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On a General Parameterization for Inverse Analysis of Heat Deposition Processes

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A general parameterization for inverse analysis of heat deposition processes using incomplete or minimal experimental data is presented. This parameterization is considered general in the sense that it can be applied, in principle, to the inverse analysis of a wide range of different types of heat deposition processes, including welding. The structure of this parameterization follows from the concepts of model and data spaces that imply the existence of an optimal parametric representation for a given class of inverse problems. Accordingly, the corresponding optimal parametric representation lies in the model space and is determined by the characteristics of the available data sets spanning the data space and the nature of the data sampling for purposes of parameter determination via appropriate optimization techniques. The elements of the proof presented here provide an elucidation of certain aspects of inverse heat-deposition analysis that are important for practical application.

Keywords aluminum, joining, modeling processes, stainless steels, welding

1. Introduction

Recent advances in the area of dynamic data-driven application systems (DDDAS) (Ref 1, 2) have demonstrated the enormous potential benefits of inverse analysis in general. The inherent property of data-driven models exploited in these systems, which are intrinsically validated in that they encode the behavior (Ref 3, 4) of the systems they simulate, make them very attractive from a validation and verification perspective. Presented here is a mathematical analysis of a specialized approach to inverse analysis of heat deposition processes, which represents a particular category of the more general inverse problem concerning inverse analysis of heat transfer. Other investigators have also focused on various aspects of inverse problems related to heat deposition processes especially as they relate to the determination of heat fluxes via appropriate regularization of their spatial and time distributions (Ref 5). General aspects of the inverse-problem approach presented here, for the analysis of heat deposition processes, have been studied (Ref 6-9). These studies considered the specific physical characteristics of heat deposition processes that are relevant to using this inverse-problem approach for their analysis. This approach included the use of effective material properties and heat source distributions as adjustable quantities. These quantities are adjusted according to experimental data in order to constrain the temperature field self-consistently. Throughout these studies prototype analyses of welds were presented in order to demonstrate many of the details associated with practical application of this inverse-problem approach and its use for extraction of process parameters and parameters that may be correlated with material properties.

In the present study, the construction of a general parameterization is presented for the inverse analysis of heat deposition processes involving plate structures using incomplete or minimal experimental data. This parameterization is considered general in the sense that it can be applied, in principle, to the inverse analysis of all types of heat deposition processes, including welding, involving plate structures. The generality of this parameterization is examined in this study and follows from the concept of a model space that establishes the existence of an optimal parametric representation for a given class of inverse problems, i.e., inverse analysis of heat deposition processes. This property is related to the fact that inverse analyses based entirely on mathematical formulations representing physical theories are not generally well-posed in that these formulations are inherently based on direct-problem paradigms. The term "well-posed" here for an inverse problem is used in its usual Hadamard sense (Ref 10). According to it a solution exists, this solution is unique and it depends continuously on the data. In particular, the concept of a model space implies the existence of an optimal parametric representation for inverse analysis, which is not based on the existence of a complete set of representative physical theories, but rather on the characteristics, relative sizes, and completeness of data sets associated with or in practice available for that system.

A conceptual foundation of the inverse-problem approach requires modifications concerning the interpretation of mathematical representations of physical systems. Important points for such a conceptual foundation in the context of the present study are the following: (a) direct-problem analyses can be interpreted as inverse-problem analyses; (b) any mathematical representation based on basic physical principles can be interpreted as a parametric-function representation for purposes of system identification using inverse analysis; (c) all material properties are based on inverse-problem analyses that are in

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tern based on a parametric representations of various sets of experiments; (d) many aspects of the inverse heat conduction problem are ill-posed due to parameter sensitivity; and finally (e), parametric-function representations adopted for use in inverse methods tend not to be unique. Various aspects of these points as they are related to heat transfer have been given elsewhere (Ref 11-15).

This discussion continues in the next section (Section 2) with a description of the concepts and properties underlying the inverse-problem approach in general and its specific application for the analysis of heat deposition processes. The model space for heat deposition processes is discussed in Section 3 as it contains the various parameterizations available for establishing models for the associated processes. Section 4 presents a general formulation of the inverse-problem approach and representation of temperature field for inverse analysis of heat deposition processes involving plate structures. In particular, this section describes the set of basis functions available for determining the models that describe the associated temperature field for heat deposition involving plate structures. Section 5 presents a mathematical analysis of aspects of the inverse heat transfer problem as they relate, in particular, to the inverse analysis of heat deposition processes. Sections 6 and 7 present a prototype inverse analysis and its generalization, respectively, applied to deep-penetration welding of plate structures. Finally, a proof is presented in Section 8 for the existence of an optimal parametric representation of heat deposition processes. This proof establishes the feasibility of constructing a general parameterization of heat deposition processes that can be used for inverse analysis of all types of heat deposition processes, including welding. The last section presents the conclusions of this study.

2. Concepts and Properties Underlying Inverse-Problem Approach

The following concepts and properties concerning the inverse-problem approach considered here have been discussed and illustrated by various case study analyses referenced in the literature and are important for the understanding and application of this approach.

(1) The direct-problem approach to the analysis of heat deposition processes can be defined as a method in which the temperature field throughout the region of interest within the workpiece is predicted using either an explicit numerical solution of the coupled equations of energy, momentum, and mass transport or an explicit physical model based on analytical solutions to the heat conduction equation for a given set of boundary conditions. The direct-problem approach requires an a priori knowledge of the physical characteristics of the energy source and of the nature of its coupling to the workpiece. Further, this approach requires knowledge of the thermal and fluid flow properties, as a function of temperature, of the material making up the workpiece.

(2) The inverse-problem approach to the analysis of heat deposition processes can be defined as an approach in which the temperature field throughout the region of interest within the workpiece is predicted using a model representation whose form is relatively convenient or optimal for adjustment of parameters. The adjustment of parameters is according to the characteristics of the experimental data concerning the actual temperature field at various locations that are sufficiently distributed spatially and temporally through the region of interest within the workpiece. Parametric formulations can range from those that include detailed descriptions of the underlying physical processes to those characterized by interpolation functions whose forms are relatively simple.

(3) The inverse-problem approach presented here is formally equivalent to constrained parameter optimization of the simulated temperature field using parametric representations.

(4) A parametric representation based on a physical model, or direct-problem formulation, provides a means for the inclusion of information concerning the general physical characteristics of the process that is in addition to that provided by localized constraints, and therefore provides an implicit global constraint based on theory.

(5) Optimization criteria are satisfied in principle by minimization of an objective function, which is defined in terms of experimental data concerning the temperature field and associated heat deposition process that are sufficiently distributed in space and time.

(6) Procedures for minimization of the objective function can in principle be enhanced based on the observation that thermal profiles resulting from heat deposition processes can be represented by a relatively small class of geometric shapes.

(7) The upstream-to-downstream trend that is characteristic of all heat deposition processes, which for a given process follows from the relative motions of the heat source and workpiece, is a dominant feature of these processes. This upstream-to-downstream trend imposes a quasi-one-dimensional character on the temperature histories associated with heat deposition processes that can be utilized for inverse analysis.

(8) In general, information concerning material properties, fluid flow properties and the physical character of a given heat deposition process can be represented implicitly via a specified distribution of temperature values over a closed surface bounding a given region of the workpiece.

(9) The inverse-problem approach is well-posed, in general, for practical application owing to the availability of experimental information concerning the temperature fields of a wide range of heat deposition and joining processes. These processes include deep-penetration laser and electron-beam welding, all modes of conventional welding, friction stir welding, multipass welding, consumable electrode welding, and heat deposition processes such as laser or electron beam free-form fabrication. A fundamental aspect of these types of processes is that relatively large quantities of information concerning their character are "directly" observable.

(10) The uniqueness and sensitivity of the simulated temperature field relative to parameter optimization are dominant characteristics of the inverse heat conduction problem. The inverse heat conduction problem must be well defined relative to these aspects in order that it is not ill-posed.

(11) The concept of an apparent (or effective) heat source distribution as viewed from the perspective of a given region of interest within the temperature field represents a significant aspect of the inverse-problem approach for its application to the analysis of heat deposition processes. The inverse model to be applied is determined by the physical characteristics of the region of interest and not the characteristics of the regions bounding it.

(12) The types of experimental information that are useful for inverse analysis of heat deposition processes, e.g., welding, are solidification cross sections (transverse, longitudinal, and top-surface cross sections), thermocouple measurements, relative position and spatial character of energy source, energy per distance (a global constraint), top-surface shape features of the weld or as-deposited consumable element, and any information related to the temperature history of the heat deposition process including transformation temperatures that can be deduced from analysis of microstructure.

(13) Inverse analyses tend to compensate for fragmented or incomplete information concerning the detailed characteristics of a given heat deposition process.

(14) Models that are structured for inverse analysis tend to be insensitive to strong nonlinearities or sharp transitions in scale.

(15) Models that are structured for inverse analysis tend to be more efficient computationally than model representations based entirely on first principles or prior knowledge, i.e., direct-problem approaches.

(16) Direct-problem formulations tend not to be "data-driven," but require that the input of information be accomplished only through the assignment of values of physical parameters. These formulations are inherently not structured for the representation of overdetermined systems or systems whose characterization is in terms of large data sets.

(17) Direct-problem and inverse-problem formulations posses an interrelationship that is important with respect to analyses based on the inverse-problem approach. An aspect of this interrelationship is that all direct-problem based parametric representations may be adopted for inverse analysis, and that in general, direct-problem analyses can be interpreted as inverse-problem analyses. This interrelationship implies that a reasonable starting point for the formulation of an inverse-problem based parametric representation is to adopt a direct-problem based parametric representation as an initial ansatz for further modification (or optimization) according to the characteristics of the experimental data concerning the field quantities of interest.

(18) The general solution to an inverse problem is not a model of the system whose characteristics are considered for analysis, but rather a set of models that are consistent with both the data and a priori information concerning the system.

(19) The inverse-problem approach to the analysis of physical processes, or systems in general, has been applied to a wide range of applications. Among the many inverse problems associated with the analysis of physical systems, the inverse heat transfer problem defines a particular class of problems that are characterized by a particular range of system-response properties. Our inverse-problem approach considers a specific category of the inverse heat transfer problem, i.e., those associated with heat deposition processes. Further discussion concerning the inverse-problem approach in general can be found elsewhere (Ref 16-22).

In what follows we extend our development of an inverse-problem approach and present further examination of its general aspects and methodology. This extension is based on the concept of a model space, which is defined below. It is significant to note two aspects of inverse analysis that provide in general for the further development of its methodology. First, the problem of parameter optimization (Ref 23, 24) is to be considered separate from that of determining an optimal parametric model representation. These problems are related, however, in that an optimal parametric representation will provide for a well-conditioned parameter optimization. Second, the uniqueness and sensitivity of field quantities simulated by inverse analysis relative to parameter optimization are characteristics of the inverse problem that determine what is to be considered an optimal parametric representation of a given system. That is to say, what specific parametric representation provides for an inverse analysis that is well-posed.

3. Model Space for Heat Deposition Processes

Following the inverse-problem approach, a system is represented by a model and associated set of adjustable parameters. The particular choice of a model (or equivalently, model and associated set of parameters) is termed a "parameterization" of the system. The choice of a particular parameterization to be used to describe a system, however, is in general not unique. In order to address the property of nonuniqueness of system parameterization, inverse problem theory has adopted the concept of "model space," where each point of this space represents a "conceivable" model of the system (Ref 17). Given a model space of a specific system, quantitative inverse analysis of the system is further enhanced by isolating the regions of model space that correspond to parameterizations that are both physically consistent and sufficiently general in terms of their mathematical representation. A physically consistent and sufficiently general parameterization of heat deposition processes is significant for the following reasons. First, temperature distributions calculated by inverse methods represent a mapping from data space into parameter space. It is therefore preferable to adopt a parametric-function representation whose form tends to minimize any bias resulting from its mathematical form. Second, a set of parameters associated with a physically consistent representation can in principle be used to extract relationships between parameters, which can provide further insight related to physical characteristics. Third, control and optimization of heat deposition processes associated with a specific application requires a quantitative assessment of process characteristics over a wide range of values of process parameters, e.g., beam current, accelerating voltage, and chemical composition of the interacting environment. System identification for purposes of process control and optimization is only realizable by specification of a parametric representation, which establishes a correspondence between model and process parameters over a sufficiently wide range of values. Fourth, a sufficiently general parametric representation can be adjusted to include influences due to incomplete information concerning the system.

Next, it is noted that specification of a given system parameterization that is complete in the sense that, in principle, it can be applied to the inverse analysis of all types of processes within a given class of applications (e.g., heat deposition processes, including welding) is equivalent to (or implies) the specification of a complete set of basis functions. It follows that one may establish a correspondence between an optimal system parameterization and an optimal set of basis functions for parametric-function representation.

4. Formulation of Inverse-Problem Approach and Representation of Temperature Field

The inverse problem concerning analysis of physical processes, in general (Ref 4), and the inverse heat transfer problem, in particular (Ref 5), may be stated formally in terms of source functions (or input quantities) and multidimensional fields (output quantities). Other investigators have also focused on various aspects of inverse problems related to heat deposition processes especially as they relate to the determination of heat fluxes via appropriate regularization of their spatial and time distributions (Ref 6). In general, the formulation of a heat conductive system occupying an open bounded domain Ω with an outer boundary Γ_o and an inner boundary Γ_i involves the parabolic equation

$$\frac{\partial T(\hat{x},t)}{\partial t} = \nabla \cdot (\kappa(\hat{x},t)\nabla T(\hat{x},t)) \quad \text{in} \quad \Omega \times (0, t_f), \tag{Eq 1a}$$

with initial condition

$$T(\hat{x},0) = T_0(\hat{x}) \quad \text{in } \Omega, \tag{Eq 1b}$$

and heat flux exchanges through the outer and inner boundaries Γ_o and Γ_i as follows:

$$-\kappa(\hat{x},t)\frac{\partial T(\hat{x},t)}{\partial n_{\Gamma_o}} = c(\hat{x},t)(T(\hat{x},t) - T_a(\hat{x},t)) \quad \text{on} \quad \Gamma_0 \times (0,t_f) \tag{Eq 1c}$$

$$-\kappa(\hat{x},t)\frac{\partial T(\hat{x},t)}{\partial n_{\Gamma_i}} = q(\hat{x},t) \quad \text{on} \quad \Gamma_i \times (0,t_f). \tag{Eq 1d}$$

Here $\hat{x} = (x,y,z)$ is the position vector, n_{Γ_o} and n_{Γ_i} are the normal vectors onto boundary Γ_o and Γ_i, respectively, t is the time variable, t_f is the final time, $T(\hat{x},t) = T(x,y,z,t)$ is the temperature field variable, $\kappa(\hat{x},t) = \kappa(x,y,z,t)$ is the heat conductivity field variable, $c(\hat{x},t) = c(x,y,z,t)$ and $T_a(\hat{x},t) = T_a(x,y,z,t)$ are specified functions, and $q(\hat{x},t) = q(x,y,z,t)$ is the heat flux on the inner boundary Γ_i. Determination of the temperature field via solution of Eq 1a-d constitutes the so-called forward or direct initial-boundary value problem. The interest here, however, is focused on a specific formulation of the inverse problem and can be stated as follows: Effectively reconstruct the heat flux field $q(x,y,z,t)$ on the inner boundary Γ_i, and the resulting temperature field $T(x,y,z,t)$ for all time $t \in [0, t_f]$ when Γ_i is totally or partially inaccessible. In order to reconstruct the heat flux, some extra information on the temperature $T(x,y,z,t)$ is needed (i.e., known values experimentally acquired) (Ref 4, 6).

A parametric representation based on a physical model provides a means for the inclusion of information concerning the physical characteristics of a given process. It follows then that for heat deposition processes involving the deposition of heat within a workpiece or plate structure of given thickness, consistent parametric representations of the temperature field are given by

$$T(x,y,z) = T_A + \sum_{k=1}^{N_k} T_k(\hat{x},\hat{x}_k,V_k) \quad \text{and} \quad T(\hat{x}_n^c) = T_n^c \tag{Eq 2}$$

where the quantity T_A is the ambient temperature of the workpiece and the locations $\hat{x}_n^c$ and temperature values T_n^c specify constraint conditions on the temperature field. The functions $T_k(\hat{x},\hat{x}_k,V_k)$ are steady state solutions to the heat conduction equation for given sets of boundary conditions (Ref 25). The quantities $\hat{x}_k = (x_k,y_k,z_k)$, $k = 1,...,N_k$, are the locations of the elemental heat sources of a given strength $C_k(\hat{x}_k)$, which is defined below. The sum defined by Eq 2 specifies numerical integration over the discrete elements of a distribution of sources that can be characterized by individual elements. Formally, Eq 2 is a linear combination of solutions to the heat conduction equation. The quantities V_k are the effective relative speeds of the elemental heat sources comprising the heat-source distribution.

The formal procedure underlying the inverse method considered here entails the adjustment of a temperature field $T(x,y,z)$ defined over the entire spatial region of the workpiece at a given time t. This approach defines an optimization procedure where a temperature field spanning the spatial region of the workpiece is adopted as the quantity to be optimized. The temperature field spanning the spatial region of the workpiece is optimized by minimization of the value of the objective function defined by

$$Z = \sum_{n=1}^{N} w_n\left(\max\{T(x,y_c,z_c)\} - T_n^c\right)^2, \tag{Eq 3}$$

where T_n^c is the target maximum temperature for positions y_c, z_c, transverse to the motion of the energy source relative to the workpiece, which is along the x coordinate.

A consistent assumption is that V_k (for all k) is equal to the translational speed of the heat source. For steady-state heat deposition within a structure of finite thickness a consistent parametric representation of the time-independent temperature field is given by

$$T_k(\hat{x},\hat{x}_k,V_k) = C_k(\hat{x}_k)\exp\left(-\frac{V_k(x-x_k)}{2\kappa}\right) \times \left[\sum_{i=-\infty}^{\infty}\left(\frac{1}{R_i}\right)\exp\left(-\frac{V_kR_i}{2\kappa}\right) + \sum_{j=-\infty}^{\infty}\left(\frac{1}{R_j}\right)\exp\left(-\frac{V_kR_j}{2\kappa}\right)\right] \tag{Eq4}$$

where

$$R_i = \left[(x-x_k)^2 + (y-y_k)^2 + (z-2iD-z_k)^2\right]^{1/2} \tag{Eq 5}$$

and

$$R_j = \left[(x-x_k)^2 + (y-y_k)^2 + (z-2jD+z_k)^2\right]^{1/2} \tag{Eq 6}$$

The quantity D is the thickness of the workpiece and $\hat{x}_k = (x_k, y_k, z_k)$, where $k = 1,...,N$, are the locations of the elemental heat sources of strength C_k. The diffusivity is defined as $\kappa = k_c/\rho C_p$, where k_c, ρ and C_p are the thermal conductivity, density and specific heat, respectively.

$$C_k(\hat{x}_k) = C_k^1(x_0, y_0, z_k) C_k^2(\hat{x}_k, x_0, y_0) \quad \text{(Eq 7)}$$

where the functional forms of $C_k^1(x_0, y_0, z_k)$ and $C_k^2(\hat{x}_k, x_0, y_0)$ are the Beer-Lambert law and Gaussian function, respectively. This follows for $C_k^1(x_0, y_0, z_k)$ since deposition-type processes (e.g., transmission of electrons or photons) can be represented with respect to penetration by the modified Beer-Lambert law, which is given in Napierian form by

$$-\ln\left[C_k^1(z_k, x_0, y_0)\right] = \mu C z_k f_1 + f_2 \quad \text{(Eq 8)}$$

where z_k is the distance from the surface of the workpiece, μ is the extinction coefficient, C is the concentration of the ambient medium, f_1 is a path-length factor, which accounts for increases in path length caused by scattering within the material, and f_2 is a geometry factor, which accounts for instrument geometry, e.g., shape or spatial profile of beam source. Similarly, a sufficiently general representation of the transverse character of heat sources $C_k^2(\hat{x}_k, x_0, y_0)$, is that of a Gaussian function, i.e.,

$$\begin{aligned} &-\ln\left[C_k^2(\hat{x}_k, x_0, y_0)\right] \\ &\quad = A \exp\left[-\alpha_1(z_k)(x_k - x_0)^2 - \alpha_2(z_k)(y_k - y_0)^2\right] \end{aligned} \quad \text{(Eq 9)}$$

4.1 Discussion

First, the parametric representations defined above may be adopted as physically consistent models of the underlying processes, i.e., pure thermal diffusion, for regions of the workpiece that are defined by various types of boundary conditions which are obtainable from various types of data sets. Second, these representations may also be adopted, however, for mapping out the temperature field at positions within the melt pool, given that one has information concerning temperature values at positions that are close to or within the region of the energy source. In this case, the parametric representation defined above can be adopted as three-dimensional interpolation functions for calculating the temperature field between upstream (the region of coupling of the workpiece to the energy source) and downstream (the region of the workpiece at and below the temperature of the solidification boundary) values of the temperature.

The input of information into the inverse model defined by Eq 2-9, i.e., the mapping from data to model space, is effected by: the assignment of individual constraint values to the quantities T_n^c (see Eq 2); the form of the function adopted for parametric representation; specifying the shapes of the upstream and downstream boundary surfaces which bound the temperature field within different regions of the workpiece; and specifying the shape of and temperature-field values at the top boundary surface of the workpiece. Specifying the shapes and temperature field values of boundary surfaces is equivalent to assigning a set of constraint values T_n^c.

At this point it is significant to note that constrained optimization of the calculated temperature field, via minimization of an objective function such as Eq 3, requires in principle a reasonable number of trial iterations in order to find the appropriate neighborhood within parameter space containing the optimal set of parameter values. This follows regardless of the specific parameter optimization procedure applied. Further iterations are then required in order to subsequently adjust these parameters relative to some designated tolerance on the calculated minimum of the objective function. For cases where the number of elemental heat sources is large (e.g., a continuous surface distribution of heat sources) even a reasonable number of trial iterations can result in a substantial computational cost due to the large number of calculations at each iteration. Minimization of computational cost can be effected, however, by sampling temperature field values at only a limited number of locations within the simulated temperature field spanning the workpiece. These locations would be expected to be in principle either near or at locations at which constraint conditions on the temperature field are specified. Specification of the best locations within the simulated temperature field for imposing constraint conditions presents interesting problems concerning the optimal sampling of data sets spanning the data space for heat deposition processes.

Following the inverse-problem approach the thermal diffusivity can be interpreted as either a phenomenological quantity or an effective thermal diffusivity whose value is related to the average material properties of the workpiece. The inverse-problem approach presented here adopts the thermal diffusivity defined as an adjustable parameter, as well as the distribution of heat sources. This flexibility is supported by the following observations. The linear combination of solutions to the heat conduction equation defined by Eq 2 should be applicable for three different types of representations: an approximate physical model representation; a three-dimensional interpolation function for assigning temperature values over the full range of spatial locations of interest; and a generating function for assigning temperature values over either upstream or downstream boundary surfaces.

A large quantity of inverse analyses of steady-state heat deposition processes, including welding, have been based on the model defined by the parameterization above. This has been the case due to the fact that a large class of heat deposition processes can be modeled to a very good level of accuracy by an effective heat source distribution moving through a workpiece of finite thickness or of effectively semi-infinite cross section. This would include all types of welding processes involving plate geometries. For welding processes characterized by nonplanar or irregular top surface shapes, such as consumable electrode and multipass welding processes, this model has still provided the basis for quantitative inverse analysis. This is due to the fact that the regions of interest in many weld analyses, e.g., the heat affected zone (HAZ), are characterized by temperature fields whose spatial-temporal forms are not determined uniquely by spatial characteristics of the energy source or of the top surface geometry of the workpiece. A significant implication of this fact is that with respect to quantitative characterization of the HAZ, for example, there is nothing in principle to be gained by detailed modeling of the energy source or of influences due to nonplanar top surface boundary conditions.

5. Mathematical Analysis

In this section mathematical aspects of the inverse heat transfer problem are examined as they relate, in particular, to inverse analysis of heat deposition processes. Although this examination is somewhat formal in terms of mathematical analysis, its significance is considerable for practical application of inverse analysis using the parametric representations presented here. The basis functions defined above represent a complete set of functions for inverse analysis of heat deposition processes in that the temperature field can in principle be decomposed into a linear combination of these functions. Given this, important properties of inverse heat-deposition analysis can be deduced by an examination of the dominant components of these basis functions. In what follows, we extract the dominant component of the basis functions given above for steady state heat deposition. Our mathematical analysis of these components provides a foundation for establishing a formal statement of the inverse heat deposition problem that is explicitly distinct from that of the inverse heat transfer problem. This formal statement is important, in that certain misunderstandings concerning the objective of inverse heat-deposition analysis can be eliminated.

Combining Eq 2 and 4, it follows that for $x > x_k$, $y = y_k$, and $z = z_k$,

$$T_S(x) = \sum_{k=1}^{N_k} C_o(x_k) k_o(x - x_k) = C_o * k_o \qquad \text{(Eq 10)}$$

where the sum in Eq 10 is the discrete form of the convolution of the functions C_o and k_o that is represented by the notation $C_o{*}k_o$,

$$T_S(x) = \lim_{D\to\infty} \left\{ \sqrt{\frac{x - x_k}{\pi}} (T(x, y_k, z_k) - T_A) \right\}, \qquad \text{(Eq 11)}$$

where $C_o(x_k) = 2C(x_k, y_k, z_k)$ and

$$k_o(x - x_k) = \frac{1}{\sqrt{\pi(x - x_k)}} \exp\left(-\frac{V_k(x - x_k)}{\kappa} \right). \qquad \text{(Eq 12)}$$

Let $\tilde{f}(s)$ be the Laplace transform of $f(x)$, defined here by the convention

$$L[f(x)] = \tilde{f}(s) = \int_0^\infty f(x) \exp(-sx) dx, \qquad \text{(Eq 13)}$$

it follows from the convolution theorem $L[C_o * k_o] = \tilde{C}_o(s)\tilde{k}_o(s)$ that

$$\tilde{T}_S(s) = \tilde{C}_o(s)\tilde{k}_o(s) \qquad \text{(Eq 14)}$$

where

$$\tilde{k}_o(s) = \frac{1}{\sqrt{s + \alpha_o}} \quad \text{and} \quad \alpha_o = \frac{V_k}{\kappa}. \qquad \text{(Eq 15)}$$

The discrete integral equation defined by Eq 10 represents the system-response characteristics of the dominant components of heat transfer for steady-state heat deposition processes. Referring to the Laplace transform of the kernel function k_o of Eq 10, it is observed that this function can be characterized as a well defined low-pass filter. That is to say, relative to a systems theoretic representation adopting the function T_S as a system output, the high-frequency components of the system input, C_o are filtered out by the kernel function k_o.

The integral equation Eq 10 is significant in that its structure represents a formal statement of the inverse heat transfer problem (or in general, inverse diffusion problem) for steady state processes. Simply stated, the inverse heat transfer problem entails, for steady state processes, a determination of the function C_o given measurements of the function T_S. It is significant to note that this formal statement of the inverse heat transfer problem is responsible for dominant influences concerning general perspectives toward inverse analysis and its relationship to the direct-problem approach. Notable among these perspectives is that the inverse heat transfer problem is ill-posed. This follows from the properties of the kernel function k_o that are such that the recovery of the function C_o, which describes the structure of the heat source, from data concerning T_S, becomes progressively more difficult as $x - x_k$ increases. This property is due to the fact that physically the process of diffusion is an entropy increasing process resulting in the progressive loss of information.

The inverse heat deposition problem, however, represents a particular category of the more general inverse heat transfer problem. In particular, the inverse heat deposition problem entails a determination of the temperature field for spatial regions within specified upstream and downstream boundaries. Simply stated, the inverse heat deposition problem seeks knowledge of the characteristics of the "deposit" and not of the source. Accordingly, with respect to the system theoretic representation given by Eq 10, the function C_o does not represent system input, but rather adjustable quantities for characterization of the function T_S within bounded regions of space. It follows that in contrast to the inverse heat transfer problem, as stated formally, the inverse heat deposition problem is in principle quite well-posed.

6. Prototype Inverse Analysis

Presented in this section is a prototype analysis of a deep-penetration welding process whose input power is adopted as a variable process-control parameter. The significance of the inverse-problem approach for this type of analysis is that the strength of the coupling of the energy source to the workpiece can be a function of the power. This implies the existence of additional process parameters that are in principle difficult to specify relative to analysis based on a direct-problem approach. This analysis considers a set of laser welds of 21-6-9 stainless steel that were made using a Diode-Pumped Continuous Wave (CW) Nd:YAG laser at a welding speed of 45 ipm (1.905 cm/s), and using helium as a shielding gas (See Fig. 1). The production of these laser welds is described in Ref 26. The cross section of the workpiece is 0.12×0.68 in. (3.05×17.23 mm) and the top of the keyhole is located 0.28 and 0.4 in. from the two edges of the workpiece. The constraint conditions (y_c, z_c) on the transverse cross section of the solidification boundary as a function of rates of energy input are as shown in Table 1.

In the section that follows this prototype analysis is adopted for construction of a generalization concerning the parametric representation of heat deposition processes. This generalization will contribute to the development of a proof for the existence of an optimal and general parametric representation for inverse analysis of heat deposition processes.

Shown in Fig. 2(a-e) are two-dimensional slices of three-dimensional temperature fields calculated according to the inverse analysis procedure described above. This calculation

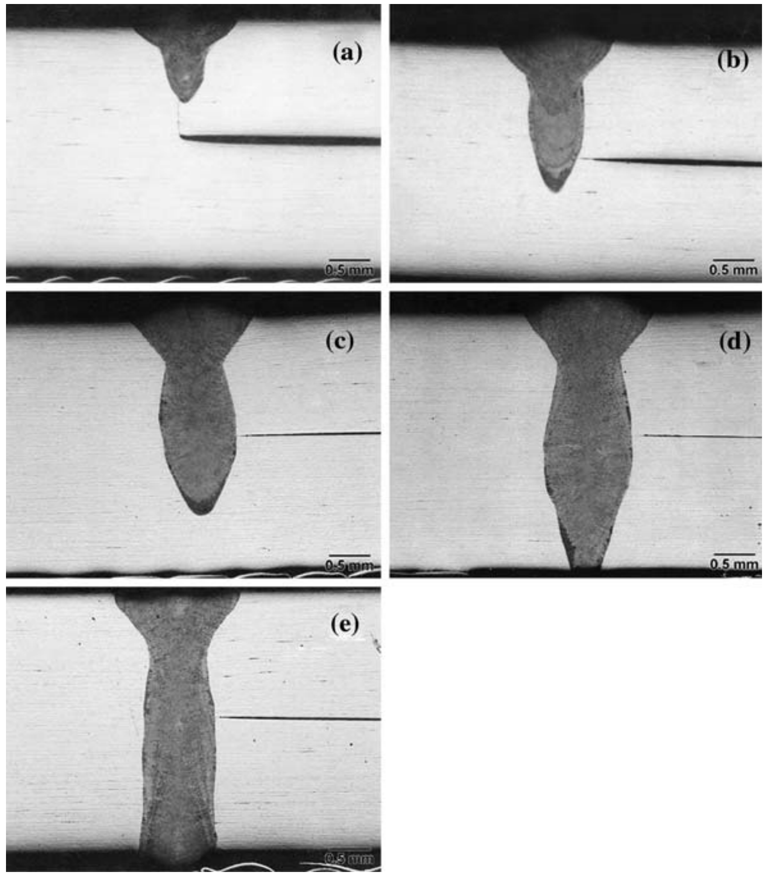

Fig. 1 Transverse cross sections of deep-penetration welds corresponding to different rates of energy input. (a) 500 W, (b) 750 W, (c) 1000 W, (d) 1250 W, and (e) 1500 W

Table 1 Constraint conditions (y_c, z_c) on the transverse cross section of the solidification boundary as a function of rates of energy input

500 W	750 W	1000 W	1250 W	1500 W
(y_c mm, z_c mm)	(y_c mm, z_c mm)	(y_c mm, z_c mm)	(y_c mm, z_c mm)	(y_c mm, z_c mm)
(0.6875, 0.0)	(0.813, 0.0)	(0.688, 0.0)	(0.75, 0.0)	(0.6875, 0.0)
(0.5, 0.125)	(0.313, 0.438)	(0.313, 0.5)	(0.375, 0.5)	(0.563, 0.188)
(0.25, 0.313)	(0.375, 0.875)	(0.438, 0.938)	(0.438, 0.875)	(0.438, 0.313)
(0.375, 0.5)	(0.25, 1.313)	(0.438, 1.313)	(0.5, 1.438)	(0.313, 0.563)
(0.125, 0.813)	(0.0, 1.75)	(0.313,1.88)	(0.438, 2.063)	(0.313, 0.813)
(0.0, 1.0)		(0.0, 2.375)	(0.313, 2.5)	(0.375, 1.063)
			(0.188, 2.938)	(0.375, 2.0)
				(0.375, 2.25)
				(0.438, 2.75)

adopts a temperature-independent diffusivity $\kappa = 5\times10^{-6}$ $m^2\ s^{-1}$ and an adjusted spatial distribution of the effective heat source so that the calculated cross sections of the solidification boundaries, as a function of power input, satisfy the above constraint conditions. This analysis is characteristic of inverse analyses that adopt a parameterized direct-problem formalism, e.g., Eq 4, a priori information concerning material properties, e.g., an assigned value of the diffusivity $\kappa = 5\times10^{-6}\ m^2\ s^{-1}$ and speed of energy source $V_k = 1.905$ cm/s, and a priori information concerning the specific type of heat deposition process, e.g., heat source distributions that are characteristic of deep-penetration welding (using electron or laser beams), for parameter optimization according to experimental measurements. The results of this particular analysis are significant in that for the specific process considered one is able to construct a multidimensional temperature field $T(\hat{x},\ Q_{\mathrm{HDP}})$, where Q_{HDP} is the rate of energy deposited on the surface of the workpiece, but not necessarily coupled into it volumetrically.

7. Generalization of Prototype Analysis

The temperature fields shown in Fig. 2(a-e) are results of an inverse analysis that assumes variation of the process parameter Q_{HDP}, adjustment of the effective heat source distribution, a model parameter, and a priori information concerning the specific type of material on which energy is deposited, the

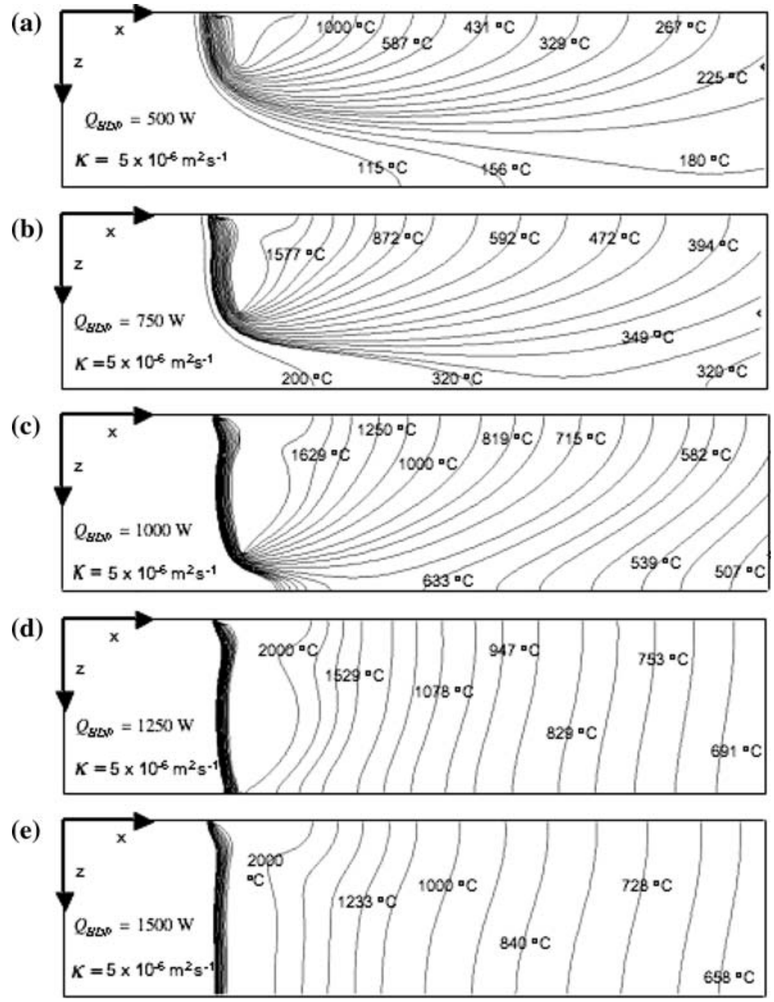

Fig. 2 Longitudinal slices of three-dimensional temperature fields at midplane of model deep-penetration welds, i.e., along *zx*-plane at $y = 0$, corresponding to different rates of energy input and $\kappa = 5\times10^{-6}$ m^2 s^{-1}. (a) 500 W, (b) 750 W, (c) 1000 W, (d) 1250 W, and (e) 1500 W

specific type of heat deposition process, and the geometry and thickness of workpiece. We now adopt this analysis in order to construct a more generalized parametric representation that is extendable in principle to inverse analysis of any type of heat deposition process for variable material properties and geometries. An analysis of the structure of this more generalized parametric representation will be shown to support the notion that construction of an optimal parametric representation for inverse analysis of heat deposition processes is feasible.

Shown in Fig. 3(a-e) and 4(a-e) are two-dimensional slices of three-dimensional temperature fields obtained by the procedure used for calculating the temperature fields in Fig. 2(a-e) for thermal diffusivities $\kappa = 1\times10^{-5}$ m^2 s^{-1} and $\kappa = 5.29\times10^{-5}$ m^2 s^{-1}, respectively, and for the same process and constraint conditions. Referring to Fig. 2(a-e), 3(a-e), and 4(a-e), one notes that these temperature fields define a multidimensional temperature field $T(\hat{x}, \kappa, Q_{\mathrm{HDP}})$.

7.1 Discussion

The multidimensional temperature field $T(\hat{x}, \kappa, Q_{\mathrm{HDP}})$. defined by Fig. 2(a-e), 3(a-e), and 4(a-e) adopts the diffusivity κ, with respect to inverse analysis, as a variable parameter of heat deposition processes. This follows in that for inverse analysis an a priori assumption of a specific value of the diffusivity κ is not in general necessary for calculation of the temperature field. Similarly, referring to Eq 4, it follows that the deposition speed V and workpiece thickness D can also be adopted as variable parameters, and that for the same process and constraint conditions assumed for the temperature fields in Fig. 2(a-e), 3(a-e), and 4(a-e), one can construct a multidimensional temperature field $T(\hat{x}, \kappa, V, D, Q_{\mathrm{HDP}})$.

At this point, it is to be noted that the multidimensional temperature field $T(\hat{x}, \kappa, V, D, Q_{\mathrm{HDP}})$ is a function of the characteristics of the specific heat deposition process through its dependence on the parameter Q_{HDP}. It follows that construction of a general parametric representation of the temperature field of heat deposition processes is possible if this dependence can be eliminated. The mathematical analysis of heat deposition processes presented below establishes a foundation for construction of a general parametric representation that is in principle independent of the type of process.

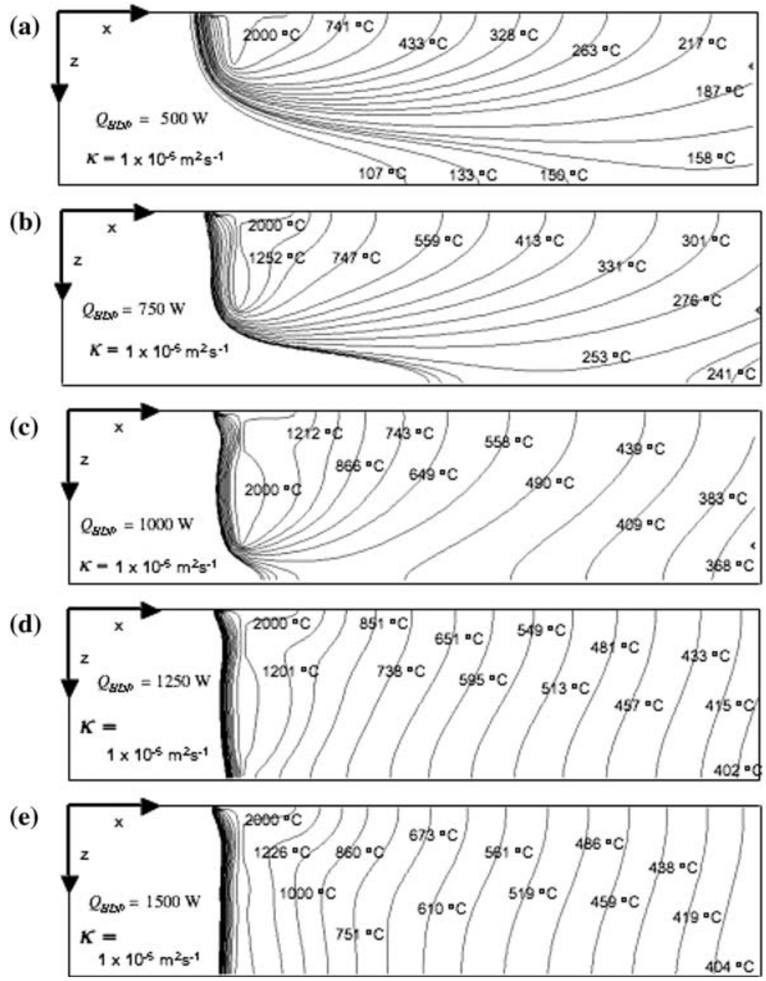

Fig. 3 Longitudinal slices of three-dimensional temperature fields at midplane of model deep-penetration welds, i.e., along *zx*-plane at $y = 0$, corresponding to different rates of energy input and $\kappa = 1\times10^{-5}$ m^2 s^{-1}. (a) 500 W, (b) 750 W, (c) 1000 W, (d) 1250 W, and (e) 1500 W

8. Proof for Existence of a General Parametric Representation of Heat Deposition Processes within Plate Structures

The set of basis functions and analysis presented above provide the essential components for construction of a proof of the existence of an optimal parametric representation for inverse analysis of heat deposition processes. This proof is considered somewhat partial, however, in that certain aspects of its development must be made more precise and investigated in more detail with respect to practical application. The essential components of the proof are as follows:

(1) Equation 4 provides a complete basis set of functions for representation of the temperature field for heat deposition processes within plate structures. That is to say, any temperature field associated with steady-state heat deposition within plate structures can be represented by a linear combination of these functions.

(2) In the case of heat deposition processes, characteristics of the temperature field are poorly coupled to the characteristics of the energy source. The characteristics of the temperature field that are associated with these processes are strongly coupled only to upstream boundaries on this field, e.g., the solidification boundary. This property follows from the low-pass spatial filtering property of the basis functions Eq 4.

(3) Given the set of basis functions Eq 4, the temperature field associated with a heat deposition process is completely specified by: the shape and temperature distribution of a given upstream boundary on the domain of the temperature field; the diffusivity κ and speed of deposition V; and the lengths of the spatial dimensions D_i of the workpiece.

(4) The shape and temperature distribution of a specified upstream boundary is determined by the rate of energy deposited on the surface of the workpiece Q_{HDP} and the strength of coupling of the energy source to the workpiece γ. As demonstrated by prototype analyses above, for any given upstream boundary, e.g., solidification boundary, there exists a multidimensional temperature field $T(\hat{x}, \kappa, V, D_i)$, such that

$$\gamma Q_{HDP} = Q_{WCH}(T(\hat{x}, \kappa, V, D_i)) \qquad \text{(Eq 16)}$$

where Q_{WCH} is the energy that has been coupled into the workpiece and is given by

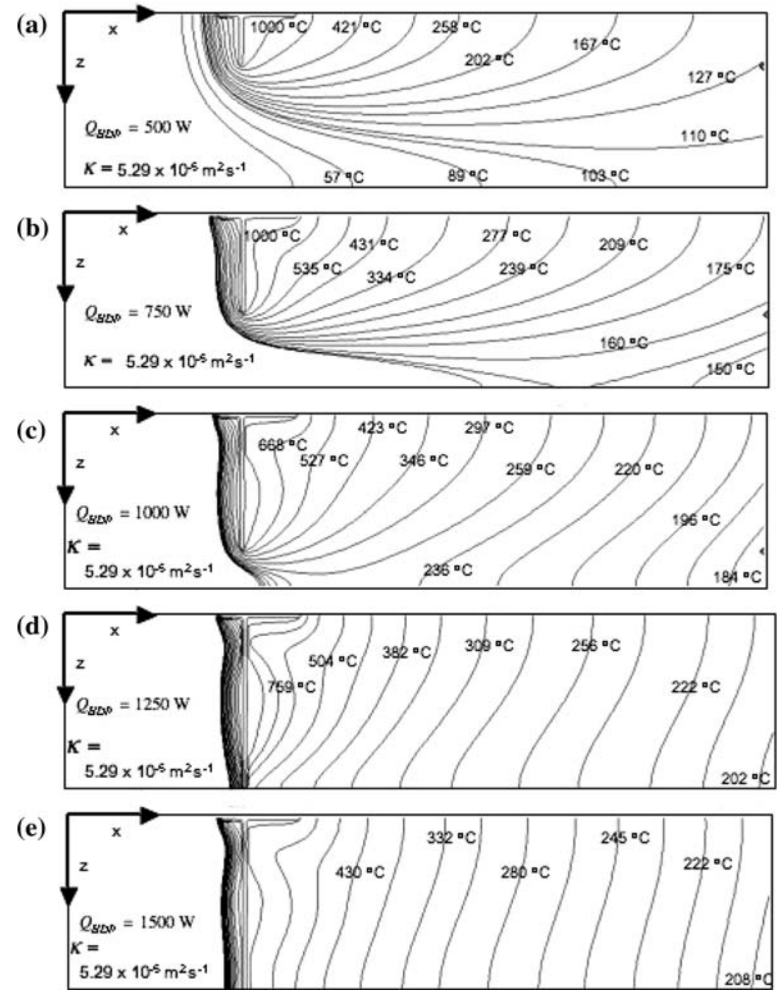

Fig. 4 Longitudinal slices of three-dimensional temperature fields at midplane of model deep-penetration welds, i.e., along *zx*-plane at $y = 0$, corresponding to different rates of energy input and $\kappa = 5.29\times10^{-5}$ m^2 s^{-1}. (a) 500 W, (b) 750 W, (c) 1000 W, (d) 1250 W, and (e) 1500 W

$$Q_{\mathrm{WCH}} = \int_{x_1}^{x_2}\int_{y_1}^{y_2}\int_{z_1}^{z_2}\left[\int_{T_A}^{T(x,y,z)} \rho(T)C_p(T)dT\right]dxdydz \quad \text{(Eq 17)}$$

for energy deposition within a sample volume $V_S = (x_2 - x_1)(y_2 - y_1)(z_2 - z_1)$. Referring to Eq 16, it is to be noted that although a characterization of the quantity γ is dependent on the nature of the heat deposition process, a general characterization of Q_{WCH} is well-posed based on the geometric structure of energy deposition profiles.

(5) In that an upstream boundary S_b is defined by its shape and the distribution of temperatures on its surface $T_b(\hat{x}_S)$, it follows that one can define a multidimensional temperature field $T(\hat{x},\ \kappa,\ V,\ D_i,\ T_b(\hat{x}_S),\ \ \hat{x}_S \in S_b)$.

Remark. At this stage it is significant to note that the multidimensional temperature field $T(\hat{x},\ \kappa,\ V,\ D_i,\ T_b(\hat{x}_S),\ \ \hat{x}_S \in S_b)$ represents a parametric representation of heat deposition processes to the extent that any of the different possible types of upstream boundary surfaces, i.e., $T_b(\hat{x}_S)$, $\hat{x}_S \in S_b$, associated with these processes can be represented using a convenient parametric representation. This stage of our proof is not rigorously precise, but based on a simple plausibility argument. Accordingly, added to the essential components of the proof is the following conjecture.

(6) The existence of a convenient and general parameterization of upstream boundary surfaces, $T_b(\hat{x}_S)$, $\hat{x}_S \in S_b$, bounding the temperature fields associated with heat deposition processes is conjectured based on the obvious fact that all heat deposition processes are characterized by thermal and energy deposition profiles whose general form can be represented by a small class of geometric shapes. This conjecture is plausible based on the fact that the observed volumetric distributions of energy from all types of heat deposition processes, within the upstream region of their associated temperature fields, can be represented by linear combinations of the basis functions given by Eq 8 and 9. This includes martini-glass structures at one or both ends of the solidification boundary and structures characterized by centralized bulging.

Remark. Having established a convenient parametric representation of the different possible types of functions

$T_b(\hat{x}_S)$, $\hat{x}_S \in S_b$ that specify the upstream boundary surface, the inverse problem is then that of the inverse determination of boundary-surface shape and boundary values, i.e., $T_b(\hat{x}_S)$ and S_b, where $\hat{x}_S \in S_b$ (see Ref 27, 28).

The arguments (1)-(6) establish a plausible foundation for the existence of an optimal parametric representation $T(\hat{x},\ \kappa,\ V,\ D_i,\ T_b(\hat{x}_S),\ \ \hat{x}_S \in S_b)$ for inverse analysis of heat deposition processes.

9. Conclusion

The main objective of this research was to establish a general mathematical framework for the eventual construction of an optimal parametric representation of heat deposition processes for the purpose of inverse analysis of such processes. Certain general aspects of inverse analysis and, in particular, of inverse analysis of heat deposition processes have been reviewed. We have constructed a parametric-function representation such that any temperature field associated with heat deposition processes involving plate structures can be represented by a linear combination of these parametric functions. We have shown using mathematical analysis that a parametric representation based on a detailed characterization of the energy source is likely not optimal for inverse analysis of heat deposition processes. A set of arguments have been constructed that support a proof for the existence of an optimal, and to some extent, general parametric representation of the temperature field associated with heat deposition processes.

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