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(2-01) p. 1 of 4

ANNOUNCEMENT

UNITED STATES DEPARTMENT OF ENERGY (DOE)
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OMB Control No. 1910-1400

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The Lincoln Electric Company

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Novel Optimization Methodology for Welding Process/Consumable Integration

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ANNOUNCEMENT

UNITED STATES DEPARTMENT OF ENERGY (DOE)
Scientific and Technical Information (STI) For Financial Assistance Recipients and Non-M&O/M&I Contractors

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J. Description/Abstract *(from page one)*

Advanced materials are being developed to improve the energy efficiency of many industries of future including steel, mining, and chemical, as well as, US infrastructures including bridges, pipelines and buildings. Effective deployment of these materials is highly dependent upon the development of arc welding technology. Traditional welding technology development is slow and often involves expensive and time-consuming trial and error experimentation. The reason for this is the lack of useful predictive tools that enable welding technology development to keep pace with the deployment of new materials in various industrial sectors. Literature reviews showed two kinds of modeling activities. Academic and national laboratory efforts focus on developing integrated weld process models by employing the detailed scientific methodologies. However, these models are cumbersome and not easy to use. Therefore, these scientific models have limited application in real-world industrial conditions. On the other hand, industrial users have relied on simple predictive models based on analytical and empirical equations to drive their product development. The scopes of these simple models are limited. In this research, attempts were made to bridge this gap and provide the industry with a computational tool that combines the advantages of both approaches. This research resulted in the development of predictive tools which facilitate the development of optimized welding processes and consumables. The work demonstrated that it is possible to develop hybrid integrated models for relating the weld metal composition and process parameters to the performance of welds. In addition, these tools can be deployed for industrial users through user friendly graphical interface. In principle, the welding industry users can use these modular tools to guide their welding process parameter and consumable composition selection. It is hypothesized that by expanding these tools throughout welding industry, substantial energy savings can be made. Savings are expected to be even greater in the case of new steels, which will require extensive mapping over large experimental ranges of parameters such as voltage, current, speed, heat input and pre-heat.

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Novel Optimization Methodology for Welding Process/Consumable Integration

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Executive Summary

Advanced materials are being developed to improve the energy efficiency of many industries of future including steel, mining, and chemical, as well as, US infrastructures including bridges, pipelines and buildings. However, the rapid deployment of these materials is often hampered by the lack of appropriate welding technology to join these materials. Development of welding technology is slow and often involves expensive and time-consuming trial and error experimentation. The trial and error experiment is needed since it is often difficult to know a-priori how the material – process effects interact to determine the final performance of the welded structure.

The ability to develop welding process, process parameters and consumables without extensive trial and error experimental work to achieve the needed performance level is an enabling technology that will address the need for rapid deployment of new materials. The goal of the current research pertains to the development of an integrated weld process model which will facilitate development of optimized welding processes and consumables in the welding industry.

Literature review showed two kinds of modeling activities. Academic and national laboratory efforts focus on developing integrated weld process models by employing the detailed scientific methodologies. However, these models are cumbersome and not easy to use. Therefore, these scientific models have limited application in real-world industrial conditions. On the other hand, industrial users have relied on simple predictive models based on analytical and empirical equations to drive their product development. The scopes of these simple models are limited. In this research, attempts were made to bridge this gap and provide the industry with a computational tool that combines the advantages of both approaches.

The work focused on Fe-C-Mn-Si low alloy steel materials and gas metal arc welding (GMAW) with solid and cored electrodes for fillet weld geometry. A modular approach was adopted since it allows for use of the individual models as stand alone tools and for continuous improvement and extension of the integrated tool to other welding processes and alloy systems as new information becomes available and the individual models are refined for greater accuracy. As a part of this research, the following software modules were developed.

1. Numerical Heat Transfer Fluid Flow Model for fillet weld geometry: This model allows for the prediction of fillet weld pool shape and also spatial thermal histories by considering convection and conduction as a function of welding process parameters. The access to this model is available to the industry via remote terminal servers.
2. Artificial Neural Network Model for Weld Pool Shape and Cooling Rate: This is faster than the numerical model, however, captures the predictive power of the same. This model is currently available to the public via the Internet.
3. Paraequilibrium Thermodynamic and Kinetic Model for Steel Transformation: This model allows for the prediction of transformation temperatures and also the continuous cooling transformation diagram as a function of steel composition.
4. Model for transition from bainite to acicular ferrite: In certain welds, a brittle bainitic microstructure is replaced by the tough acicular ferrite. The mechanism for this transition as a function of inclusion characteristics was explained using a kinetic model.
5. Artificial Neural Network Model for Weld Metal Properties: Using published literature and data from industries, an artificial neural network model was developed. This model

allows for the prediction of yield strength, toughness, ultimate tensile strength and elongation as a function of weld metal composition and process parameters.

With the development all five modules, the primary goal of the proposed research was attained. Seamless integration of all five modules was not achieved. Complete integration was not possible due to limitations in the computational tools. However, limited integration was achieved in coupling some of the modules. In addition, some of the modules are available via the Internet.

The next goal of the proposed research was to use these tools to optimize the welding processes and consumables to achieve the required properties. Since the integrated tool was not available, the optimization methodology was demonstrated by coupling the artificial neural network (ANN) model for properties with commercial optimization software. The optimization lead to a weld metal composition which will lead to optimized charpy toughness at -20 ^{o}C. This weld metal composition was in agreement with published literature.

The above mentioned project activities demonstrated that it is possible to develop hybrid integrated models for relating the weld metal composition and process parameters to the performance of welds. In addition, these tools can be deployed for industrial users through user friendly graphical interface. In principle, the welding industry users can use these modular tools to guide their welding process parameter and consumable composition selection.

It is hypothesized that by expanding these tools throughout welding industry, substantial energy savings can be made. Savings are expected to be even greater in the case of new steels, which will require extensive mapping over large experimental ranges of parameters such as voltage, current, speed, heat input and pre-heat. There are indirect environmental benefits of this research worthy of consideration. In chemical industries, poor weld quality may compromise the integrity of the welded products. This can leads to spillage of chemical products and can result in plant interruptions that may result in energy-intensive startups and environmental impacts. By expanding these hybrid models to predict the defect formation, one can design the welds against such catastrophic failures.

Some of the software modules will be commercially distributed to the public so that the welding industries can reap the advantages of the predictive software. The hybrid integrated software tool developed in this project will be continuously evaluated. After achieving sufficient confidence, improving the user interface, enhancing the robustness and with independent evaluations, the software tool may be offered to the welding industry.

This project also indicated many challenges that still need to be considered. The following recommendations are made to address these challenges.

- Develop operational characteristics models to evaluate the arc stability and also fume generation
- Extend the model to slag based systems
- Develop computational tools to allow for easy integration of software modules
- Expand the optimization goal to include all the properties, i.e., strength, toughness, elongation, and creep-rupture properties to expand the application of these models to high-temperature use in energy and chemical industries
- Develop similar hybrid models for industries associated with welding, namely casting, forming, heat-treatment and surface processing

Introduction

Problem Statement

Energy has displaced national defense as the primary driver of innovation in most, if not all, industry sectors today, Figure 1. The need for both reduced consumption from conventional energy sources and more efficient alternatives in energy supply is changing approaches to design and construction in all sectors. Industry segments within the energy sector, both upstream (e.g. drilling & offshore) and downstream (e.g. power generation), are driven by the need for greater efficiency in their delivery of energy to the industrialized economies of the world. The nature and availability of these energy sources influence all associated industry sectors and segments further downstream, Figure 2. Welding is a key enabling technology in all industry segments and plays a critically important role in their ability to implement more energy efficient and cost effective designs and fabrication methods. The ability to optimize both the welding processes and the welding consumables in a reliable and efficient manner is crucial to ensure that the US welding industry, as well as the associated industries that it supports, remains competitive in a global marketplace.

Effective use of welded constructions is an essential element in enhancing the economic competitiveness of many US industries. Arc welding is particularly important in steel fabrications for heavy industry, which includes farming equipment and machinery, process equipment for manufacturing and mining, and infrastructure for petroleum refining and distribution. Consequently, *Welding* is a critically important *Supporting Industry* for several *Industry of the Future* segments. The *Steel* and *Chemicals* segments have identified the need for research initiatives in welding to support their energy initiatives.

The Steel Industry Roadmap [1] recognizes the need to integrate welding process/consumable development with steel development as a top priority. In terms of new products, the steel industry expects a greater focus on mechanical performance (i.e. ductility, yield/tensile ratio, fracture toughness, notch toughness, hydrogen control and weld quality) as the shift is made to higher strength steels. Weld metals that match or nearly match the base steel performance will be needed where they do not exist today. This is true for all applications discussed in the roadmap – bridges, shipbuilding, rail cars, pipe, construction and industrial equipment and tanks. Weld integrity was sited as a particular concern in tanks for hazardous chemicals storage. Weld process control is considered extremely important in this application where automation often is not feasible.

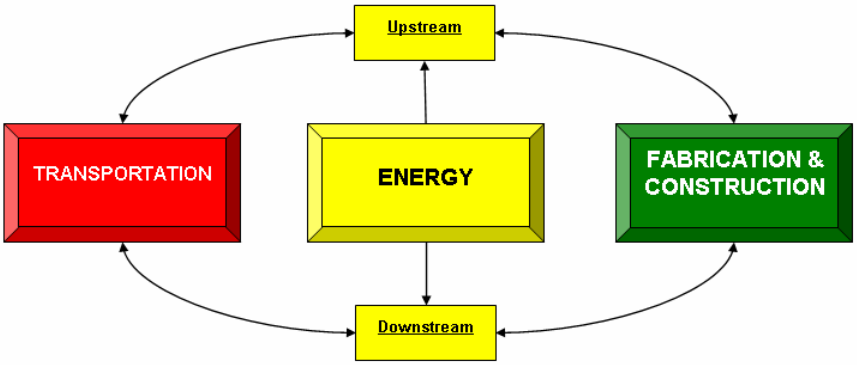

Figure 1: Energy as Central Driver for Industrial Development Across Sectors

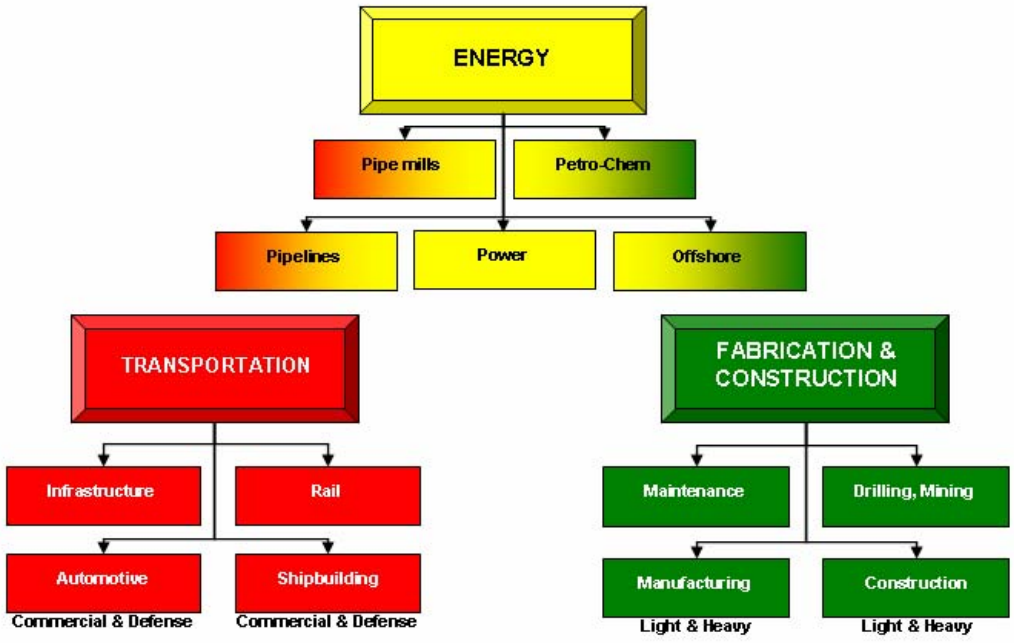

Figure 2: Industry Segment Overview

The Chemical Industry Materials of Construction Roadmap [2] also recognizes the need to develop joining methods with the deployment of new materials as a "most critical" problem area. While not limited exclusively to welded metal construction, welding process and consumable development will play a significant role in the successful implementation of new carbon steels and alloys in the chemical industry.

It is clear from the Roadmaps that advances in welding processes and consumables development have not kept pace with other advances in materials and manufacturing practices. Historically, this results from an almost totally empirical approach to welding process optimization and consumable design, which lags the development of new materials. This, in turn, is due mainly to the absence of predictive tools that can consider collectively the effect of welding process parameters and welding consumables on operational characteristics and weldment properties. In general, the welding industry is far behind the industries it supports in the use of predictive tools that have accelerated the demand for new materials that enable implementation of alternative designs for energy efficiency. If the *Steel* and *Chemicals* industry segments in the U.S. are to realize their visions in the development and deployment of new alloy systems, the welding industry must respond quickly with welding process/consumable combinations suitable for their fabrication. Modeling is an essential tool in the development of new methodologies to introduce new welding processes/consumables efficiently and reliably.

Development of new methodologies is consistent with the Welding Technology Roadmap [3], which seeks to facilitate the transition of welding from an empirical based to a physical based process. It is recognized that improved knowledge of process control and filler metals are "companions to the development of new materials for use in welded applications." Weld process and product modeling, both elements in this work, are considered to be a "top priority" as a tool in helping designers and welding engineers relate weld microstructure and related properties to specific welding processes. It is also anticipated that the same models could be used as process

control tools. The ultimate benefits to industry are sited as the "ability to weld materials previously not used, an increase in the knowledge base, better quality and lower costs, and reduced energy use."

While integrated models are sited as a specific need for pipeline fabrication, all industry sectors rely on the timely development of welding process and consumables for fabrication with new materials. One example is the recent development of high performance steels (HPS) for bridge fabrication, where full advantage cannot be taken of the improvements in steel design and manufacture because a development effort for welding processes/consumables was not considered viable due to market size, time constraints and resource availability. Having better predictive tools available would certainly have made such a development effort more commercially viable.

The problem is not the total absence of predictive models. Those that do exist are powerful research tools that are limited to very specific parts of the welding process. They are not easily integrated and no single model can be used to describe the full range of physical and chemical processes occurring during arc welding. They are not used extensively in the welding industry because the models are highly complex, require specialized training to develop and test, and consume a large amount of computer time to run.

It is unlikely that the welding industry will be able to respond to the expected growth in new materials without better tools in the form of analytical methods and predictive models.

The Technology

Accordingly, this research was undertaken to develop a hybrid integrated model for GMAW that combines both fundamental approaches based on physical science principles and artificial neural networks in a modular fashion. "Hybrid" because of the combined use of empirical and physical science based models. The models are "Integrated" because the outputs from one module become the inputs for others. There is no new technology development involved. Rather, existing technology is considered and implemented in a novel way.

The bases of the hybrid integrated optimization tool are a series of artificial neural network models trained on the outputs from the physical science models supplemented by experience and empirical data. Obtaining predictions from models based on physical science principles is computationally intensive. For this reason, such models are not very useful as engineering tools irrespective of their accuracy. Neural networks answer the problem of computation time, but must be trained on accurate data sets to ensure reliable predictions. Generating such data sets empirically is often more time consuming than the first principles model predictions. Consequently, previously developed models for individual physical processes that occur in welds (e.g. heat transfer, fluid flow and metallurgical changes) were used only as starting points for development and were supplemented by a large body of empirical data in the development of neural network models. Specific expertise in the modeling of fluid flow and heat transfer in the weld pool provided detailed insight about the welding processes that could not otherwise be obtained by measurement. It is this expertise that was applied to develop the relationships among welding process variables, thermal cycle, weldment structure, and weldment properties.

The work focused on Fe-C-Mn-Si low alloy steel materials and GMAW with solid and cored electrodes. The GMAW process was selected because it does not include a slag component common to other arc welding processes. The Fe-C-Mn-Si low alloy steel system was chosen because it has the widest availability for experimental verification and is the best documented alloy system.

An important aspect of developing the hybrid integrated computational tool is the use of a

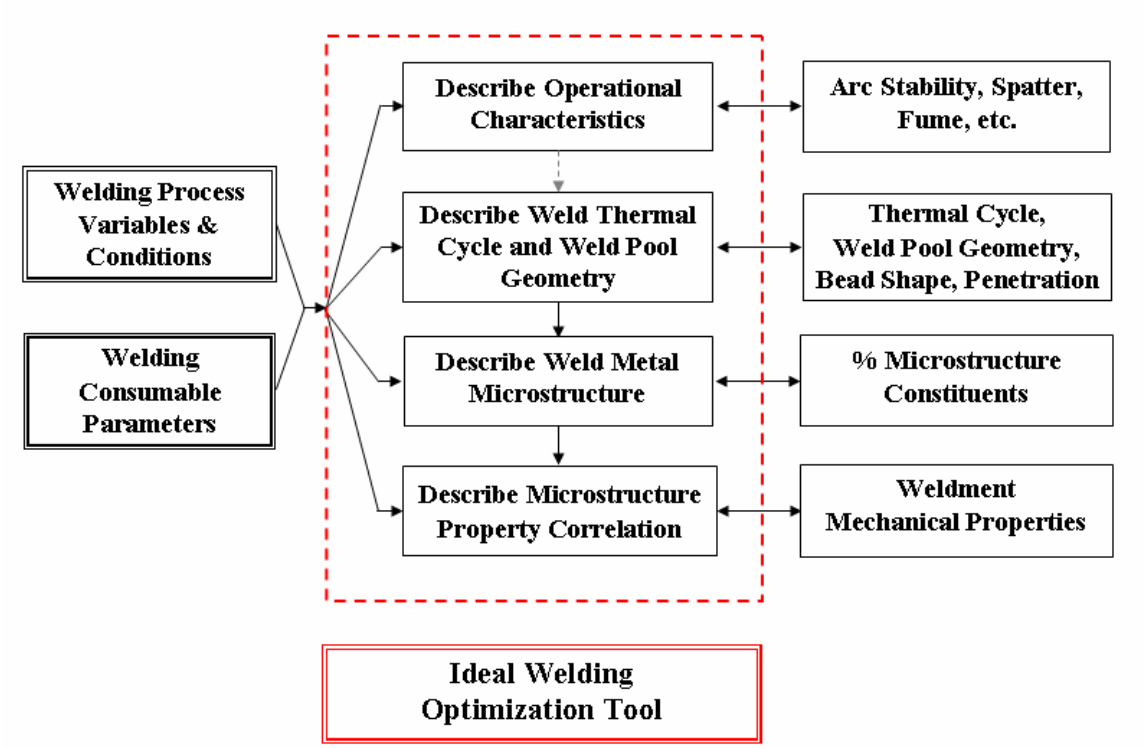

Figure 3: Model Overview and Task Integration

problem-solving environment (PSE) that facilitates the use of sub-process models located on computers at different geographical locations [4]. This is what made the collaboration among participants effective. Furthermore, it made the final integration of multiple models into a single computational tool feasible.

The modular approach, illustrated in Figure 3, allows for use of the individual models as stand alone tools and for continuous improvement and extension of the integrated tool to other welding processes and alloy systems as new information becomes available and the individual models are refined for greater accuracy. With demonstrated capability for Fe-C-Mn-Si GMAW, extension to other processes and alloy systems is considered straightforward.

The Benefits

Implementation of these new methodologies will enhance the economic competitiveness of both the U.S. welding industry and the end users in the U.S. who will be able to use the same tools to optimize the productivity and reliability of welded fabrications. The integrated tool developed under this project will have direct immediate benefit in optimizing the GMAW process with both solid and cored wire Fe-C-Mn-Si electrodes. More importantly, it will serve as a platform from which to extend the methodology to welding processes that incorporate slag and higher alloy material systems. The modular approach proposed enables a process of continuous improvement as industry needs change.

Energy Savings

The previous discussion indicates that the major benefit of this project is enabling the energy based initiatives in other industry segments, which is not possible to quantify. However, it is

possible to estimate potential energy savings simply due to a reduction in the number of test welds needed to "optimize" a welding process for use in an application or develop a new welding product.

Welding consumable selection and fabrication indeed requires significant energy requirements due to the need for extensive experimental weld production and testing for each steel and joint configuration. Typical energy spent on welding 1 m of steel plates using GMAW (assume 20 volts, 300 amps, average speed: 0.002 m/s = $3x10^6$ J/m) will be $3x10^6$ J or 2843.6 BTU. A typical weld consumable design for given steel and given joint configuration would likely involve production of at least 30 experimental welds to attain an "optimum" welding consumable. This requires 85,308 BTU of energy just for production of test welds. It is important to note that this energy estimate is only for a single combination of steel and weld joint geometry. In general, for each application, a welding engineer may recommend 2-3 as candidates. This leads to a total use of 255,924 BTU for each application. Although, one may consider this energy as small in comparison to steel making or chemical processing, weld consumable selection occurs for each grade of steel and each application through out the life of that steel product. This estimate is based on the notion that three steel grades will satisfy the requirements of the industry. In practice, this estimate is often increased due to weldability problems that are not perceived in the initial stage of design. Since welding process and consumable development frequently lags commercial introduction of new base material developments, the need for welded fabrication often leads to time-consuming and expensive weldability experiments after construction starts.

This leads to recurring energy costs which could be controlled by using integrated models to limit the number of experimental welds. Since the hybrid integrated model is based on fundamental theories to the extent possible, it will be able to aid future advanced materials development itself to avoid the paradox of advanced materials with no good weldability characteristics, thus reducing the magnitude of experimental weld production and evaluation. Estimating a reduction in the number of experimental welds to 5 from 30 leads to (~80%) energy savings of 204,739 BTU per joint configuration. If we assume, an average of 100 joints per industry per year, this leads to energy savings of 2,047,390 BTU per year industry. Savings are expected to be even greater in the case of new steels, which will require extensive mapping over large experimental ranges of parameters such as voltage, current, speed, heat input and pre-heat.

It is important to note that most of the energy savings in the processing industry can be achieved by applying this integrated process model concept for the design of optimum material-process combination.

Environmental Benefits

There are indirect environmental benefits of this research worthy of consideration. Energy usage is reduced simply due to less experimentation during product design stage. In addition, the production of welds with optimum service conditions reduces the possibility of re-work. Essentially, this minimizes production and repair costs. In chemical industries, due to poor welds (less high-temperature resistance or corrosion resistance) the integrity of the products is compromised. This often leads to spillage of chemical products and can result in plant interruptions that ultimately result in energy-intensive startups.

Although, the failures of the welds leading to accidents are rare, they do occur due to faulty design of welds for structural applications. For example, the lack of proper operational characteristics leads to lack of penetration in welds, which in turn leads to explosion of refrigeration components due to ammonia leak [5]. Recently, NASA has recognized the potential of failures in weld in their structures [6]. Research is underway to consider the effect of inelastic conditions of weld in evaluating the failure of welded structures in buildings during

earthquakes [7]. Therefore, rigorous weld consumable design with operational characteristics to avoid physical defects, such as lack of penetration, and enhanced properties to withstand service conditions would be ideal. In this regard, the hybrid integrated model provides an efficient tool to perform weld design and optimization for improved weld integrity.

Economic Benefits

The immediate direct benefit of this project is to the manufacturer of welding product who is able to utilize the tool effectively to reduce time to market and improve profitability. While this is significant to the manufacturer, it is only a fraction of the potential benefit to US industry as a whole. In order to capitalize on the benefits of new alloys planned by the *Steel* and *Chemicals* sectors, timely introduction of fabrication methods including welding is essential. Effective utilization of the integrated model proposed by this research is expected to facilitate cost-effective development of new welding processes and consumables that will be needed in the future. By association, it will enhance the economic competitiveness of both the end user industry sectors and the domestic welding industry in the world marketplace. In addition, increased productivity resulting from welding process optimization is expected to reduce energy consumption through operational efficiencies.

One example is the recent introduction of high performance steels (HPS) for bridge construction. The use of HPS70W in lieu of 50W on demonstration projects enabled designers to maximize girder spacing and minimize weld sizes. The result was a 24-30% weight reduction and overall fabrication cost savings of 11%. Considering that the Federal Highway Administration estimates that 1/3 of the nation's 578,000 bridges are in need of repair or replacement, the cost benefit potential is substantial and will be realized only if welding process and consumable development keeps pace. The introduction of HPS100W, which offers even greater cost benefit, has been delayed because suitable welding consumables did not exist commercially. Similarly, introduction of higher strength steels for rail car fabrication in the US are stalled because of welding issues.

Commercialization

Initial commercial application of this research was accomplished by the industrial partner in this project in the development of new welding consumables for the energy sector. The individual modules were implemented as they became available. In addition, the modules were used, as appropriate, in product design activities for several of the industry segments illustrated in Figure 2. The tool is expected to be instrumental in welding product development in at least two industries where new alloy introductions are considered critical. In addition, the tool will be useful in helping specific customers with welding process optimization.

Ongoing commercial application of this research originally was to be promoted through the national laboratory (ORNL) web site. However, with the recent restructuring in the national laboratory network, it is unclear how or if this will be accomplished. Discussions have started with Edison Welding Institute for this purpose.

Access to the predictive tool for weld penetration, bead shape, and cooling rate is available at www.personal.psu.edu/axk927/research.htm. Some of the simple microstructure models are also available at http://engm01.ms.ornl.gov.

Background

State of the Art

The design of welding products that meet both operational requirements and weldment property needs is far from trivial. Operational characteristics that must be considered include arc stability, deposition rate and extent of spatter/fumes. The operational characteristics control the welding productivity and, therefore, the cost. Weldment properties include yield strength, tensile strength, ductility and toughness. The desired weldment properties are controlled by the service requirements for the final fabricated structure. Both characteristics are affected by welding process parameters such as voltage, current, travel speed, and consumable parameters such as composition, shielding gases and fluxes [8]. Traditionally, weld process modeling has focused on individual physical processes including heat transfer, fluid flow, arc-plasma interactions, gas-metal interactions, slag-metal interactions, solidification and solid-state transformations and their effects on welding characteristics, weld quality, productivity, microstructure and weld properties.

The primary limitation is that the individual processes are typically considered in isolation when, in reality, they are interrelated. The factors affecting operational characteristics and weldment properties are not independent of each other. For example, the operational conditions control the weld thermal cycle and final weld metal composition. In turn, thermal cycles and weld metal composition control the final microstructure. Finally, the microstructure controls the final properties. Therefore, it is critical to consider all of these interactions when designing weld processes and consumables.

Consequently, welding process, process parameter and welding consumable selections are rarely optimized completely. In many cases, the optimum conditions for operational characteristics may not overlap with optimum conditions for superior weldment properties. However, these inter-relationships between operational characteristics and properties are expected to be specific to particular alloy classes and welding processes and, therefore, cannot be generalized. Consequently, traditional welding design has involved extensive, expensive experimentation by trial and error. This trial and error methodology severely limits the potential for optimization of existing consumables and also the development of new consumables for new classes of structural alloys. This constraint is mainly due to the absence of predictive tools that can consider the effect of welding consumable and welding process parameters on both operational characteristics and weldment properties.

Over the past three decades, much research focused on developing an understanding of each of the above physical processes individually. The work on arc plasma – liquid metal interactions [9] showed the effect of plasma on reducing the vaporization of elements from metals. In addition, models have been developed to understand the vaporization of alloying elements and dissolution of gases in the weld pool. Other research led to the development of computational heat transfer and fluid flow models to describe the weld pool development [10]. This demonstrated the importance of the rate of change of surface tension with temperature on the weld pool flow behavior and resulting weld pool shapes. The heat transfer and fluid flow models can be used to describe complex thermal excursions of inclusions in a steel weld metal [11]. Further, slag-metal reactions and solidification partitioning were considered with regard to their influence on microstructure of low-alloy steel weld metal [12].

Fundamental aspects of inclusion formation in liquid steel have been studied and led to major breakthroughs in understanding of inclusion formation in steel weld metal [8]. This work showed that inclusion formation in steel welds can be described by overall transformation kinetic theories.

Sequential oxidation of various elements in liquid steel varies depending upon the weldmetal composition as well as the cooling rate, contrary to the fixed oxidation sequence assumed before. Based on these theories, a model was developed to describe inclusion formation as a function of weld metal composition and thermal history. In addition, experimental investigations showed fluid velocity gradients lead to rapid inclusion coarsening [13]. Recently, the effects of fluid flow on the inclusion formation have also been considered [11] using computation heat transfer and fluid flow models. Moreover, recently in-situ diffraction techniques have been used for tracking the phase transformation in heat-affected-zones and the weld metal regions [14,15].

The relationship between crystallographic conditions and weld solidification characteristics is being modeled [16]. Bhadeshia et al devoted extensive efforts to describe the microstructure development with theories of phase transformation [17]. Preliminary studies are underway to relate the weld microstructure to properties [18,19]. Currently, there are no physical models that describe some simple welding characteristics such as spatter and fumes as a function of consumable and process parameters in a quantitative manner. Although the above work addresses each of the physical processes and some limited interactions between them, there is no comprehensive predictive tool that considers all of the interactions in an integrated and quantitative way.

Objectives

The primary objective of this work is to develop a hybrid integrated computational tool for GMAW process and consumable optimization based on a combination of physical process and artificial neural network models. The tool was intended to describe both operational characteristics and weld metal properties from welding process and consumable input variables. Specifically, this hybridized model is intended as an engineering tool that can be used to:

1) optimize the welding process for productivity and quality, and
2) integrate and streamline the development of new welding processes and consumables.

Further, the model is intended as a framework for modeling other welding processes and consumables.

In order to achieve the objective of integrating both weld process and material models into a single development tool, several major technical issues were addressed. These correspond with the modules illustrated in Figure 3, and are intended to build on one another as follows:

1) Description of operational characteristics as a function of welding process (GMAW), process parameters (voltage, current, travel speed, plate thickness, etc.) and consumable variables (solid or cored electrode, composition, shielding gas, diameter, etc.).
2) Description of weld thermal cycles and weld pool geometry as a function of welding process parameters.
3) Description of microstructure development as a function of thermal history, composition, dissimilar metal effects, etc.
4) Development of microstructure-property correlation.

Although successful development of an operational characteristics model is not technically required for the thermal cycle and weld pool geometry segment, it is necessary for the development of a fully integrated computational tool. Since operational characteristics are

1) often difficult to quantify in ways that relate to the commercial acceptance of a welding process or consumable, and
2) predictive models require quantitative metrics,

a decision would be needed early in the program as to the utility of this first module.

The thermal cycle, microstructure and microstructure-properties modules were to be developed concurrently. The key measure of success would be in their integration at the end. The

advantage to the modular approach is that each increment of work will be useful as a predictive tool for optimization of some part of the welding process. If, for some reason, verification of any one module failed, the other modules could be used.

Project Team

The collaboration among a national laboratory, a strong research university, and an industrial partner committed to the welding industry was essential for leveraging all of the skills needed to develop effective tools that ultimately could be implemented for commercial purposes. The national laboratory and the university offered extensive experience in modeling welding processes and weld metal systems. However, effective integration of welding process and materials models into a computational tool to facilitate welding process optimization and consumable design requires a practical working knowledge of welding processes and consumables as they are applied in practice. This expertise was offered by the welding company. Three of the principal investigators are internationally known for modeling work associated with welding and weld metal microstructures. In addition, the national laboratory has experience designing internet calculations, which have allowed industrial and academic users to evaluate and use predictive models for various purposes.

Methodology, Results and Discussion

Hybrid Model Development

At the outset, the development of a fully integrated computational tool for weld process and consumable optimization seems quite aggressive. The focus on Fe-C-Mn-Si GMAW greatly simplified the technical challenges. Since much steel fabrication is done using fillet welds, a down hand fillet weld was used for this work. A typical fillet weld macrograph is shown in Figure 4.

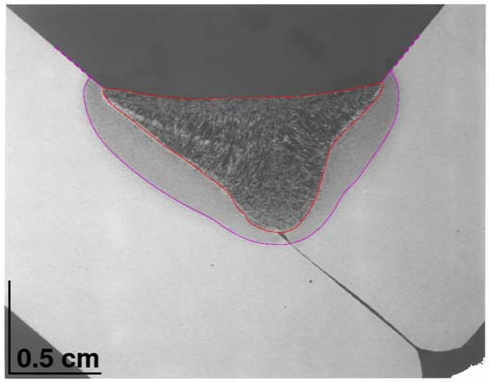

Figure 4: A macrograph of a typical filler weld

In the literature, both physical and analytical models exist for the welding process, which were supplemented by a large body of empirical data available for the alloy system. Artificial neural networks were developed from empirical knowledge and data where suitable models are not available. Beyond that, the task became one of model verification, refinement and integration. The underlying philosophy in this research is the modular approach as previously described. This approach was preferred for several reasons.

1) It was expected to yield usable results in the shortest period of time.
2) If complete integration of all model segments was not feasible, the successful modules would be useful as individual predictors of certain aspects of welding performance. This ensures some benefit regardless of final outcome.
3) It allows for continuous improvement. As new research is done, better models can be substituted for the old and new models can be added to extend the utility of the integrated model to other welding processes and alloys.

Many of the individual process models that form the basis for the hybridized model were developed previously [9]. However, those that were not available and need to be generated and the existing models need to be enhanced. The overall integrated predictive tool will consider the interactions between these sets of physical processes. This modular approach is preferred for the following reason. At present, available fundamental models cannot consider all the physical

processes and, therefore, there is a need to use semi-empirical and empirical models such as artificial neural network models. However, as new and improved fundamental models for physical processes are developed [20], the modular approach proposed in this project allows for flexible and efficient incorporation of new developments. The specific approach for each module is discussed in detail.

Operational Characteristics Model

Although much experimental information exists on operation of welding processes, such as arc stability, deposition rate, spatter formation and fumes with different welding consumables, there is no established quantitative method to predict them. Further, previous works in this area have shown that these characteristics may not be independent of each other. Arc stability in GMAW is related to the ratio of arc-period to short-period [21], the type of shielding gas [22] and the melt-back distance. The melt-back distance is related to Joule-heating that will depend on the welding consumable composition. The deposition rate is related to the type of metal transfer for a given welding process parameter. These can be related to the arc voltage condition [23]. There are fundamental models that exist to describe molten droplet formation at the electrode tip and are related to welding current by considering electromagnetic pinch effect, surface tension, gravitation and momentum transfer due to motion of the consumable [23]. Weld spatter formation is also related to the type of metal transfer. All arc welding processes produce fumes, which pose potential health concerns and will be impacted by anticipated changes in OSHA requirements [24]. The particle size distribution and specific surface area of the particles in fumes are known to vary with different welding processes [25]. However, there are no models to describe them. The elemental evaporation models and thermodynamic stability of various species in gases can be used as a guideline only for estimating the welding fume composition [9].

Consequently, the original plan for this work was to use published experimental techniques to measure the operational characteristics quantitatively. Based on the new experimental and existing industrial data, critical operation characteristics could then be identified and analyzed. This information would, in turn, be used to develop an artificial neural network and semi-empirical models for this task. Model verification could then be done with new experimental data and independent data sets and also with extensive sensitivity analysis.

Unfortunately, several issues with available experimental techniques and measurement methods made any reasonable model development impractical.

- The relationship between many published experimental techniques and “operator appeal” is not well established.
- The complexity of the interactions described above reduces many “measurement” methods to subjective assessments (e.g. arc stability).
- Those methods that do produce quantitative measurements lack sufficient precision for model development without much larger data sets than were available.

The effort required to resolve these issues was beyond the capabilities of the resources available. The result was a shift in focus to the remaining aspects of the welding process for which modeling was considered far more feasible.

Weld Pool and Thermal Cycle Modeling

Description of thermal cycle and weld pool shape as a function of welding process parameters has been studied extensively in the past and continues to be investigated by many researchers [9,10]. Due to the enormous literature on this subject, only salient features are outlined. The models can be classified into two categories.

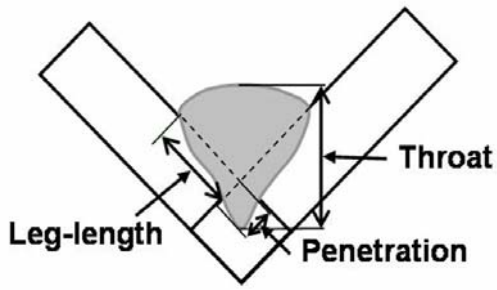

Figure 5: Geometric Parameters of Fillet Weld

The first category is the analytical models, which uses modified forms of solutions to heat transfer equations developed by Rosenthal to predict weld pool shape and thermal cycle [9]. Analytical and computer models are available to describe the thermal history at various locations of a weldment. However, these models are not easily extended to a wide range of welding processes.

The second category is the numerical heat transfer models with or without consideration of fluid flow conditions [10]. These models are based on the numerical solution of the equations of conservation of mass, momentum and energy in two or three dimensions. Although, these models are powerful and can describe fine details of the weld pool development, they are computationally intensive and require considerable expertise in the computer systems.

The complications of the numerical models increase if the consumable effect is considered [10]. Numerical models are often cumbersome, computationally intensive and often not suited for process optimization. Recent work has shown that by calibrating analytical models or coupling neural network models with experimental parameters such as weld pool width and depth [26], one can obtain sufficiently accurate results that eliminate the above-cited limitations. However, the challenge is to describe the effects of shielding gases in the solid wire electrode GMAW process and that of metal powder addition in the cored wire electrode GMAW process.

This project extended the above work and developed a generalized methodology to relate the welding process, consumable parameters and joint design to weld pool geometry and thermal cycles. The goal of this modeling is to predict the typical fillet weld pool geometry

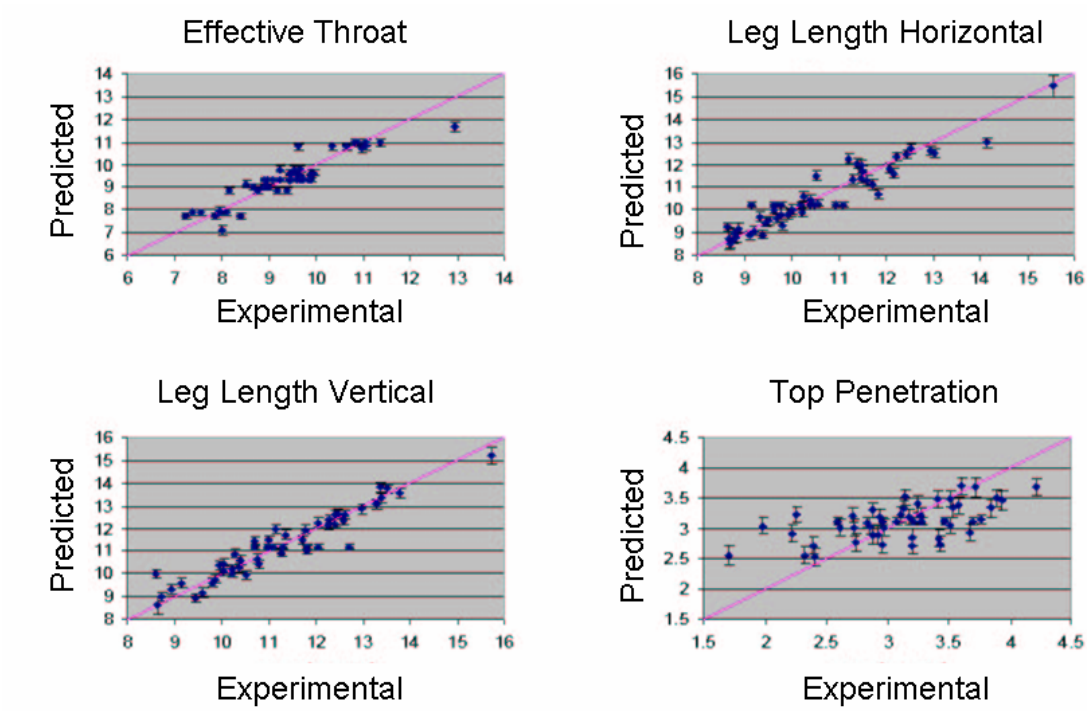

Figure 6: Comparison of Predictions with Simple ANN model with Experimental Data

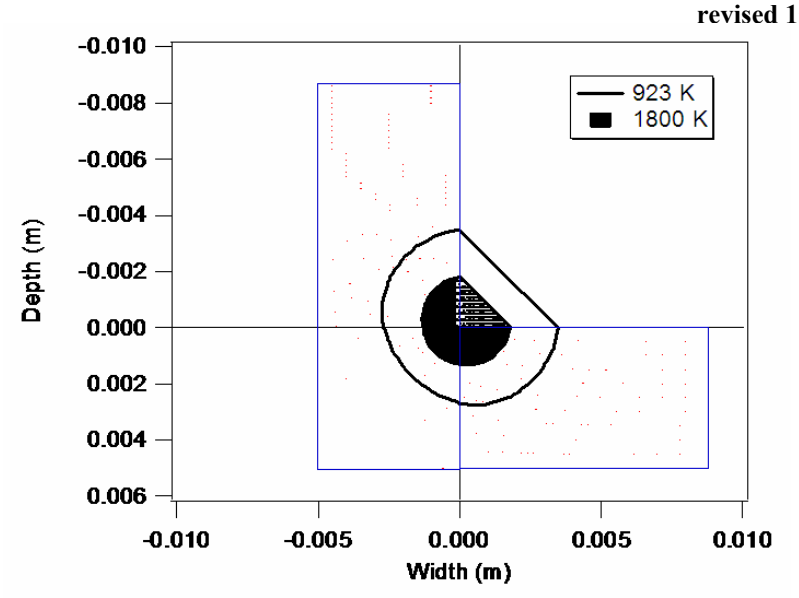

Figure 7: Typical result of analytical model

characteristics as shown in Figure 5. Additional goal is to predict the weld thermal cycles at different locations. The following discussion shows the steps taken to develop this model.

Simplified ANN Model for Weld Pool Shape

Extensive data on weld pool geometry as a function of different process parameters was used for artificial neural network (ANN) modeling of weld pool shape. Different sets of ANN models were developed to relate the six input variables to different outputs. The predictability of effective throat, leg length horizontal, and leg length vertical were good as demonstrated by the position of data points with reference to line of ideality [see Figure 6]. However, the predictability of top penetration was poor, since the predicted values show no correlation with experimental values. Careful analysis of data showed that this is related to large errors in the measured values of top penetration for a given welding process condition. Further work to address this problem was not considered viable. Therefore, the project direction was changed to the development of analytical and numerical models.

Analytical Models for Fillet Welds

The analytical models are indeed faster and will allow for rapid evaluation of process parameters. Therefore, extensive literature review was made to see if there are any simple analytical models for fillet weld geometry. The review lead to a classic paper by Jeong and Cho who have developed an analytical solution to predict the transient temperature distribution in fillet welds [27] using conformal mapping. The model was extended to the current research. Typical prediction is shown in Figure 7. The figure shows the weld pool (shaded) and also the HAZ regions. Careful analysis of the predictions showed that these models are applicable only for the HAZ region of the fillet welds. In addition, these models ignore the effect of weld pool fluid flow. As a result, the model could not be used for the weld metal regions of the fillet weld. Therefore, to allow for the realistic prediction of fillet weld pool shape with due consideration of convective fluid flow, numerical heat and mass transfer models was selected for the next step.

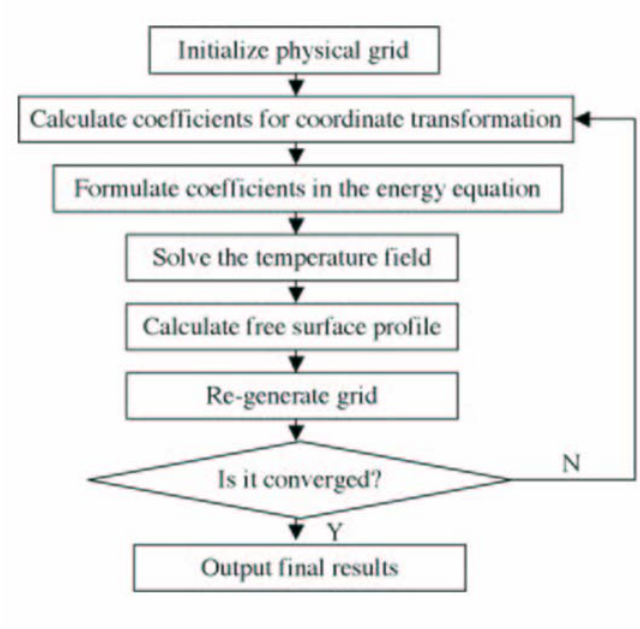

Figure 8: Schematic of the overall procedure for temperature calculation during fillet welding

Comprehensive Heat and Mass Transfer Numerical Model

The numerical methods that consider heat and mass transfer during welding were developed for bead on plate welds. While this simple geometry may be useful for research purposes, it is of little commercial significance. Consequently, a fundamental framework for weld bead shape control based on science in real welds with complex geometry and with filler metal additions became the overall focus. The basis for the computational methodology to describe the weld pool shape in fillet welds [28] is briefly described as follows.

Methodology

In the present investigation, as an initial step to understand the transport processes during fillet welding only the temperature field calculation is undertaken. Convection in the weld pool is ignored. Therefore, the calculations are strictly valid for low Peclet systems. It should be noted that conduction calculations might not always lead to an accurate prediction of the weld pool geometry. However, it can be shown later in this report that several important geometric features of fillet welds, such as the weld pool shape, leg lengths, finger penetration and the solidified surface profile can be reasonably calculated in many cases. For welding conditions with high welding speed and low heat source power, the effect of convection on the weld-pool heat transfer is usually comparable to that of conduction (i.e., Peclet number is low). For such cases, conduction calculation can provide reasonable predictions of fillet weld geometry.

A boundary fitted coordinate system is employed to solve the temperature field in the complex physical domain. The governing energy equation and boundary conditions are transformed into the curvilinear coordinate system. The transformed equations are then discretized and solved in a simple rectangular computational domain. Figure 8 is a schematic diagram showing the overall procedure for the temperature field calculation during fillet welding. The following simplifications and assumptions are used in the present study:

1) Convective heat transfer in the weld pool is ignored.
2) The heat flux from the heat source at the top surface is approximated by a Gaussian heat distribution. Furthermore, the effect of droplet sensible heat in affecting weld pool heat transfer is included by incorporating a cylindrical heat source within the weld pool.
3) The physical properties of the material such as the density and the thermal conductivity are assumed independent of temperature.

Coordinate Transformation

Calculating temperature distribution during fillet welding requires solving the energy equation in a domain of complex geometry. Therefore, it is convenient and desired to transform the complex geometry into a simple geometry and then solve the transformed energy equation in the simple geometry. As shown in Figure 9, the Z direction in the physical domain is transformed into the ζ

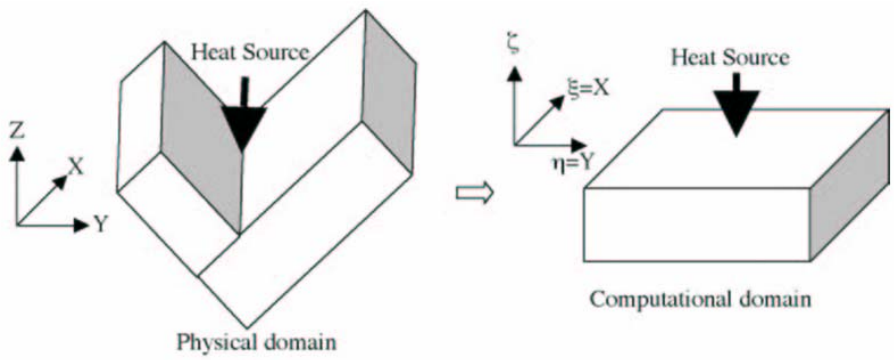

Figure 9: Schematic showing coordinate transformation

direction in the computational domain. The X and Y directions remain untransformed, since the grid system will be adjusted only in the Z direction to fit the top free surface profile. The advantage of the domain system (shown in Figure 9) is that only one coordinate direction (i.e., Z direction) needs to be transformed and, therefore, the transformation procedure is greatly simplified.

Simulation of Metal Droplet Transfer

During fillet welding, the electrode's tip melts and forms metal droplets. The transfer of metal droplets into the weld pool delivers excess heat to the molten pool and is responsible for the characteristic pool shape with finger penetration at high arc currents. In this study, the heat transfer from the metal droplets was approximated by considering the existence of a cylindrical volumetric heat source in the weld pool. Then, energy transported by the droplets was assumed to be uniformly distributed in the cylindrical cavity. Three parameters are required to define the cylindrical heat source:

- the depth of the cylindrical cavity.
- the radius of the cylindrical cavity, and
- the power density (J/m3-s) of the cylindrical source.

The parameters such as the droplet size, shape, velocity, and transfer frequency are prerequisite to calculate the dimension of the cylindrical source.

Typical Calculations

The 3-D heat transfer and fluid flow code developed at PSU was modified to implement the solution of energy equation in the curvilinear coordinate system discussed in the previous sections. Two case studies were carried out to validate the model using the experimental results of fillet welding from the industrial partner. The materials properties are summarized in Table 1 and the welding parameters in Table 2. The droplet parameters and the dimension and power density of the cylindrical volumetric heat source used in the calculation are also given in Table 2.

Table 1: Physical properties of the low carbon steel used in the calculation

Physical Property	Value
Liquidus Temperature, T_L, (K)	1785.0
Solidus temperature, T_S, (K)	1745.0
Density of liquid metal, ñ, (kg/m^3)	7.8×10^3
Thermal conductivity, k_S, (J/m·s·K)	25.1
Thermal conductivity, k_L, (J/m·s·K)	125.5
Specific heat of solid, C_{PS}, (J/kg·K)	703.4
Specific heat of liquid, C_{PL}, (J/kg·K)	808.1
Surface tension coefficient (N/m)	1.2

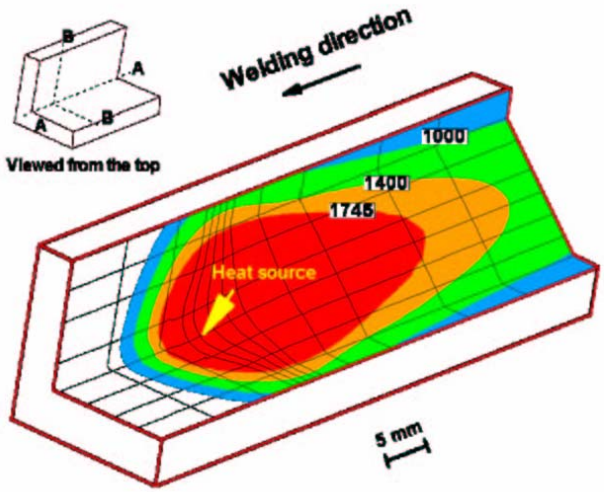

Figure 10: Calculation of temperature field at the top surface.
The temperatures are given in Kelvin. The solid line represents the grid system used in the calculation

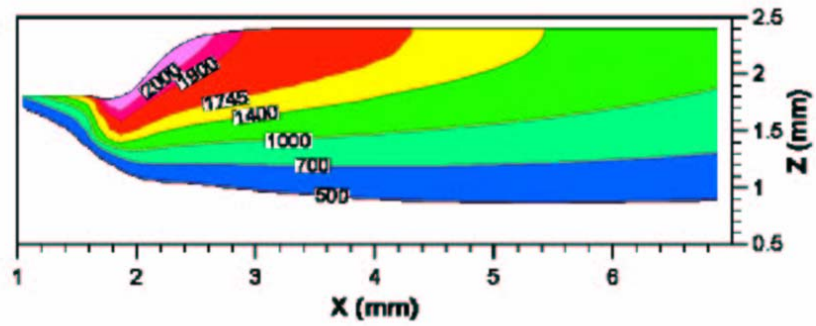

Figure 11: Calculated temperature field, longitudinal section A-A in Figure 10.
The temperatures are given in Kelvin.

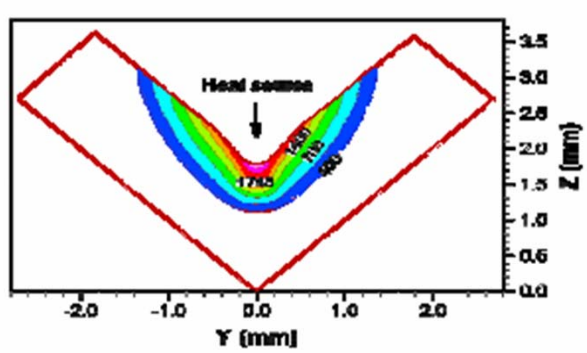

Figure 12: Calculated temperature field just under the heat source, section B-B in Figure 10.
Temperatures are in degrees Kelvin.

Table 2: Welding parameters used in the calculation

Welding parameter	Case #12	Case #23
Arc current (A)	312.0	286.8
Arc voltage (V)	33.0	31.0
Arc efficiency (%)	40.0	53.0
Arc radius (mm)	5.0	5.0
Welding speed (mm/s)	6.35	6.35
Wire radius (mm)	0.6604	0.6604
Wire feeding rate (mm/s)	169.3	169.3
Droplet radius (mm)	0.8	0.8
Droplet transfer frequency (Hz)	105	92
Droplet velocity (m/s)	1.2	1.2
Radius of the cylindrical heat source (mm)	1.6	1.6
Depth of the cylindrical heat source (mm)	4.5	4.0
Power density of cylindrical heat source (J/mm^3-s)	33.6	33.6
Note: In these experiments, the torch angle is 270° and the part angle is 180°.		

Table 3: Welding process parameter range used in the development of ANN

Variables	Minimum	Maximum	Mean
Arc current (Amp)	**200.0**	**410.0**	**326.3**
Arc voltage (V)	**25.0**	**42.0**	**33.8**
Welding speed (mm/s)	**4.2**	**8.5**	**6.4**
Wire feeding rate (mm/s)	**120.0**	**290.0**	**199.6**
Arc efficiency	**0.3**	**0.6**	**0.5**
Arc radius (mm)	**4.0**	**6.5**	**5.1**
Arc distribution factor	**0.5**	**3**	**1.4**
Droplet efficiency	**0.1**	**0.2**	**0.13**
CTWD (mm)	**17.5**	**30.0**	**23.4**
Wire radius (mm)	**0.5**	**0.9**	**0.7**
Effective thermal conductivity (J/m-sec-K)	**83.6**	**543.4**	**298.5**
Effective viscosity (Kg/m-sec)	2.0×10^{-2}	21.0×10^{-2}	7.9×10^{-2}
Density (Kg/m3)	**7000.0**	**8500.0**	**7742.1**
Solidus temperature (K)	**1690.0**	**1790.0**	**1741.7**
Liquidus temperature (K)	**1745.0**	**1815.0**	**1784.6**
Enthalpy of solid at melting point (kJ/Kg)	**731.5**	**1149.5**	**1002.4**
Enthalpy of liquid at melting point (kJ/Kg)	**1045.0**	**1463.0**	**1280.2**
Specific heat of solid (J/Kg-K)	**543.4**	**794.2**	**677.0**
Specific heat of liquid (J/Kg-K)	**689.7**	**919.6**	**789.7**
Thermal conductivity of solid (J/m-sec-K)	**14.6**	**40.5**	**26.9**
Coefficient of thermal expansion (1/K)	**0.0**	1.7×10^{-5}	9.1×10^{-6}
$d\gamma/dT$ of pure material (N/m-K)	-5.5×10^{-4}	-2.5×10^{-4}	-4.2×10^{-4}

A 53 × 66 × 34 grid system was used in the calculation and the corresponding solution domain had dimensions of 100 mm in length, 54 mm in width and 45 mm in depth. The calculation converged within 5000 iterations, which took about 4~5 minutes in PC with 2.8 GHz CPU and 512 Mb Memory.

The calculated temperature field viewed from various directions is shown in Figures 10, 11, and 12 where the weld pool boundary is represented by the 1745 K solidus isotherm. As shown in these figures, the weld top surface is severely deformed due to the effect of the arc force. The liquid metal is pushed to the rear part of the weld pool, which forms weld reinforcement during solidification. The isotherms are largely elongated due to the high welding speed.

The same model was further developed to consider the convective conditions too and the detailed are presented in various publications [28, 29, 30, 31]. The evaluation of these predictions is presented in the next section.

Comprehensive Artificial Neural Network Based on Comprehensive Numerical Model

Although the above heat transfer and fluid flow model was comprehensive and showed good correlation with experimental data, the use of these models was not straightforward. The model has to be run over the network and took several minutes to set up and run. This limited the use of these models by the welding engineers at the participating industry. Therefore, alternative approach, which has similar predictive power, however, simple to use was needed. To address this need, the numerical heat transfer and fluid flow model was run for wide range of welding process parameters. The input parameters for the neural net included arc current, arc voltage, welding speed, wire feed rate, arc efficiency, arc radius, arc distribution factor, droplet efficiency, contact tip to work distance, wire radius, material type, effective thermal conductivity, effective viscosity, density, solidus, liquids, enthalpy of solid at melting point, enthalpy of liquid at melting point, specific heat of solid, specific heat of liquid, thermal conductivity of solid, coefficient of thermal expansion, and the magnitude of surface tension with temperature. The output of the model is penetration, actual throat, leg-length, length of pool, peak temperature, and the maximum cooling time between 800 to 500 ^{o}C. The neural net was developed using genetic algorithms. The final artificial neural net was coded into a simple Java application. The graphical user interface and a typical use scenario of the model are shown in Figure 13. This tool has similar predictive power as that of comprehensive numerical heat transfer and fluid flow mode, but, it is easy to use and fast. The only limitation is that the model is applicable only to the welding process parameter ranges [see Table 3] which are used as input to develop this artificial

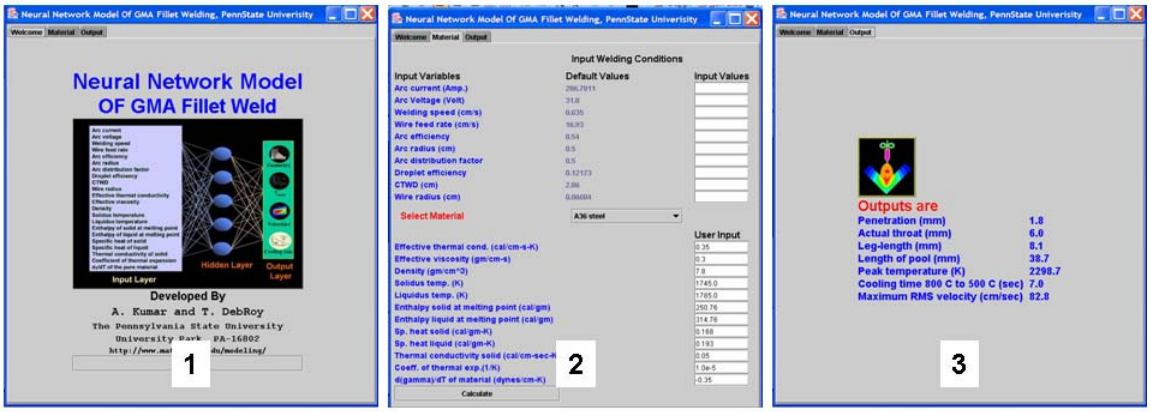

Figure 13: The graphical user interface for ANN that is based on comprehensive heat transfer and fluid flow model.

The numbers correspond to steps taken to calculate weld pool shape using this tool.

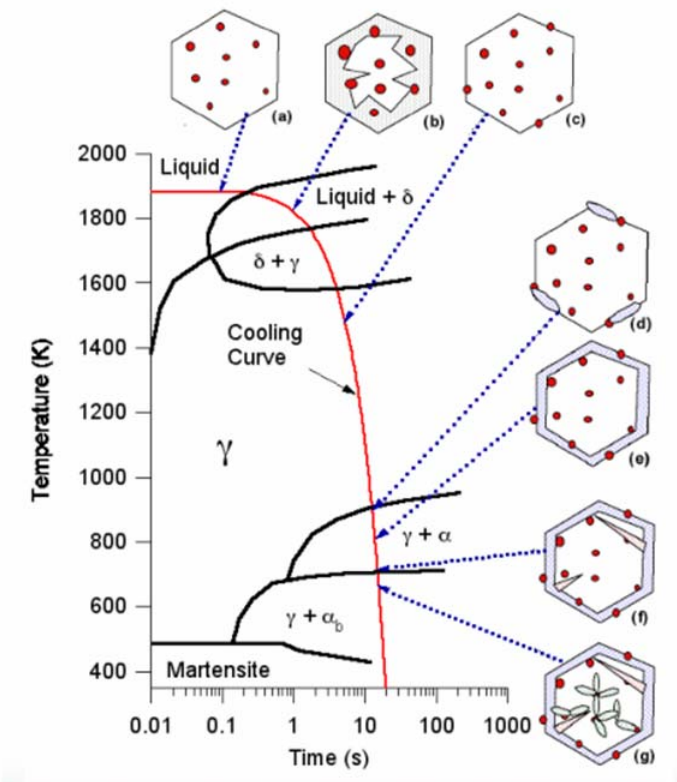

Figure 14: Schematic Illustration of Various Phase Transformation That Lead To Final Weld Microstructure

neural net.

Microstructure Model Development

Similar to weld thermal cycle and pool shape prediction, extensive knowledge exists on relating weld thermal history to microstructure development in steel welds [17,19,32, 33]. Models have been developed that are based essentially on relating thermal history to weld metal hardenability. Bhadeshia et al used quasi-chemical models to relate the driving force for formation of ferrite from austenite to the hardenability of steel [17]. These driving force values were used to calculate paraequilibrium conditions between austenite and ferrite. Diffusivity data were used to calculate growth rates of ferrite in austenite. With these calculations and the weld thermal cooling curve, the microstructure development in Fe-C-Mn-Si low alloy steel welds was described. In other methods, the cooling time between 800 to 500°C and carbon equivalence was used to estimate the volume fractions of ferrite, bainite and martensite [32].

This model will utilize the thermal history data predicted by the previous module and will estimate the volume fractions of microstructural phases. As mentioned earlier, the model will be developed in a modular fashion in order to be able to couple it with the modules for operational characteristics and thermal cycle. Model development will involve some experimental characterization using optical microscopy.

Microstructure Modeling Methodology

The microstructure modeling methodology was developed to describe various reactions that occur in the weld as shown in Figure 14. The phase transformations including (a) inclusion formation, (b) solidification to δ-ferrite, (c) austenite formation from δ-ferrite, and (d to g) decomposition of austenite to various α-ferrite morphologies (i.e. allotriomorphic ferrite, Widmanstätten ferrite, Bainite and acicular ferrite) were considered. The inclusion model used the published model presented in the literature [34,8]. The solidification models are based on kinetic and interface-response function theories [35, 36] and solid-state transformation are based on paraequilibrium transformation of austenite to ferrite [37, 38]. It is important to note that microstructure evolution at high-temperature affects the transformation at low temperature. For example, inclusion formation affects the acicular ferrite formation [39]. Therefore, the cooling rate experienced by the weld metal affects the microstructure evolution.

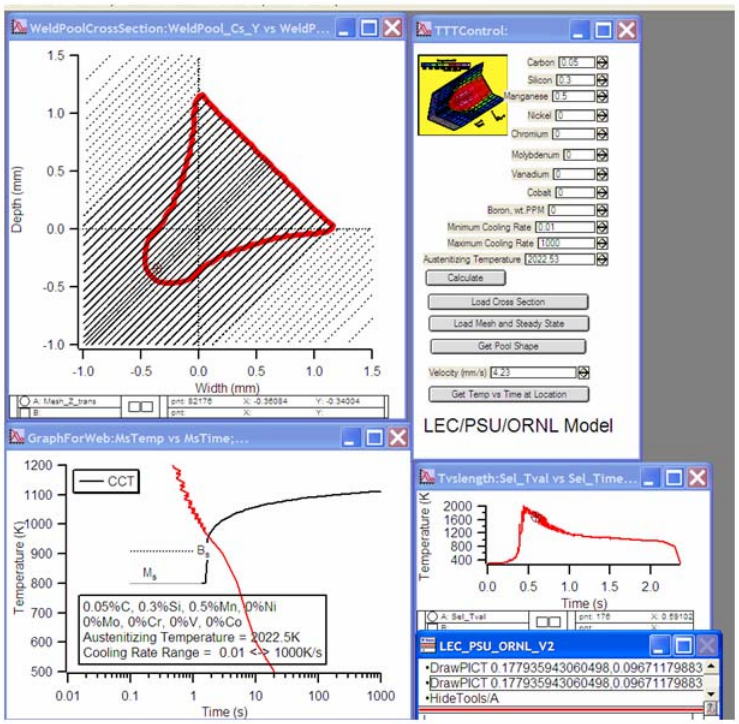

Figure 15: Interface for linking of Comprehensive Numerical Heat Transfer Model with Microstructure Model

Linking of Thermal Model with CCT Diagram Model

To predict the microstructure, there is a need to know the change in cooling rate as a function of location within the weld metal region. Since the artificial neural net model calculates only the maximum cooling rate, we cannot get spatial variation of cooling rate. Therefore, there is a need to interface the phase transformation models with predictions from comprehensive numerical heat transfer and fluid flow models. This interfacing was performed with graphical software IgorPro. The interface is shown in Figure 15. This computational tool reads the output result from numerical model presented in earlier section and plots the weld pool shape. In addition, if the user moves the cursor to a particular location, it extract the predicted thermal cycle. Later, the computational tool calculates the continuous cooling transformation model based on paraequilibrium transformation models. Finally, thermal cycles and the continuous cooling diagrams are overlaid on each other. This tool is very useful, since the user can interrogate the spatial variation of cooling rate and change in weld metal composition too. If the cooling rate is faster than the critical rate, the model would predict the formation of martensite. This tool can be used for designing new weld metal composition, for a given weld pool shape and spatial variations of cooling rate.

Although, this model is powerful, it also suffers from the disadvantage of needing to run numerical heat transfer models to obtain the spatial variation of cooling rate. To address this limitation, use of a simple microstructure model [see Figure 16] can be resorted before the use of detailed models. These simple microstructure models are already developed by ORNL and are available at Internet [40]. This microstructure model is based on carbon equivalence developed by Ion, Easterling and Ashby [41].

Modeling Transition from Bainite to Acicular Ferrite

During the model development for microstructure, there was an absence of predictive models to describe the transition from bainitic microstructure to acicular ferrite microstructure [42]. This phenomenon is observed in certain weld metals when small change in inclusion characteristics occurs. For example, in a C-Mn steel weld metals when the inclusions are not titanium rich, the predominant microstructure is bainitic [see Figure 17a]. However, with the addition of small titanium content, the weld metal contained titanium rich compounds on the inclusion surfaces and also lead to the predominantly acicular ferrite microstructure. To describe this transition, a phase

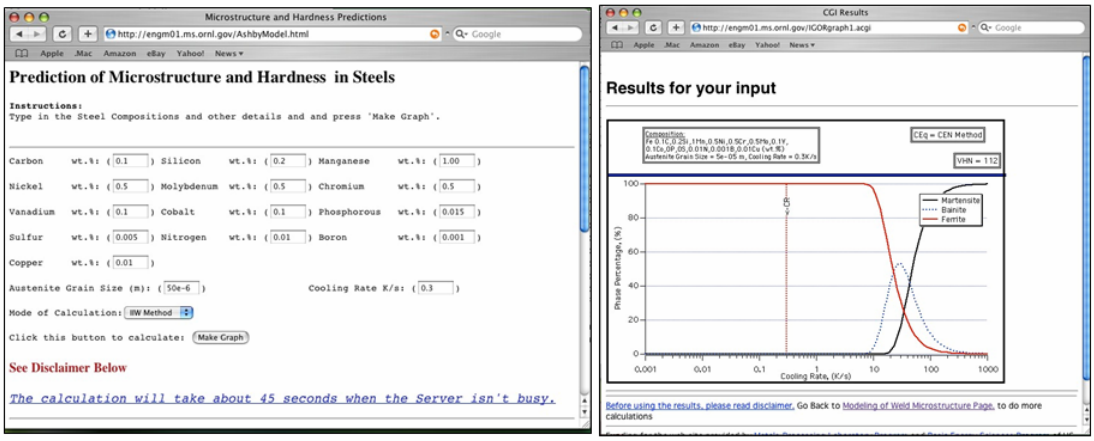

Figure 16: Internet based simple microstructure calculation as a function of composition and average cooling rate

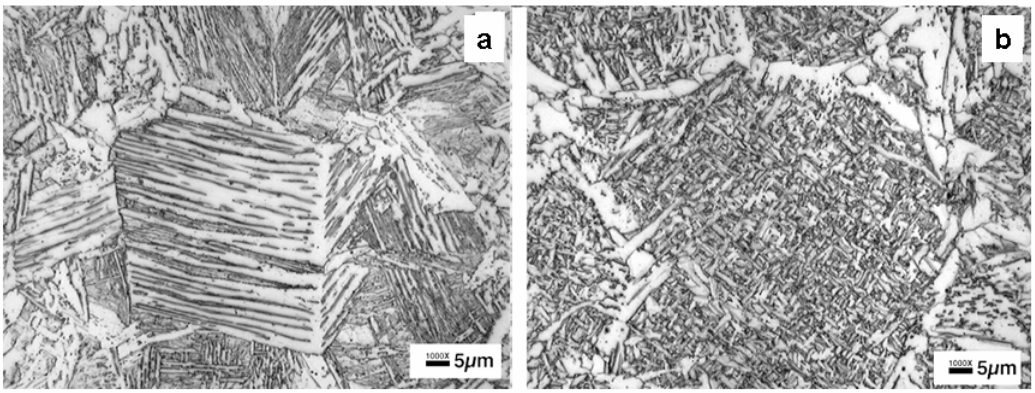

Figure 17: Microstructural Transition from bainite to acicular ferrite due to a change in inclusion content

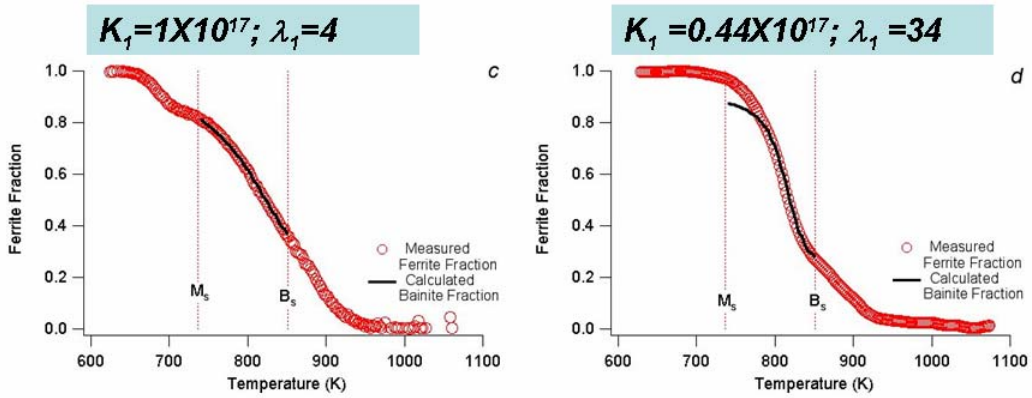

Figure 18: Comparison of predictions from bainite / acicular ferrite transformation kinetic model

transformation model for bainite and acicular ferrite was developed. This model considers the nucleation site density (K1) and autocatalysis factor (λ). The calculations indicated that the autocatalysis factor for acicular ferrite is higher than that of bainitic microstructure. The comparison of model and experimental data are shown in Figure 18.

Process-Microstructure-Property Correlation Models

A quantitative description of microstructure-property correlation is one of the crucial links to the hybrid integrated tool. Past work on relating microstructure to properties can be classified into three categories. The first is based on developing analytical equations describing strength parameters and using work hardening and dislocation pileup theory [43]. The second is based on developing semi-empirical relations between microstructure and flow properties [19]. The third approach is based on developing artificial neural networks to describe complex relations between microstructure and all properties such as yield, tensile and toughness [44]. The first two methods are based, to a large extent, on fundamental relations. However, the application of these methods to the complex, multiphase microstructure of low-alloy steel weld metal is complicated and necessitates further detailed research.

Recent Basic Energy Science welding research has shown that it is indeed possible to relate the local microstructural changes to weldment strength properties in a quantitative way [45,19]. However, this research is in its infancy and further work is necessary before it can be used as an optimization tool. Therefore, artificial neural networks was developed to relate the welding process parameter, composition and post weld heat treatment to the mechanical properties including yield strength, ultimate tensile strength, elongation and toughness. Based on experimental information available from the industrial partner, published literature [46], a generalized quantitative methodology was developed to relate microstructure to properties such as strength, ductility and toughness. This neural net was also coded into a simple graphical user interface and is shown in Figure 19. This model has been extensively tested by the participating industry and the results of the comparisons are presented in the next section. At this point, all the individual modules that are needed for hybrid model development have been developed. This indeed satisfies the primary aim of the overall goal of the proposed research.

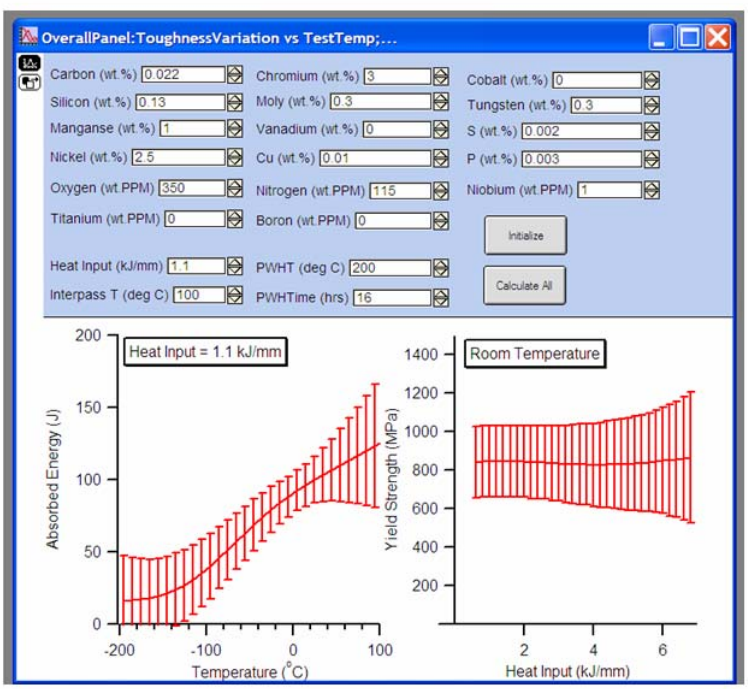

Figure 19: A user-friendly ANN model for weld metal strength and toughness

Model Integration

The next goal was to integrate all the individual software modules into a single application. This step was indeed proved to be

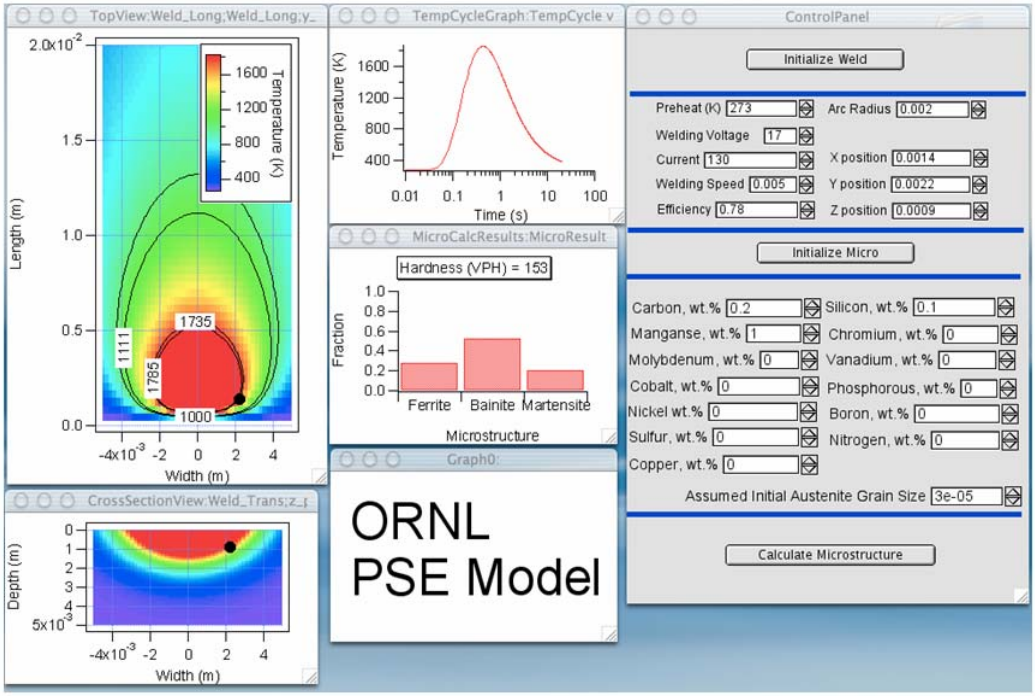

Figure 20: A Simple Problem Solving Environment Model for weld microstructure and hardness as a function of steel composition and weld cooling rate

challenging and lead to lot of obstacles. The obstacles were related to the lack of computational infrastructure to do this effectively over three organizations. The shortcomings are listed below:

- Lack of seamless coupling of these software modules
- Need for dedicated expertise in running the model as well as Internet Technology
- Lack of flexibility to interrogate the software model sensitivity very easily
- Lack of computational tools that can run over different computational platforms

It has been demonstrated [47] that these obstacles can be overcome by using Java based client-server tools. This was accomplished using the concepts that relate to problem solving environments (PSE). However, the resources needed to do the same for the current project was beyond the allocated funds. Therefore, attempts were made to develop these integrated models with limited scope to demonstrate the applicability of the concept. This simple integration or PSE model was developed with IgorPro software for butt welds. This model calculates the weld heating and cooling using simple Rosenthal type equations and the microstructure was calculated using Ion, Ashby and Easterling model. The interface is shown in Figure 20. Using this tool, the industrial user can evaluate the following questions.

- What will happen to weld pool shape if the welding velocity increases?
- With the same increase in welding speed, what microstructure will result for a given chemical composition?
- What will be the hardness for the same condition?
- How can the process parameters be changed to obtain the desired microstructure?

In principle, the above tool can be expanded by coupling the same with ANN for the fillet weld pool shape [see Figure 13] and also paraequilibrium CCT model [see Figure 15].

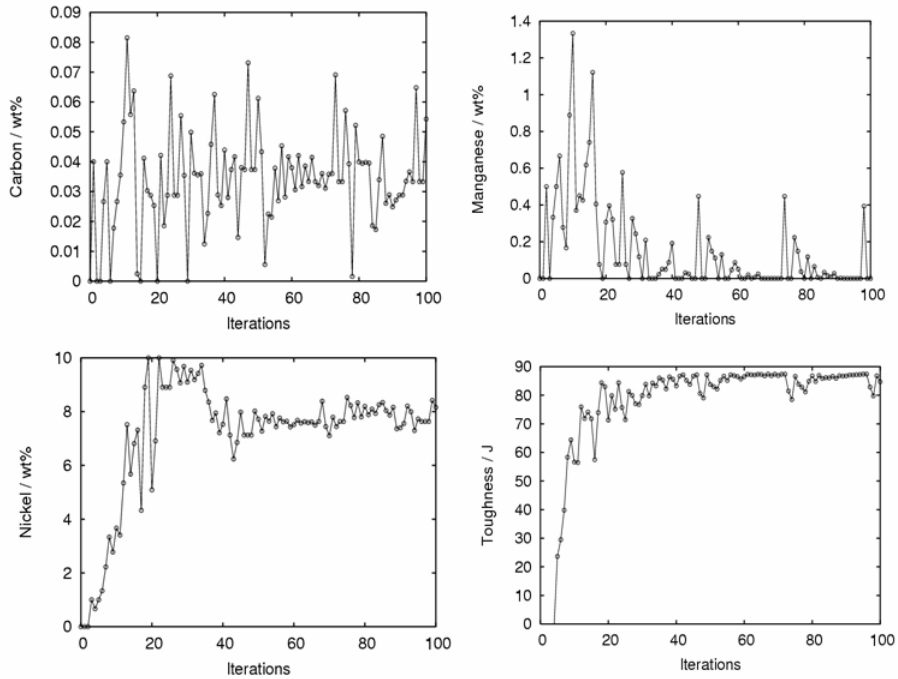

Figure 21: The graphs show that Downhill simplex optimization finds the optimum in only 67 iterations unlike any of the other optimization methods.

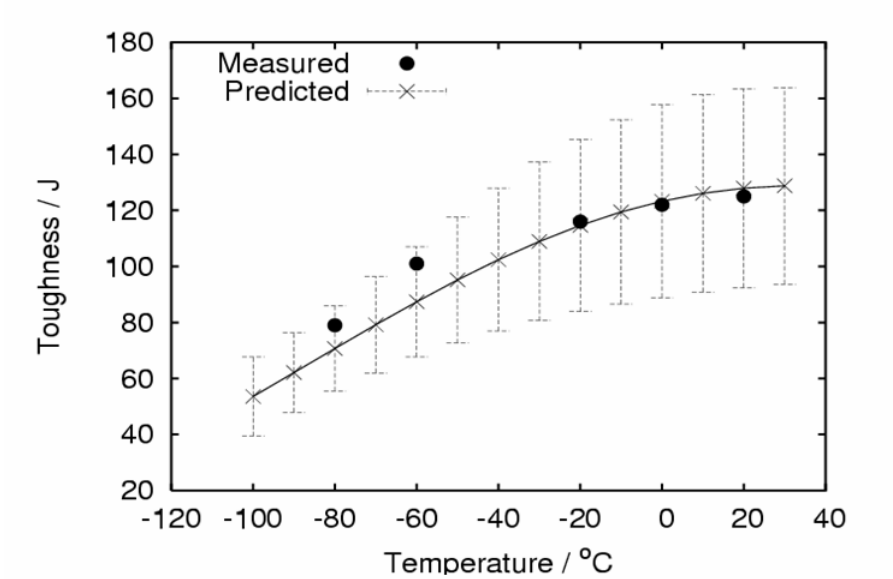

Figure 22: Comparison of Charpy toughness predicted using artificial neural network models and measured Charpy toughness values.

Optimization of Weld Metal Composition for Maximizing Toughness

If one can integrate all the software modules into one single computerized model, we can use the same to perform optimization. The optimization will allow the industrial user to achieve the optimum welding composition and process parameter to achieve the desired weld pool shape microstructure and mechanical properties. As mentioned earlier, the current research was not able to develop a fully integrated model due to computational issues. However, to demonstrate the feasibility of such technology, the optimization exercise was performed with the ANN model for toughness prediction [see Figure 19]. The charpy toughness model relates the welding process, process parameters and steel composition to toughness.

A commercially available optimization tool (EPOGY) was used for this exercise. The EPOGY software was given a target of achieving the maximum toughness at -20 ^{o}C. The EPOGY tool was instructed to change the concentration of carbon, manganese and nickel. The EPOGY tool was able to attain this goal by increasing the nickel content for a given welding process. The sensitivity to the optimization methodologies were also evaluated in this demonstration.

The optimization exercise utilized both linear and non-linear optimization routines. The linear methods tried to relate the inputs (welding process parameters and consumable design variables (Ni, Mn and C)) to the output (toughness) in a linear way and find the optimum. This method however failed to relate the trend in which the toughness varies with the change in inputs, thus supporting the widely accepted idea that composition and process parameters related in a non-linear way to toughness. Next, the following non-linear methods were evaluated namely

- downhill simplex,
- genetic optimizers, and
- sequential quadratic programming (SQP) methods.

Among the three methods, downhill simplex optimizers captured the trend in only 67 iterations when compared to the genetic and SQP which took 323 and 1836 iterations, respectively. Further, an advanced hybrid optimizer was also evaluated. The hybrid optimizers use any of the optimization techniques either linear or non-linear methods in a random way to find the global optimum. In the present case, the hybrid optimizers arrived at the optimum after 1600 iterations. However, the regions of the input space that was explored by each optimization technique varied. Nevertheless, all the techniques reported the same optimum composition. For the present case, considering the lowest number of iterations taken by the downhill simplex method, it is considered to be the best. But, downhill simplex did not explore all of the input regions. Hence, the possibility of getting into a local optimum is always there. In this case, hybrid optimizers may be relied upon.

A typical optimization run to arrive at optimum carbon, manganese and nickel concentrations using downhill simplex method is shown in the Figure 21. The predicted weld composition and its calculated toughness data are compared with already published data [see Figure 22] and were in good agreement.

Experimental Evaluations

During the course of this research, many experimental welds were produced and their physical characteristics as well as chemical and mechanical properties were measured. Microstructures were characterized and reconciled with the weld thermal cycle predictions and predicted vs. measured properties.

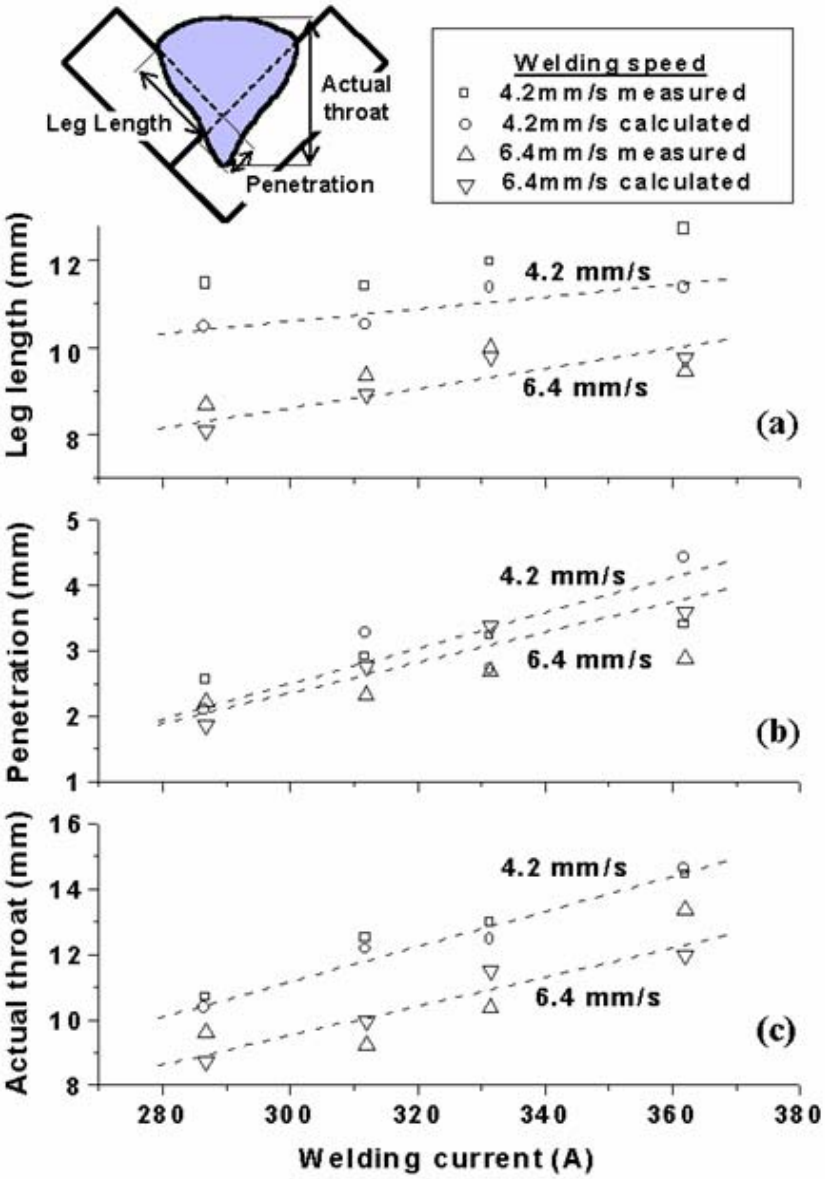

Figure 23: Weld bead geometric parameters as a function of the current and welding speed: (a) leg length, (b) penetration, and (c) actual throat.

The dashed lines are plotted by fitting the computed data.

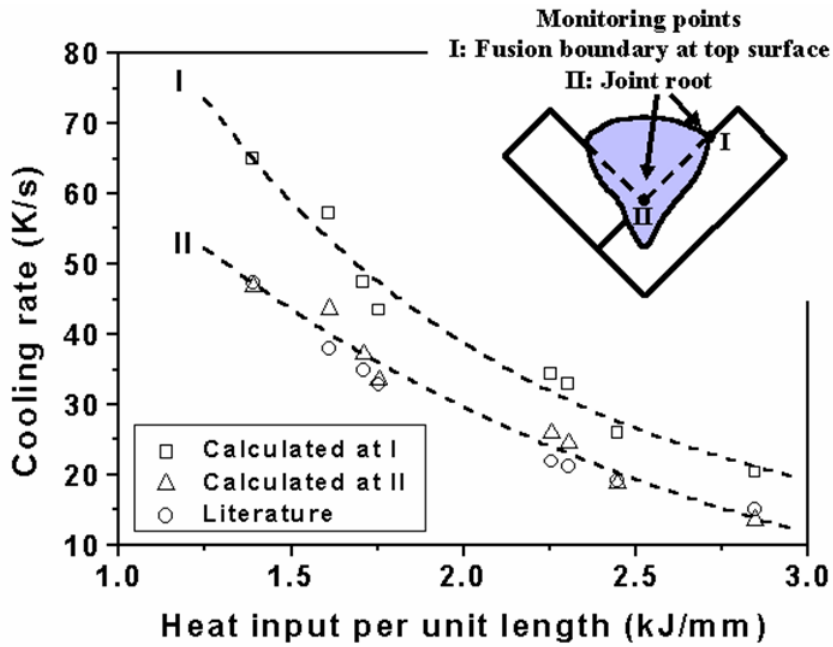

Figure 24: Comparison of cooling rate predicted by numerical model at different locations and published data at the same locations

Weld Thermal Cycles and Weld Pool Geometry

Measurements from a large body of fillet weld data for various solid wire electrodes of the Fe-C-Mn-Si type were used to supplement the numerical methods used for this model development. The welds represented the full range of operable conditions for the GMAW electrodes using Argon-CO_2 shielding gas.

Experimental verification was conducted for the weld pool geometry module by fabricating and sectioning additional fillet welds made under controlled welding conditions. These welds were made using AWS A5.18 ER70S-3 solid wire electrode. Because the relevant thermal properties do not vary for Fe-C-Mn-Si and low alloy steel weld metals, there was no need to test a broader range of materials for comparison with the bead shape and penetration profile predictions. This part of the study focused on spray transfer GMAW, Argon-CO_2 shielding gas, 29 to 35V voltage range, and 6.5 to 18.5 ipm travel speed range. Other factors studied include torch angle, part angle and contact tip to work distance. As many as three metallographic sections were prepared per weld by polishing to 1 micron and etching with 2% Nital.

The numerical heat transfer model was used to calculate the temperature field and solidified surface profile during GMA fillet welding for a variety of welding conditions. The calculated weld bead geometry was compared with that measured experimentally. It was found that the calculated shape and size of the fusion zone, finger penetration characteristic of the GMA welds and the solidified free surface profile were in fair agreement with the experimental results for various welding conditions. As shown in Figure 23, the computed values of important geometric parameters of fillet welds, i.e., the leg length, the penetration depth and the actual throat, agreed well with those measured experimentally. Furthermore, the calculated cooling rates were also in good agreement with independent experimental data, as shown in Figure 24.

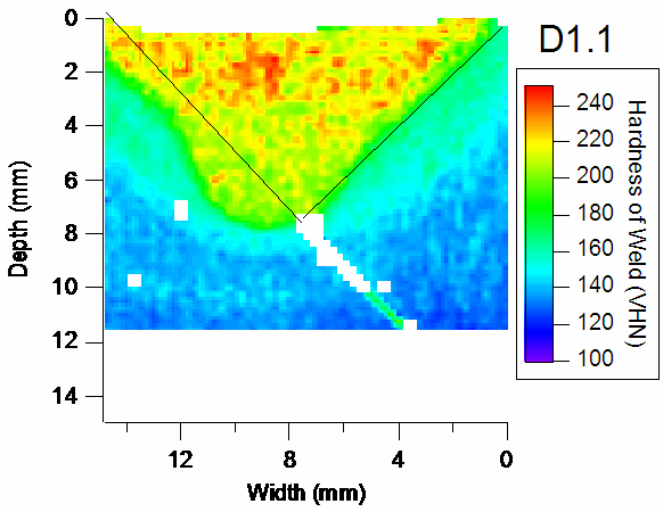

Figure 25: Spatial distribution of hardness in a fillet weld shown in an image format

Microstructure and Hardness

Groove welds were fabricated using Fe-C-Mn-Si electrodes in both solid wire and cored wire form. The purpose of the groove welds was evaluation of the microstructure development and microstructure-property correlation modules. These experimental welds were characterized with optical microscopy and electron microscopy and tested for weld metal chemical composition, strength, and Charpy V-notch toughness.

Although the modules were developed for Fe-C-Mn-Si GMAW, engineers were anxious to begin using the tools for other arc welding processes and alloy systems. Accordingly, several other weld sets were prepared using gas-shielded flux cored arc welding (FCAW-G), shielded metal arc welding (SMAW). A few test welds were prepared using GMAW with higher alloy level electrodes. In addition, a limited number of welds were used to evaluate the preheat/post-heat features of the modules.

The calculated cooling rates [see Figure 24] for the fillet welds showed interesting phenomena.

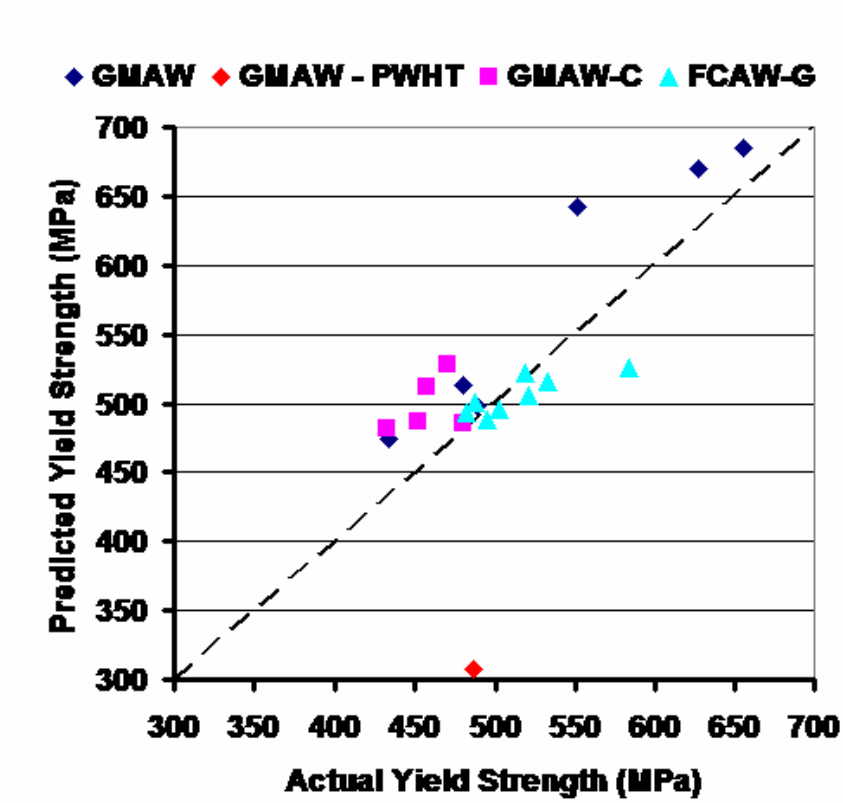

Figure 26: Comparison of predicted yield strength and measured yield strength

Different markers correspond to different welding processes.

The cooling rates in the region II are lower than region I. Simple evaluation of the same with the microstructure and hardness model [see Figure 16] indicated that this must lead to harder microstructure in region I compared to Region II. To evaluate this prediction, hardness measurements were made as a function of spatial location. These measurements were made with an automated hardness tester. The measured results are shown in an image format in Figure 25. The measurements show that the hardness near the surface (including the region I) are harder than the hardness near the root of the weld (including the region II). This measurement is indeed in agreement with the predicted trend.

Mechanical Property Correlation

The mechanical property ANN model has been extensively evaluated by the industrial user in this research. Comparison of the predicted yield strength with experimental measurements is shown in Figure 26 and shows good agreement. It is interesting to note that the ANN model predictions were applicable to both GMAW as well as FCAW.

Accomplishments

The current research project indeed achieved the goal of developing software modules to predict the fillet weld pool shape, thermal cycles, microstructure, and properties for GMAW of steels.

The research developed an innovative approach to develop an artificial neural network models that maintain the essence of comprehensive heat and mass transfer model for rapid and easy prediction of fillet weld pool shape.

The models allow for the industrial users to predict the microstructure and hardness as a function of weld cooling rate and spatial location within the weld metal region.

The results of this research, methodology of the research, the scientific findings have been published in open literature. In addition, some of the software modules are available to be downloaded from Internet location.

The design of welding consumable composition by coupling welding model and optimization tools was demonstrated.

This project demonstrated that the hybrid model is the right approach to transition the academic and scientific models of welding process, microstructure and properties to the welding industries quickly.

Conclusions

The current research project developed hybrid integrated model to predict the weld pool shape, weld cooling curve, microstructure, hardness and mechanical properties.

A new approach was developed to predict the fillet weld pool shape using co-ordinate transformations and by solving conservation of mass and momentum of liquid steel as a function of welding process parameters.

Numerical heat transfer and fluid flow model calculations were used to develop an artificial neural net model to predict the weld pool shape and cooling rate as a function of material and process parameters. This model maintains the accuracy of the numerical model and also rapid to evaluate by the industrial users. The predictions by these models were in good agreement with the experimental measurements.

Microstructure development in these welds was predicted by using paraequilibrium

transformation theories. The microstructure model was coupled with the predictions from numerical heat transfer and fluid flow models.

A user-friendly artificial neural net data that relates the welding process parameters and weld metal composition was developed and was delivered to the industry. The predictions of yield strength and toughness are in good agreement with the measurements.

The concept of integrating individual software modules was demonstrated. In addition, the concept of optimizing welding process parameters and consumable composition using these models was demonstrated.

Some of the software modules have already been released through Internet to public. The software tools will be evaluated extensively within the participating industry. After achieving sufficient confidence, improving the user interface, enhancing the robustness and with independent evaluations, the software tool will be marketed to the welding industry.

Recommendations

Most of the objectives proposed in the research have been attained. However, the research also indicated many challenges that still need to be considered. Some of the challenges have already been presented in the above sections. The following recommendations are made to address these challenges.

- Develop operational characteristics models to evaluate the arc stability and also fume generation
- Extend the model to slag based systems
- Develop computational tools to allow for easy integration of software modules
- Expand the optimization goal to include all the properties, i.e., strength, toughness, elongation, and creep-rupture properties to expand the application of these models to high-temperature use in energy and chemical industries
- Develop similar hybrid models for industries associated with welding, namely casting, forming, heat-treatment and surface processing

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