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ANNUAL REPORT ON THE COLLABORATIVE PROGRAM OF RESEARCH IN ENGINEERING SCIENCES

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**Energy Laboratory of the
Massachusetts Institute of Technology**

**in collaboration with
Idaho National Engineering Laboratory**

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MASTER

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INTRODUCTION

In 1985, the Energy Laboratory of the Massachusetts Institute of Technology (MIT) and the Idaho National Engineering Laboratory (INEL) began a collaborative program of energy-related engineering research. This program was extended for another three years starting in January 1991. The program continues to pursue three broad goals: to perform quality research on energy-related technologies involved in industrial processes and productivity; to demonstrate the potential of collaborative programs between universities and the national laboratories; and to encourage the transfer of the technology developed to the industrial sector. This annual report describes progress at MIT under the MIT/INEL program during the past year.

RESEARCH PROGRESS SUMMARIES

Highlights of research activities and accomplishments during the past year include the following:

Modeling and Control of Droplet Based Thermal Processes: Multivariable Control of Gas-Metal Arc Welding

In previous work, a basic approach to the problem of control of welding processes using multivariable adaptive control theory was established and a set of non-stationary process transfer functions for both the thermal and geometric aspects of the process, capturing the non-linear dynamics and statics, were developed. In addition, depth estimators based on real-time inverse heat transfer solutions and surface temperature measurements have been developed.

However, it has become increasingly apparent through the modeling and experiments, that the process has insufficient latitude to respond to realistic disturbances in a multivariable fashion. In particular, the heat and mass transfer processes involved are far too coupled to allow independent regulation of weld geometry or thermal properties. Accordingly, process modifications to enhance the "reachability" of the process, including transverse and longitudinal high frequency weaving of the heat source to vary the input heat distribution, are being developed.

In current work, this problem of three-dimensional heat distribution control is being generalized using both a distributed parameter control theory and a novel heat source design. While many simplistic inverse heat transfer and distributed parameter control research efforts have been reported, none deal with the problem in the face of variable geometries and high degrees of model uncertainty. Efforts in this are focussed on just such uncertainties and on realistic geometries.

Finally, a new welding process that seeks to decouple heat and mass transfer by using a stream of superheated filler material to both heat and fill the joint has been developed. This "stream welding" process relies upon very precise control of the temperature and flow rate of the metal stream. This control is achieved by a novel continuous-flow arc furnace that has a small thermal mass, thereby allowing rapid temperature changes in the filler material. Preliminary tests with this apparatus are now underway.

Metal Transfer Control in Gas-Metal Arc Welding

The objective of this project is to find new control methods to improve metal transfer in gas metal arc welding -- a widely used manufacturing process. A lumped-parameter mathematical model of the system is being developed with the goals of being suitable for real-time control system design, yielding additional physical understanding, and being readily usable by researchers and engineers.

A novel gas metal arc welding experiment, which modifies the fundamental way metal is transferred in the welding process, has been designed and constructed. The experiment uses mechanical energy as a new control input to the welding process. The metal electrode is vibrated axially during welding at the desired frequency of drop detachment in order to force the detachment of metal drops. The experiment is being used to explore new modes of metal transfer and for testing algorithms for detecting and controlling these modes.

The mathematical model being developed captures the instantaneous dynamics of drop detachment. Hitherto, dynamic electrode melting models have only sought to capture the average of the process. The model being developed in this project captures the instantaneous geometric evolution of drops melting on the end of an axially moving electrode. This model also has potential uses for droplet systems other than welding.

Fundamentals of Elastic-Plastic Fracture: Three-Dimensional and Mechanistic Modeling

A methodology for predicting constraint-sensitive plane strain ductile fracture in engineering structures is being developed. At low toughness, the elastic T-stress and K provide a rigorous and straightforwardly calculable two-parameter fracture mechanics. Applications include pressurized thermal shock. At loads giving moderate to large-scale yielding, a modification to the standard effective crack length formulation accounting for effects of T-stress on plastic zone size gives simple and accurate estimates of J, compliance, and crack tip constraint based solely on elastic K and T calibrations. In fully plastic cracking of low to moderate strength structural metals, asymptotic elastic-plastic crack tip fields fail to dominate the strain over microstructural length scales, suggesting the utility of rigid/plastic models. Such fully

plastic cracking is based on limit analysis and a micromechanical model of crack tip opening angle that is sensitive to constraint and an effective slip angle at the crack tip. The corresponding material constraints are being determined from bending and tension tests of both standard and novel design.

All of these models are being incorporated into line-spring finite elements for surface-cracked plates and shells, providing simple and extraordinarily accurate analysis and simulation of these important engineering flaws.

Comminution of Energy Materials

Comminution of energy materials is energy intensive; one of the principal sources of inefficiency in many classes of devices is the presence of excessive fines within the coarse medium. The fines cause an unwanted shielding of the coarse medium and impose multiple passes on the feed (e.g., roller tables, ball mills) resulting in frictional losses. This study investigates the mechanics of rapid fines removal to provide design criteria for a new generation of comminution machines with a significantly elevated comminution efficiency.

It is well known that dense, size-distributed particulate media have a natural tendency to segregate in the presence of flow and gravity, although these effects remain poorly characterized and are typically viewed as a hindrance. Here, the aim is to understand and incorporate these phenomena to improve comminution efficiency. Using a cylindrical rotary crusher, the research studies particle segregation by means of unsteady fluidization in vertical and near vertical configurations. In the conceptual device, the time scale of the unsteadiness in the period of rotation. The goal is to achieve full separation in minimal time to accommodate a large and efficient comminution throughput.

Experiments have been conducted with bidisperse mixtures of silica spheres (50-3000 micrometers in diameter) in water with impulsively started fluidization. The results of numerous experiments are summarized with the following observations:

- segregation of bidisperse mixtures can be achieved with impulsive fluidization, even for systems in which the fines are sufficiently large to prevent their percolation through the coarse matrix. It has been found that separation critically depends on the initial formation of an upward-propagating pocket within which segregation occurs: coarse particles rain down through it, while fines remain fluidized, leaving a fines-free bed of coarse particles below. Segregation is markedly reduced in the absence of this structure.
- the limiting factor to the speed of segregation and hence fines throughput is the speed of the leading edge of the pocket. This interfacial speed is directly

linked with the rate at which coarse particles can become detached from the above binary dense-pack. The present work is addressing the mechanics of this process theoretically and experimentally.

The program aims to develop the theoretical base of understanding for particulate segregation phenomena in a variety of configurations to help improve processes in which segregation is either desired, as it is here, or unwanted, as in mixers for example.

Synthesis and Optimization of Integrated Chemical Processes

The goal of this research program is to develop new systematic methods for the synthesis and optimization of chemical processes. As the chemical industry is one of the largest consumers of energy in the US, it is important to find efficient and creative computer-aided design strategies for developing new manufacturing processes, and retrofitting existing plants.

The general philosophy of this research is to develop, in an university environment, innovative generic methodologies for solving problems of industrial importance. These methods are then demonstrated by using prototype software to solve problems typical of those encountered in industry.

Research is currently considering two topics. A long term program that focusses on synthesis techniques for achieving increased energy efficiency through better heat and work integration is culminating with an investigation of the simultaneous synthesis and optimization of the chemical process, its heat exchange network, and the utility system. Secondly, a new initiative is addressing the need for process design and optimization technologies for batch/semi-continuous processes. Such processes are of increasing industrial importance for the manufacture of high value-added specialty products and pharmaceuticals, which have relatively short product life cycles. Research is therefore focussing on the development of computer-aided design tools for rapid and efficient process development.

PROGRAM MANAGEMENT

Management of the program rests with a program manager from each of the two institutions. The INEL Program Manager, Dr. Donald Keefer, coordinates the INEL research program which is administered through the Idaho Operations Office of the Department of Energy. The Principal Investigator of the MIT Program is Prof. David Hardt, assisted in day-to-day management by Dr. Elisabeth Drake. The INEL and MIT Program Managers interact with each other and with a program monitor in the Office of Basic Energy Sciences, Division of Engineering and Geosciences, Department of Energy.

Because the program entails objectives which go beyond the research results normally expected in such an effort, a committee system has been established to ensure that all objectives are met. Technical Advisory Committees, consisting of experts in the various fields of research, attend an annual overall program review meeting to assess the technical progress of the projects, as well as to evaluate program direction and management. [Reviews are held at alternate years at MIT and the INEL. The 1993 review was held at INEL.] The Committees provide both oral and written reports of their findings to the Program Managers. The DOE program monitors also attend the oral presentations. The written reports are subsequently transmitted to the Principal Investigators of each project. Views expressed by the Committees are taken very seriously and frequently serve as a basis for changes in research techniques, new avenues of approach, and altered management procedures. Membership of the Technical Advisory Committees, as of July 1993, is shown in Table 1.

A Steering Committee, consisting of representatives selected from the Technical Advisory Committees, has the charter of reviewing research progress, program management, quality of inter-laboratory collaboration, responsiveness to industry's long term needs, and potential new research areas. In addition, technology developed in the program is examined for appropriateness for transfer to industry. The Steering Committee is intended to identify candidate technology and establish mechanisms for transfer to industrial use. It also provides a forum in which MIT and INEL Principal Investigators and industry representatives can interact directly to assist in achieving program goals. Steering Committee members, as of July 1992, are indicated by a "*" in Table 1.

TABLE 1. TECHNICAL ADVISORY COMMITTEES
(as of July 1993)

Sensing and Control of Droplet Based
Thermal Systems

Mr. Howard B. Carey
Hobart Brothers Company

Dr. Hugh Casey*
Los Alamos National Laboratory

Dr. George E. Cook
Vanderbilt University

Mr. Richard Morris
David Taylor Research Center

Prof. David Olsen
Colorado School of Mines

Dr. Paul W. Ramsey
Ramsey and Associates

Synthesis and Optimization of Integrated
Chemical Processes

Prof. Lorenz T. Biegler
Carnegie Mellon University

Fracture Mechanics/Comminution/NDE

Dr. John Gudas
David Taylor Research Center

Prof. John B. Ketterson
Northwestern University

Prof. Robert McMeeking
University of California at Santa Barbara

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

Dr. Sam S. Palusamy*
Westinghouse Electric Corporation

Dr. Edward Zywick
Lawrence Livermore Laboratory

* Steering Committee Member

Modeling and Control of Droplet Based Thermal Processes: Multivariable Control of GMAW

Principal Investigator
David E. Hardt
Research Associate
Jae-Bok Song
Steven Lee
Christopher Ratliff
Uppendra Ummethala

Progress Report for the Year Jan. 1, 1993 - Dec. 31, 1993

Abstract

Work on Multivariable Control of Gas-Metal Arc Welding during this period has concentrated on three main topics: the development of the process herein called "stream-welding" to permit greater decoupling of the heat and mass transfer, a beginning effort to develop a more fundamental understanding of the basic temperature distribution control problem presented by welding, and finally the preparation of a cooling rate/fill experiment to permit comparison of INEL intelligent control approaches and our own adaptive control methods.

The Coupled Output Problem

Our previous work has demonstrated the highly coupled nature of welding outputs during conventional GMAW (for a summary see Hardt, 1992). In particular the outputs of width, depth, fill, heat affected zone and centerline cooling rate tend to be closely coupled even for significant variations of inputs such as wire feedrate and travel speed. This arises from the distributed nature of the heat diffusion as well as the coupled mass and heat transfer from the welding torch. In our earlier work we began to address this problem with the two torch and scanned torch work of Doumanidis and Hardt(1990), and the high frequency weaving in Masmoudi and Hardt(1992).

In the current work we are looking at more fundamental approaches to this problem looking both at the welding source and the basic heat diffusion problem, the latter from a distributed parameter control perspective.

• Stream Welding

Last year we began examining process modifications that completely decouple the base material heating from the filler material heating, and further attempted to control droplet production and placement. In particular we were exploring the concept of "spray welding" whereby the filler material and the welding heat is provided by superheated metal droplets. The concept was based on existing patents (Singer, 1986) and a new process developed at MIT by Prof. Jung-Hoon Chun at MIT Passow and Chun, 1991) capable of producing drops of very uniform size and heat content.

The basic concept was to precisely control the heat content of the filler material and its flowrate as well. In addition, these two could be changed independently. The heat transfer problem involved in splatting droplets is quite complex and not yet solved in the literature (see Lee, 1993) therefore

we have taken an empirical approach to this part of the research. This means that a source for molten material at a precise temperature that could also produce a continuous stream of droplets is required. Since we also wanted to minimize the amount of additional heat needed to produce the weld, the ability to considerably superheat the metal was necessary.

Accordingly, a small volume (about 3 cc) arc furnace was designed that permits continuous replenishment of the metal using a conventional metal feed system controlled by the reservoir height. The temperature of the reservoir is likewise controlled by varying the arc current in an closed-loop fashion based on a thermocouple measurement of the metal temperature. The molten material is then ejected from the bottom of the crucible. A patent disclosure for the device has been filed with MIT, owing to the novel combination of small metal mass (permitting rapid temperature changes) and the feedback systems permitting crucible fill and temperature regulation.

A working version of this furnace has been constructed and is undergoing initial tests, and is shown in Fig. 1. Details of the construction and some performance data is found in Lee (1993). The design temperature is 2200°C, so that steel can be superheated, however, the highest temperature achieved to date is 1700°C owing to limited current in the existing power supply.

Fig. 1 Cross Section of the High Bandwidth, Continuous Flow Arc Furnace Used for Stream Welding

At present the feedback loops for active control of this furnace are under test, however, using a single charge of tin (to keep initial temperatures low) simple stream welding tests have been performed, and excellent sidewall penetration was observed in simple vee groove welds.

Lastly, we have for now abandoned the concept of spraying in favor of leaving the exit stream from the furnace unperturbed. Thus the metal fills the weld in a continuous stream, provided it is not far from the exit to the weldment. Thus the name "stream welding".

• Distributed Parameter Control Problem

One of the most basic inputs in welding is the heat distribution from the source, be it arc, laser or other high flux density source. In prior work we have attempted to vary the input distribution to the weldment by moving the torch longitudinally or transversely during welding. In this work we have begun considering the general problem of controlling any type of a heat input distribution to create a desired *temperature distribution history* throughout the volume of the weldment.

An initial exploration of the literature shows that while some work has been done in the basic mathematics of describing three-dimensional heat diffusion both as an inverse heat transfer problem and as a distributed parameter control problem, there is no published work that treats the general problem of high-bandwidth tracking control of two- or three-dimensional heat transfer in solids with complex shapes and with variable boundary conditions. It is this problem to which this work is addressed.

Initially we have explored classical distributed parameter control theory as a means of controlling two-dimensional and three-dimensional temperature distributions. Such efforts assume basic parabolic equations and attempt to devise control laws based on these descriptions. However, such approaches are applicable only to highly idealized sources, measurement and simple geometries, and it is anticipated that they will not be directly applicable to the problem at hand.

To date we have concentrated on two approaches. The first is modal decomposition of the heat transfer equations, which permits rapid solution of the terminal distribution problem, but cannot deal with complex geometries or variable boundary conditions. In the second we have developed a straightforward finite difference approach that treats the nodes as states in a large dimension state variable problem. When treated as a linear problem this allows simulation of the two and three dimensional problem, but is not very useful for analysis.

Comparison of Intelligent and Adaptive Control Methods

At MIT we have concentrated on the use of adaptive control methods, typified by use of a linear system identifier running continuously, and tuning of the controller continuously based on this identification. An alternative method is being developed at INEL, that uses fuzzy linguistics and non-linear (neural networks) for the same task. In this task we have been developing a standard experiment to compare these two methods. The problem is simultaneous control of cooling rate and fill, a problem addressed by Einerson et al (1992) at INEL. To date we have developed the hardware for such an experiment, and have completed initial modeling experiments identifying the control latitude of the process.

Proposed Plans for the Year Jan. 1, 1993 to Dec. 31, 1993

For the stream welding task, it is planned to work up to steel welding, and to conduct an exhaustive set of welding test, with and without weldment heating, to determine the basic characteristics of welds made this way. Inevitably improvements to the arc furnace will be required, and one goal will be to reduce the ultimate size of the furnace to make it possible to use in more typical welding situations. In addition we will want to maximize the bandwidth of the furnace to permit rapid changes in the stream temperature during welding.

The thermal control task will pursue characterization of the basic resolution the process based on the source and heat transfer properties of the weldment. This will allow us to establish the degree of control possible in a given welding situation. This will include maximum gradients, rates of change in temperatures, and ability to estimate temperature distributions internal to the weldment.

In addition we will conduct a canonical experiment controlling temperature distribution in a 2D solid with a rapidly scanned GTAW torch as the source. Both thermocouples and IR measurements will be made, the former in internal points and the latter on external surfaces.

Finally, it is expected that the intelligent control - adaptive control comparison will be completed this year, with the implementation of first a simple linear control scheme, followed, by a linear adaptive methods, and finally by the intelligent control method of Einerson et al (1992).

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• Recent Publications

1. Masmoudi, R. , and Hardt, D.E., " High-Frequency Torch Weaving for Enhanced Process Controllability: Effect on Coupling of Pool Width and Heat Affected Zone Width" *Proc. Third International Conference on Welding Research*, ASM, Gatlinburg, June, 1992.
2. Hardt, D.E., "Welding Process Modeling and Re-Design for Control" *Proc. 4th US/Japan Symposium on Flexible Automation*, San Francisco, July, 1992.
3. D.E. Hardt, M. B.Hale, "Multi-Output Process Dynamics of GMAW: Limits to Control", *Proc. Third International Conference on Welding Research*, ASM, Gatlinburg, June, 1992.
4. Hardt, D.E., Eagar, T.W., Lang, J.H., and Jones, L., "Welding Process Decoupling for Improved Control", *Proc. 12th BES Conference. Department of Energy*, Argonne, May, 1993.
5. Song, J.B., and Hardt, D.E., "Adaptive Control of Weld Geometry in GMA Welding", *Proc. American Control Conference*, San Fran. June, 1993.
6. Song, J.B., and Hardt, D.E. "Adaptive Control of Gas Metal Arc Welding" to be published, *ASME J. of Dynamic Systems Measurement and Control*, 1993.
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Metal Transfer Control in Gas Metal Arc Welding

PERSONNEL

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ABSTRACT

The objective of this project is to find new control methods to improve metal transfer in gas metal arc welding -- a widely-used manufacturing process. A lumped-parameter mathematical model of the system is being developed with the goals of being suitable for real-time control system design, yielding additional physical understanding of the process, and being readily usable by researchers and engineers.

A novel gas metal arc welding experiment, which modifies the fundamental way metal is transferred in the welding process, has been designed and constructed. The experiment uses mechanical energy as a new control input to the welding process. The metal electrode is vibrated axially at the desired frequency of drop detachment while welding to force the detachment of metal drops. The experiment is being used to explore new modes of metal transfer and for testing algorithms for detecting and controlling these modes.

The mathematical model being developed captures the instantaneous dynamics of drop detachment. Hitherto, dynamic electrode melting models have only sought to capture the average of the process. The model being developed in this project captures the instantaneous geometric evolution of drops melting on the end of an axially moving electrode. This model has potential uses for droplet systems other than welding.

GOALS

Our research is part of the MIT/INEL collaboration on sensing and control of droplet-based thermal processes. This collaboration is attempting to improve arc joining processes by using new control techniques such as "intelligent" control and by finding new arc processes that are more controllable than those currently available.

The objective of our portion of this effort is to find new control methods to improve electrode to base plate metal transfer in gas metal arc welding -- one of the most widely used arc welding processes. Central to our efforts is the development of a mathematical model of the physics of the metal transfer process with the goals of this model (1) being suitable for real-time control system design, (2) yielding additional physical understanding of the process, and (3) being readily usable by other researchers and engineers.

Additionally, through experimental work, we are pioneering the combination of advanced real-time control techniques with new welding process modifications in order to further develop the mathematical model, a control system, and possibly realize a commercially viable new welding process. Such a new process may yield decreased energy use, increased operator safety, decreased environmental impact, and improved quality and productivity.

PROGRESS

After initial test during the summer of 1992, we implemented additional sensors and software features in our electrode vibration welding equipment during the fall of 1992. The features were in preparation for quantitative experiments to study the behavior of this new process. In particular, we implemented circuitry to coordinate the high-speed video system with the DSP control system. Also, the software capability to collect 20 channels of data, 4000 points deep, at the system sampling rate (typically 2 kHz) was implemented.

Initial results using our experiment show that it is possible to greatly affect the metal transfer process. For example, using 1/16" electrode wire, it is possible to accelerate drops off the electrode of a size that are only seen above 300 amps in normal welding with only 200 amps. Additionally, we have found that using vibration makes it possible to maintain a stable arc at much lower currents. This result is a consequence of not allowing large drops to form on the end of the electrode. We have observed the formation of the drop using laser backlighting and a high-speed (> 1000 frames/sec) video system.

The spring and summer of 1993 were devoted to developing a dynamic model to predict the detachment times and accelerations of drops as they are shaken off the end of the electrode, so that it will be possible to predict when the vibration frequency and amplitude are properly tuned for one drop emitted per vibration pulse. The model has the form of a damped nonlinear spring-mass system. We would like to emphasize that the geometry captured by this model is useful for other processes where drops are being driven off a solid surface. In welding, the forces acting on a deforming drop are somewhat complicated and we have derived several new analytic expressions for these forces from first principles.

We model deformations of the drop as being ellipsoidal or some combination of ellipsoids and hyperboloids. The dynamics of the drop concern only the center(s) of mass of the shapes and, thus, the shapes are not truly self-consistent. That is, the forces are

determined using the shapes, but the shapes are directly determined by the continuum of forces in the drop. This approximation is necessary as a continuum approach would result in complicated sets of nonlinear partial differential equations that would be too time-consuming to solve for the type of model we are constructing.

The nonlinear dynamic equations are of the form:

$$\dot{m} = M(\tau)$$

$$\dot{V}_u = (F_{ext1} + F_{int1}) / m_u$$

$$\dot{z}_u = V_u$$

$$\dot{V}_l = (F_{ext1} - F_{int1}) / m_l$$

$$\dot{z}_l = V_l$$

The states defined here are total drop mass, upper center of gravity (cg) velocity, upper cg position, lower cg velocity and lower cg position. During some periods of time, there is only a single cg. The primary "external" forces acting on a welding drop are gravity, the drag of the arc plasma flowing past the drop, a magnetic body force due to the welding current, and interfacial tension when the drop is detaching. "Internal" forces include the changing surface energy and viscous energy loss in the drop as it deforms.

As the drop deforms along axis of symmetry z , the surface tension force can be computed as:

$$F_s = -\sigma \frac{dA}{dz}$$

where σ is the coefficient of surface tension and A is the surface area of the drop.

Assuming only irrotational flow in the drop, the viscous force simplifies with no further approximations to:

$$F_v = -\frac{64}{9} \pi \eta \frac{a^2}{C} (v_u' - v_l)$$

where η is the first coefficient of viscosity and a is the ellipse dimension in the x direction. Lifting the assumption of irrotational flow is a challenge we wish to pursue in the future.

Computation of the body force generated by the current flowing through the drop is subject to a number of assumptions. In particular, it is necessary to assume some current density profile along the surface of the drop. Experimental measurement of this current density is very difficult and results are not available in the literature. Assuming a density, the magnetic stress tensor can be integrated throughout the volume of a drop. Unfortunately, this operation produces elliptic line integrals of the second kind and so it is impossible to report an analytic solution here, other than to say that the force is of the form:

$$F_m = \mu_0 \pi J(S) P(S)$$

where $J(S)$ is the surface current density as a function of the surface S and $P(S)$ is a purely geometric coefficient. This body force is applied to the cg of the drop even though it is a distributed body force acting on the fluid. The computation of the line integral for this force at each time step slows our simulation and we hope to find suitable approximations of it. We note that our analytic solution for the magnetic force in a deforming ellipsoid correctly reduces to the known analytical solution of the spherical case.

We have implemented this drop simulation using Matlab m-files which are somewhat slow, but highly portable and thus easily shared with other researchers and engineers. It has been our experience that the results presented for many process models are difficult to reproduce due to relatively non-portable implementations and insufficient reporting of parameters and techniques. We are striving to contribute portable and useful models to the control community.

At the time this document is being written (August 1993), the initial simulation development is almost complete. Comparisons with results obtained with the vibration experiment will be first presented at the peer review in March 1994.

PROPOSED PLANS FOR THE YEAR JAN. 1, 1994 - DEC. 31, 1994

In 1994, we plan to begin work on the topics described in Tasks 1 and 3 of our March 1993 proposal to DOE. These topics are (1) continued development of our process control model for metal transfer control in gas metal arc welding, (2) experimentation with light sensing for drop transfer control, (3) implementation and testing of control algorithms designed using our process model, and (4) beginning the design and development of a semi-transferred plasma arc welding system.

We will continue to develop our process control model by including thermal dynamics. Prior to this step, the growth rate of the drop in our model has been assumed to be simply proportional to the arc current. Our earlier studies dealt with the more basic issues of steady-state heat transfer in the electrode and drop detachment rates in the standard (non-vibrated) gas metal arc welding process. This work identified factors limiting heat transfer to and through the drops, and the basic mechanisms for drop detachment. In particular, it was found that in order to accurately predict electrode melting rates at higher welding currents, it was necessary to include a modified electrode geometry in the thermal analysis. This geometry change consisted of a tapering of the normally cylindrical end of the electrode. Therefore, we will include the process of electrode tapering in our model and study how this geometry variation, along with the geometry of the deforming drop, affects heat flow in the drop and electrode.

In our previous work, the electrode vibration controller has used the electrode feed speed as a feedback signal. This feedback signal is an average indication of the metal transfer process, but for maximum performance from the system, a technique is needed to detect the separation of individual drops from the electrode. The arc voltage (which is measured to control the electrode feed motor in constant-current welding) contains the desired information, but, due to noise and the fact that the current supply regulation is not ideal, the information is difficult to extract. A promising new source of information is the intensity of the arc light. Relatively clean signals of drop detachment have been observed by other researchers when monitoring arc light intensity at high detachment frequencies. We will apply this new sensor to the MIT vibration welding system and study its usefulness for the control of electrode behavior.

With a method of drop separation detection, and decoupling of the electrode melting and the base-plate heating processes using vibration, a metal transfer controller will be developed which controls the instantaneous metal transfer rate. The goal of the controller will be to maximize the stable transfer of metal for a given base-plate heating, which will result in a productivity gain for the process. In addition, since the time the metal drop spends in the arc is minimized, a reduction of welding fumes should result, thus making the welding process cleaner.

A unique capability of the vibration-enhanced gas metal arc welding system at MIT is the ability to control the drop acceleration and the arc current independently. Using this

capability, we will study the importance of drop acceleration on weld penetration in order to determine the usefulness of electrode vibration as an additional input for controlling the shape of the weld pool.

Finally, we will begin the development of a new arc process we call *semi-transferred plasma arc welding*. In this process, only a portion of the arc is transferred to the base-plate and the rest is used solely for melting the electrode. The heat supplied to the substrate can be varied by a factor of 20 (from 1,000 W/cm² to 20,000 W/cm²) which will complete fusion of the droplets with the substrate without the production of a molten pool of excessive volume. This process provides excellent independent control of the electrode melting rate and base-plate heating. We will be developing a power supply, welding head, and computer control system to explore the scientific and industrial usefulness of this process. Later plans include the development of a physical process model of the system.

RECENT PUBLICATIONS

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Fundamentals of Elastic-Plastic Fracture: Three-Dimensional and Mechanistic Modeling

PERSONNEL

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ABSTRACT

Tractable multiple-parameter elastic-plastic fracture mechanics methodologies are being developed and applied to provide improved descriptions of crack front fields and cracking behavior. The so-called T -stress of linear elastic fracture mechanics has been shown to be a useful correlator of varying crack-tip stress triaxiality, and efficient numerical procedures for calculating T have been developed and implemented. Simplified models of fully plastic plane strain cracking have been developed which predict a marked sensitivity of crack tip opening angle ($CTOA$) to the triaxiality of stress at the crack tip and to the angle at which a dominant shear band intersects the crack plane at the moving tip. For single-face-cracked specimens, these parameters have been linked through slipline and least upper bound (LUB) methods to the ratio of tension to bending moment carried by the uncracked ligament. A set of traditional and novel tension and bending specimen designs have been formulated for purposes of experimentally determining a given material's dependence of $CTOA$ on crack tip stress and slip angle.

GOALS

The principal objective of this research is to develop improved techniques for predicting the structural integrity of cracked, ductile structures (i.e., those fabricated from lower strength materials, including weldments, that contain partial-penetrating surface flaws and are subjected to essentially monotonic loading). Current technology for predicting ductile fracture can be highly conservative (e.g., use of deep-crack bend toughness data to predict the behavior of shallow defects), but the degree of conservatism is not

determined. Carefully-crafted (but tractable) simplified engineering models of ductile fracture, based on (a) the underlying physics of fracture processes and their dependences on stress and local deformation and on (b) appropriate mechanics analyses of the dependences of crack-tip stress and deformation on geometry, loading type and magnitude, and material resistance to plastic flow, can be formulated and successfully applied to obtain more reliable predictive capabilities.

PROGRESS

1. Wang [8] showed convincingly how the T -stress correlation accurately defines evolving loss of crack-front stress triaxiality along both shallow and deep surface crack fronts, in both tension and bending, and at load levels from small-scale yielding to limit load. Moreover, these excellent correlations can be accurately matched by using simple line-spring models [5] of the structure. There is simply no precedent for such detailed information regarding the fields of stress and deformation along 3-D crack fronts as obtained from so simple an engineering tool.

2. Lee and Parks [4] have refined the limit surfaces of shallow-cracked single-face-cracked specimens subject to combined tension and bending. The improved definition of the yield surfaces and the $CTOD$ greatly enhance the accuracy with which the line-spring models fully plastic shallow-cracked structures [5].

3. Robust, accurate, and simple means have been developed to calculate the T -stress in engineering structures. A general approach [9] based on a finite element domain integral form of an interaction integral is an applicable post-processor for any crack geometry. For the special case of part-through surface cracks in plates or shells, the line-spring has been adapted to calculate T [11]. Current extensions of the continuum form give T for transient thermal loading. A recent result is that for sufficiently shallow cracks, a thermal shock provides negative T at peak levels of induced K_I . This has major bearing on the thermal shock problem, since the local stress at peak K_I will be reduced, and less likely to cause cleavage fracture [12].

4. Kim and McClintock have developed a novel application of the least upper bound method of limit analysis to estimate crack-tip *stress state*. Briefly, the method consists of determining the least upper bound circular arc for a given loading of an uncracked ligament, including the angle θ , with which the arc intersects the crack plane and the displacement offset across the arc in terms of remote kinematics. It is proved that, if one assumes that the tangential traction on the optimal arc is the shear yield strength and that the normal stress across the optimal arc obeys a Hencky equilibrium equation, then the single unknown (corresponding to a reference value of the normal stress at a reference position on the arc) can be chosen to provide a traction distribution along the arc which precisely equilibrates the global loading. Moreover, using the crack tip

orientation of the optimal arc, the crack tip stress triaxiality (e.g., the normal stress σ_z across the optimal arc at the crack tip) can be estimated in terms of the reference stress level. Comparison with detailed finite element limit analyses [4] shows the results to be extremely accurate for deep single-edge-cracked geometries under combined tension and bending. This provides a three-parameter characterization of the fully plastic stress and displacement fields for a growing crack, analogous to the K_I for linear elastic structures or the J for initiation in a plastic structure.

5. Hauf, et al [2] have developed an extended effective crack length formulation, wherein the added correction term depends not only quadratically on K_I/σ_y , but also on $\tau \equiv T/\sigma_y$. The motivation for the modification is the marked sensitivity of plastic zone size and orientation to τ in small-scale yielding. The plastic zone is particularly enhanced for $\tau < 0$, and effective crack length formulations for specimens with $T < 0$ give more accurate estimates of J , compliance, and local stress triaxiality. The method is based solely on elastic calibrations of K_I and T , and has been found accurate up to typically 85 – 90% of limit load in a wide range of geometries.

6. McClintock et al [6] have developed a rigid-plastic model of *CTOA* for plane strain crack growth based on localization by hole growth, and on the parameters θ_s and σ_s emerging from either slipline or least upper bound fields. The model predicts a strong functional dependence of *CTOA* on σ_s , which is consistent with experimental observations [1]. In turn, the dependence of (σ_s, θ_s) on the ratio of tension to bending supported by the ligament can be determined from sliplines or least upper bound methods, thus providing a rational modeling path from the structural level to the crack tip. We have identified a series of experimental specimens which can be used to experimentally determine a given material's dependence of *CTOA* on (σ_s, θ_s) . Tests are being prepared on a mild steel. Together with item 4 above, this provides a fully plastic mechanics of crack growth.

7. Lee has recently implemented a line-spring model of fully-plastic through-thickness penetration of part-through surface-cracks which admits the functional dependences of *CTOA* noted above. The predicted shapes of ductile crack growth fronts are in good agreement with those observed experimentally. Further detailed comparison with experiments which have been performed at INEL is underway. Another model of line-spring-based crack extension has been implemented for certain structural crack configurations (axisymmetric surface crack in a pipe under tension; long compliant strip under tension) by Kim. These results emphasize the role of large displacement (by rotation and translation) in thin elastic structures under tension so that the uncracked ligament is entered under the resultant force.

PROPOSED PLANS FOR THE YEAR JAN. 1, 1994 — DEC. 31, 1994

- Completion of T -stress-based analysis of transient thermal loading of shallow cracks.
- Calibration of the micro-mechanical model for $CTOA$ through testing of the unequally-grooved tension and bending specimens.
- Begin finite element analysis of the simulated undermatched weldment specimens being tested by Epstein at INEL.
- Include higher order weight functions for T -stress (generated and provided by Sham of RPI) into linespring finite elements for analysis of both K_I and T in surface-cracked plates and shells subject to transient thermal or residual stress.
- Begin exploratory slipline and least upper bound analyses of plastically heterogeneous crack configurations (mismatched weldments).

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COMMINUTION OF ENERGY MATERIALS

PERSONNEL

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ABSTRACT

Comminution of energy materials is an energy intensive process, and one of the principal sources of inefficiency in many classes of devices is the excessive presence of fines within the coarse medium. These processes impose multiple passes on the feed (e.g. roller tables, ball mills) which result in frictional losses and an unwanted shielding of the coarse medium. This study constitutes an investigation of the mechanics of rapid fines removal to provide design criteria for a new generation of comminution machines with a significantly elevated comminution efficiency. It is well known that dense, size distributed particulate media have a natural tendency to segregate in the presence of flow and gravity, although these effects remain poorly characterized and are typically viewed as a hindrance rather than a means of improving comminution efficiency.

Here, we aim to understand and incorporate these to achieve our goal. Using a cylindrical rotary crusher as the motivating conceptual design, the research focuses on particle segregation by means of unsteady fluidization in vertical and near vertical configurations. In the conceptual device, the time scale of the unsteadiness is the period of rotation, and it is of significant interest to this application to achieve full separation in minimal time to minimize the machine period and accommodate a large and efficient comminution throughput.

Experiments have been conducted with bidisperse mixtures of silica spheres (50-3000 micrometers in diameter) in water with impulsively started fluidization. The results of numerous experiments are summarized with the following observations:

- segregation of bidisperse mixtures can be achieved with impulsive fluidization, even for systems in which the fines are sufficiently large to prevent their percolation through the coarse matrix. It has been found that separation critically depends on the initial formation of an upward propagating pocket.
- the limiting factor to the speed of segregation and hence fines through-put is the speed of the pocket. It is directly linked with the rate at which coarse particles can become detached from the binary dense-pack. The present work addresses the mechanics of this process, both theoretically and experimentally.

PROGRESS

During this period, the impulsive fluidization work was initiated having established an understanding of steady fluidization within stationary beds in the prior year. In this past year, the activity was broken down into:

- developing the experimental method and video data acquisition,
- using image based data reduction to provide useful quantities rapidly,
- identification and characterization of the new phenomenon by which segregation has been found to occur,
- preliminary investigation of complex configurations such as tilted channels, and time varying channel widths

Impulsive fluidization was studied in vertical acrylic test-sections (1x4cm cross-section) that were initially filled with water saturated coarse and fine particles. The mass fractions were chosen to ensure that the fines filled the pore space of the coarse pack. The sizes of coarse and fine particles studied was 2,3,4mm and .2,.3,.4mm respectively. A typical sequence of events is shown in Figure 1. In all tests, it was found that no percolation of the fine species occurs within the coarse medium, and the mixture always moves as a plug until it is depleted from below. This is contrary to published findings of percolation studies which suggest that if the fines are smaller than approximately 1/7th of the bed particle size, they should percolate through one another.

In this process, it was found that separation critically depends on the initial formation of an upward propagating pocket within which segregation occurs: coarse particles rain down through it while fines remain fluidized, leaving a fines-free bed of coarse particles below. Segregation is markedly reduced in the absence of this structure even when the fines are small enough to percolate through the coarse bed. Conversely, even mixtures with a

coarse/fine particle size ratio of 2 were successfully segregated. This constitutes a new size segregation phenomenon that is viable even at high solid fractions.

Speed and Quality of Segregation:

The quantities most relevant to the processes of interest are the time taken to clear the fines and how well the fines have been cleared. The parameter that governs the clearing time is the speed at which the moving plug is depleted from below, as this interface must traverse the plug to induce separation. The speed of this interface was measured for a broad range of particle sizes, and is shown in Figure 2. It was surprisingly found to only depend weakly on the coarse particle size, unlike the settling speed of individual particles. The removal fraction which represents the fraction of the original quantity of fines removed during this process is shown in Figure 3. These data clearly show the importance of the fluidization flow rate. If the mean velocity is greater than the terminal velocity of the fines, nearly complete removal is assured.

Complex Geometries:

Real devices and machines are rarely vertical with a constant cross section. To address this reality, preliminary test were carried out in inclined geometries as well as ones where the cross-section changes with time, as is the case with our motivating design.

Effect of inclination:

Inclination was found to have an adverse effect on segregation contrary to the behavior of inclined (Boycott) settlers. The passage of the "segregation pocket" was visible but it was consistently restricted to the upward facing side of the channel, resulting in poor segregation on the lower side.

Effect of wall motion:

In our motivating design, the wall gap changes as a function of time. To model this, the original test section was modified with one laterally moving wall. Similar impulsive fluidization experiments were conducted with a range of outward wall speeds. The motion of the wall was found to be beneficial in reducing and even eliminating the rise of the plug during segregation. High rises are undesirable as they would necessitate larger machines to contain the material.

Applications and Industry Involvement

A number of processes require transport of solids at high concentration for which separation is typically not possible without dilution (e.g. ceramic slurry molding, powder metallurgy). This new phenomenon, although originally motivated by comminution, is also of

direct application to the design of a new class of separation machines for media of high solids loadings, that have the capability of dividing a medium into two fractions according to a threshold size. The applications of this work to the design of separation machines is natural, and a patent will be sought for devices based on this new segregation phenomenon. Further research into the mechanics of this process remains necessary for optimization purposes and to address effects associated with size distribution, particle shape and non-uniform pocket formation.

PROPOSED PLANS FOR THE YEAR JAN. 1, 1994 - DEC. 31, 1994

This program has not been integrated with a counterpart activity at INEL and therefore is not being continued as part of the collaborative program. A separate independent proposal has been submitted for continuation funding.

PUBLICATIONS AND CONFERENCE PRESENTATIONS

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Kytömaa H.K. and Schiaffino, S.A. "A new enhanced method of fast segregation of fully saturated particulate media," DuPont, Wilmington, Delaware, August 13, 1993.

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Figure 1. Sequence of video images spaced by 1/6th of a second of an impulsively fluidized mixture of fine and coarse glass spheres (0.2 and 0.4 mm respectively). The fine particles are dark and the coarse particles are transparent. The frames show the initial upward motion of the mixture, followed by the wave-like progression of a particle free region in which segregation between the two species occurs. This sequence also reveals the sudden nature of the final separation stage (frame 18) in which the fines break through in an apparently unstable manner. This mechanism is a potentially useful method of rapid removal of fine particulate in comminution processes.

Figure 2 Depletion velocity of the rising plug, as measured by an observer moving with the velocity of the plug (U_l).

Figure 3 Normalized fine particle removal fraction.

Synthesis and Optimization of Integrated Chemical Processes

PERSONNEL

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ABSTRACT

This research is aimed at developing improved computer based methodologies for the design of integrated batch and continuous processes. Work is underway in two major areas: each constitutes a separate doctoral thesis project.

The first area is Synthesis of Heat and Work Integration Systems for Continuous Processes. The classical approach to complete flowsheet synthesis has been to decompose the problem into chemical process design, heat exchanger network design, and utility system design. The solution obtained using this sequential approach neglects many subsystem interactions leading to inefficient use of capital, raw materials and energy. This research focusses on the development of a simultaneous methodology for total flowsheet synthesis that exploits the subsystem interactions. This year, a detailed case study involving an ethylene process has prompted the development of a novel method that simultaneously targets a refrigeration utility system for performance, capital cost, and operating costs.

The second area is Synthesis and Optimization of Batch Processes. Such processes are of increasing industrial importance for the manufacture of high value added specialty products and pharmaceuticals. In many of these markets, the ability to bring new or improved products rapidly to market is critical to competitiveness. The research focusses on the application of modelling technology to batch process development: the derivation of a large scale manufacturing process from a laboratory or pilot scale experiment. Computer based tools can both decrease the duration of the development phase, and improve the efficiency of the resulting process. In the past year, a detailed methodology that utilizes modelling technology for batch process development has been derived.

GOALS

The overall goal of this research is to develop novel systematic methods for the synthesis and optimization of chemical processes. As the chemical industry is one of the largest consumers of energy in the U.S., it is important to find efficient and creative computer-aided design strategies for developing new processes, and retrofitting existing plants. Our philosophy is to develop, in a university environment, innovative generic methodologies for solving problems of industrial importance. These methods are then demonstrated by developing prototype software and applying it to solve problems typical of those encountered in industry. At present, our specific goals are:

- (a) To improve the efficiency of energy usage in continuous processes through the simultaneous design of a process, its heat exchanger network, and the utility systems.
- (b) To create and demonstrate novel computer-aided design tools for the rapid development of efficient batch processes.

PROGRESS

Synthesis of Heat and Work Integration Systems: Juan Gomez is working on his Ph.D. thesis project entitled, "Simultaneous Optimization of a Chemical Process, its Heat Exchanger Network and the Utility System Using a Process Simulator." His objective is to develop an optimization strategy that optimizes the subsystems simultaneously by taking into account the subsystem interactions. The method combines rigorous industrial-scale process simulators and thermodynamic targeting methods. The result is the first method that can conduct this simultaneous optimization with reasonable computational expense.

Last year three realistic, industrial-scale problems were identified to test the methodology. The first was a process for the fractionation of crude petroleum. In this problem, the design of the heat recovery network in the crude preheat train is of primary importance. The second problem was the optimization of the cold end of an ethylene plant. Here, the design of the utility (refrigeration) system dominates. The third problem was the design of a process to manufacture vinyl chloride monomer. This process is dominated by the optimization of the chemical process itself. Results obtained for the crude fractionation problem showed the cost optimum is very flat, but very different from that obtained using more simplistic methods previously presented in the literature.

This year, due to the size of an ethylene plant, significant effort was devoted to develop a realistic and stable model in which to test the methodology. In order to solve this problem, it was found that a new thermodynamic targeting method to predict utility (refrigeration) system performance was needed. The method developed uses simple Rankine cycle models to predict complex and cascade refrigeration system performance, and is the

first in the literature to target not only utility system performance but also its capital and operating costs without actual design. This is similar to pinch targeting for heat exchanger network design. The saving in computer time due to the transformation to a targeting space should allow mathematical programming methods to solve the overall problem in realistic time scales. The method is currently being embedded in the optimization step of a process simulator (ASPEN PLUS) in order to solve the ethylene problem.

Synthesis and Optimization of Batch Processes: Russell Allgor is working on his Ph.D. thesis project entitled "Modeling Tools for Optimal Batch Process Development". He has recently completed his thesis proposal. Much of the previous research related to batch processes has dealt with the selection and sizing of equipment. However, we feel the design of the process to be operated in this equipment is a more relevant and important problem that it is encountered far more frequently. Moreover, the consideration of detailed operating policies at the design stage has been absent from almost all of the previous work.

In the past year, a thorough reexamination of our research goals has identified what we term batch process development problems. These deal with the manufacture of a product in an existing facility, and apply to the improvement of existing processes, toll and custom manufacture, and the introduction of new products. Batch process development requires the conversion of a description developed during process synthesis or experimentation into a detailed procedure capable of manufacturing the product on a large scale in an existing facility. Thus, the engineer must determine operating policies, select the equipment items, and derive a feasible schedule. This research is the first to propose a systematic methodology that applies process modeling technology to examine detailed operating policies at the process development stage.

A methodology has been developed that explicitly exploits processing tradeoffs at the design stage in order to make the best use of equipment, raw materials, and the time available. A two step procedure is proposed. First, a "base case design" (a feasible production scale design that meets both the production and time horizon constraints) is derived from the information provided by the process synthesis. The following sequence of steps is proposed: abstract the information provided by the synthesis stage as a hierarchical task network, derive mechanistic models for the individual tasks, develop operating policies and calculate cycle times, determine a feasible schedule on the available equipment, check for feasibility, and update the operating policies if necessary. Next, the base case is optimized by manipulating the process operating policies and schedule simultaneously. Completion of these tasks requires the application of combined discrete/continuous simulation, dynamic optimization, and scheduling technology.

The implementation and demonstration of this methodology requires the development of a software tool to support the interactive application of this broad range of tools to a common process representation. The prototyping of this modeling environment forms the next stage of the research.

PROPOSED PLANS FOR THE YEAR JAN. 1, 1994 - DEC. 31, 1994

This is the final year that this research will form part of the MIT/INEL collaborative program. A separate proposal with the same title has been submitted to the Department of Energy to fund the period 1/1/94 to 12/31/96. The proposed research under this latter proposal will be described here.

Juan Gomez plans to complete his thesis in June 1994. The final case study involving a vinyl chloride monomer plant will be completed. Russell Allgor will concentrate on the design and implementation of the software tool introduced above. The modeling environment will rely on a graphical interface that facilitates the development of models, access to numerical tools, and analysis of results. The key notion will be separate but consistent representations for the process and the plant. A plant object will represent the equipment and interconnections in a particular facility, whereas a process object will represent the task network for a particular process. Consequently, many process objects may be designed for the same plant, or a single process object can be implemented in several different plants. The object oriented concepts of inheritance and polymorphism will be employed to handle interactions between these two descriptions, and to maintain consistency. General relationships between equipment and task types will be defined, and particular instances of these general types will be used to build plant and process objects respectively. The constraints imposed on a process by a particular plant can then be inferred from these relationships, and, for example, automatically downloaded to a scheduling tool.

Further, we will be actively collaborating with industrial colleagues to identify a series of real life batch process development problems with which to test and refine the prototype software.

The application of process modeling technology to batch process development problems will rely on the efficiency and robustness of the numerical algorithms required to solve the various steps in the methodology outlined above. We are therefore adding a major new thrust that will explore the enhancement of these enabling technologies. In particular, we will explore novel algorithms that utilize a combination of symbolic and numerical information concerning a mathematical problem in order to locate a solution more robustly and efficiently. This technology is particularly suitable for application in the proposed modeling environment, because process models will be stored in a common symbolic format that can be readily accessed by any solution algorithm.

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Budget not included.
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