than traditional approaches. Although the field of process synthesis has been the subject of active research in chemical engineering over the past decade, most work reported in the literature has dealt with idealized systems. The focus of our work has been to develop algorithms that deal with constraints and nonidealities that characterize industrial processes. The objective has been to develop new generic methods and to demonstrate them with prototype software. Methods and programming techniques of artificial intelligence have been used where appropriate. The net result of the research has been an improved understanding of the nature of the problem of energy integration in process plants. The methods developed will help engineers solve realistic industrial problems.

Three doctoral theses have been completed on the project, Wilcox (1985), Viswanathan (1989), and Yoon (1990). The publications that have resulted from this work are listed at the end of this section.

Richard Wilcox's thesis, completed in 1985, dealt with the synthesis of heat and power systems in chemical plants. He established a general framework for looking at the problem of heat and work integration. He developed an algorithm for identifying the best places in a process from the standpoint of energy integration where pressure changes should occur. He also considered methods for analyzing the structural resilience (operability) of heat exchanger networks, and developed a new method, based on the transportation model formulation, for estimating the minimum utilities target in a plant with match-dependent constraints.

The goal of Murali Viswanathan's thesis, completed in 1989, was to develop improved methods to synthesize heat exchanger networks for constrained and nonideal chemical processes.

In many plants, certain heat exchange matches are forbidden because of safety or because the streams are located far apart in the plant. In the thesis, new problem formulations based on the transshipment and transportation models of operations research were developed to determine targets for the minimum utilities cost, the minimum number of heat exchanger units, and the minimum capital cost of the heat exchange equipment. The new formulations apply both to constrained and unconstrained problems.

The presence of a constraint will generally result in an increase in the minimum utilities, minimum units, or minimum heat exchanger surface required. A systematic methodology was developed to analyze the possibility of minimizing the consequences of forbidden match constraints. This is based on the use of one or more process streams to behave both as a hot and cold stream (dual stream). The net result was the discovery of new, hitherto unknown, lower cost heat exchange network structures. The strategy can be extended also to deal with preferred and restricted matches.

Synthesis and Optimization
of
Integrated Chemical Processes

Principal Investigator
Lawrence B. Evans

Presentation to
Technical Advisory Committee
and
Proposal Review Panel

July 17, 1990

We are proposing a major redirection of the project.

From: Synthesis of Heat and Work
Integration Systems

To: Synthesis and Optimization of Batch
and Semi-Continuous Processes

Figure 1. Example of a Petrochemical Process with Heat Integration.

The vast majority of previous work in computer-aided chemical engineering has dealt with continuous processes to manufacture bulk commodity products.

It is important now to begin developing computer methodologies for synthesis of batch and semi-continuous processes used to manufacture higher value specialty products.

Figure 2: Role of Process Synthesis, Optimization and Analysis

Philosophy

The role of university systems research is to develop generic methodologies for solving problems of industrial importance.

Publications from this Research

Theses

Wilcox, R. J., "Synthesis of Heat and Power Systems in Chemical Plants," Ph. D. Thesis, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, June 1985.

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Barrera, M. D. and L. B. Evans, "Optimal Selection of Equipment Units for Batch Processes," presented at the AIChE Annual Meeting, San Francisco, November 1989.

Sundaram, S. and L. B. Evans, "Synthesis of Batch Distillation sequences," presented at the AIChE Annual Meeting, San Francisco, November 1989.

Viswanathan, M. and L. B. Evans, "Simultaneous Optimization and Heat Integration of Chemical Processes in the Presence of Constraints," presented at the AIChE Annual Meeting, San Francisco, November 1989.

Publication Strategy

Publications in Preparation/Submission

Viswanathan and Evans, "Heat exchange Networks with Dual Streams"

Viswanathan and Evans, "Simultaneous Process and Heat Recovery Network Optimization with Constraints"

Yoon and Evans, "Optimal Placement of Heat Pumps and Heat Engines"

Yoon and Evans, "Simultaneous Synthesis of Plant Utilities System and Heat Recovery Network"

Barrera and Evans, "Optimization of Batch Processes"

Barrera and Evans, "Techniques for Solution of the Structure Subproblem,"

Sundaram and Evans, "Optimal Operation of Batch Distillation,"

Helget and Evans, "The Computational Architecture for a Next Generation Dynamic Simulator."

Murali Viswanathan's PhD Thesis

Goal: To develop improved methods to synthesize heat exchanger networks for constrained and nonideal chemical processes.

1. Development of targets for minimum utilities, minimum number of heat exchanger units (matches) for constrained networks.
2. Identification of heat exchange network structures involving *dual streams* that can serve as both hot and cold streams to overcome constraints and result in lower-cost networks.
3. Handling of non-point utilities that go through a temperature change.
4. Establishment of surface area targets in the presence of constraints and non-uniform heat transfer coefficients.
5. Use **of** area targeting to resolve tradeoffs **between** operating and capital cost on using dual streams.
6. Optimization of the process simultaneously with the heat exchange network in the presence of constraints.

Hyung Yoon's PhD Thesis

- Goal:** To develop methodologies that consider the effect of work interactions for a process that produces or requires significant amounts of mechanical energy.
- Previous work:** assumed plant utilities system was fixed, hot and cold utilities were available at fixed utility levels and specified cost.
- Result:** Development of a methodology to simultaneously synthesize the utility plant with the heat recovery network.
- Approach:** Use heuristics to identify alternative temperature levels for utilities and locations of heat pumps and heat engines.
- Place the alternatives in a superstructure and use MILP to select units in the optimum network.

Batch and Semi-Continuous Processes

Figure 3: Example of a Flowsheet for a Batch Process

Types of Process Units in a Non-Continuous Plant

1. Continuous units operate at steady-state and are characterized by their processing rate. Continuous units operate all the time except for occasional shutdowns for maintenance. Because they are always operating, continuous units must be preceded and followed by intermediate storage tanks in order to interact with the other units in a non-continuous system.

2. Semi-continuous units also operate at steady-state while they are running, but they do not run all the time. An example is a feed pump to a batch reactor. The pump operates only during vessel filling and is shut down for the remaining part of the operating cycle.

3. Batch units are characterized by their size or volume. Batch units have distinct filling, processing, draining, and preparation (e.g., cleaning) segments to their operating cycles. No mass crosses the unit boundaries during the processing step. The average processing rate for a batch unit is determined by dividing the batch size by the total unit cycle time.

4. ~~Semi~~-batch units are the same as batch units, except that mass may cross the ~~system~~ boundaries during the processing step. A fed-batch fermentor operates as a semi-batch unit because nutrients are fed during the fermentation part of the cycle.

The Batch Process Design Problem

A new product has been developed by the chemist in the laboratory and it is desired to make a larger quantity of the product for market testing and evaluation. The product will usually be manufactured in an existing batch plant.

Questions:

1. How will the product be made in the plant?
2. How much will it cost?
3. How soon can it be produced?

Unique Aspects for Synthesis and Optimization

1. The processes are inherently dynamic in nature. Unsteady heat and material balances are described by systems of nonlinear differential and algebraic equations, whereas continuous processes are mostly described by algebraic equations.
2. Batch manufacturing is usually done in an existing plant using standard equipment in the plant. Therefore, the design consists of selecting which equipment from inventory will be used.
3. The location of intermediate storage is an important consideration. There are four policies (unlimited, finite, and no intermediate storage and zero wait).
4. Scheduling must be considered.

Storage Policies for a Non-Continuous Process

1. Unlimited Intermediate Storage (UIS). This is an idealized case where the interstage storage is effectively infinite in size. The size of the storage does not impose any constraints on the operation of the process.

2. Finite Intermediate Storage (FIS). In this case, the storage size is bounded. The limitation might impact on the operation of the system. This case is probably the most common situation in practice.

3. No Intermediate Storage (NIS). In this case there is no storage between stages. The upstream unit can only discharge its batch when the downstream unit is available. Thus, the upstream unit may have to serve as its own storage tank while the downstream unit finishes the previous batch. While waiting, the upstream unit is prevented from starting the next batch. A NIS case might arise when successive batches cannot be mixed. For example, batches of pharmaceutical products might be processed with NIS for reasons of purity and quality control.

4. Zero Wait (ZW). In this case, the batch in the upstream stage cannot wait for a downstream unit to become ready. Thus, the upstream unit can not serve as its own storage tank. The upstream unit must not start processing the current batch until it is certain that a downstream unit will be ready when the upstream unit finishes. An unstable reaction mixture that must be quenched immediately is an example of a ZW case.

Figure 4: Gantt Chart Showing Schedule of Operation for a Two-Stage Process Processing Two Batches each of Products A and B

Steps in Batch Process Design

The starting point is the recipe that the chemist has devised for making the product in the laboratory. This recipe should be revised as necessary so it is suitable for making the product at the larger scale. The remaining steps are:

- (a) Assign recipe tasks to stages of processing, i.e. to types of equipment units.
- (b) Select values of the operating variables and times for these tasks.
- (c) Select or size all equipment units and determine the number in parallel for each stage.
- (d) Locate and size intermediate storage (if any).

Research Problems to be Addressed

1. What should be the computational architecture to solve the problem of dynamic simulation inherent in batch process modeling?
2. What is the best approach to solving the problem of optimizing batch process design and operation?
3. How should the batch process synthesis problem be formulated and solved?

Important Criteria for a Next-Generation Dynamic Simulator

1. Models of the individual elements of the flowsheet should be in modular form and generalized for any chemical system.
2. The system should be able to use existing software to compute physical properties efficiently.
3. The system should be able to incorporate existing dynamic models that are already programmed.
4. The system should take advantage of parallel computing architectures, but the code should not require it.
5. The system should be able to handle large flowsheets.

Strategy for Batch Process Optimization

Approach:

Partition the decision variables into two sets:

- (1) Performance variables consisting of operating times and operating variables, and
- (2) Structural variables that determine which equipment units and storage tanks are to be used at each stage.

The performance subproblem (fixed structure) has continuous decision variables.

The structure subproblem (fixed performance) has discrete variables.

The goal of the research is to develop solution strategies for solving each subproblem and the two together.

Batch Process Synthesis

Main Tasks:

1. Representation -- determining the general structure of the separation system.
2. Evaluation -- use appropriate models to evaluate and compare alternatives.
3. Strategy -- developing a model for systematically generating alternative structures for evaluation.

Figure 5: Distillate Composition Profiles for Separation of a Three-Component Mixture of A, B, and C by Batch Distillation

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