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Validation Experiments to Application: A Model Based Approach

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Relation of Validation Experiments to Applications

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Abstract

Computational and mathematical models are developed in engineering to represent the behavior of physical systems to various system inputs and conditions. These models are often used to predict at other conditions, rather than to just reproduce the behavior of data obtained at the experimental conditions. For example, the boundary or initial conditions, time of prediction, geometry, material properties, and other model parameters can be different at test conditions than those for an anticipated application of a model. Situations for which the conditions may differ include those for which 1) one is in the design phase and a prototype of the system has not been constructed and tested under the anticipated conditions, 2) only one version of a final system can be built and destructive testing is not feasible, or 3) the anticipated design conditions are variable and one cannot easily reproduce the range of conditions with a limited number of carefully controlled experiments. Because data from these supporting experiments have value in model validation, even if the model was tested at different conditions than an anticipated application, methodology is required to evaluate the ability of the validation experiments to resolve the critical behavior for the anticipated application. The methodology presented uses models for the validation experiments and a model for the application to address how well the validation experiments resolve the application. More specifically, the methodology investigates the trade-off that exists between the uncertainty (variability) in the behavior of the resolved critical variables for the anticipated application and the ability of the validation experiments to resolve this behavior. The important features of this approach are demonstrated through simple linear and non-linear heat conduction examples.

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Nomenclature

a	parameter vector for Taylor Series
d	decision variable
d	vector of decision variables
F	model validation experiments
F	vector of models for validation experiments
G	model for target application
G	vector of models for target application
k	thermal conductivity
o	convergence rate (code verification context)
q	flux
p	number of singular values retained
q	number of nonzero singular values
r	number of flux measurements, ratio of grid refinement (Appendix)
s	number of important model parameters for the application
S	matrix of singular values
T	temperature
t	time
U	orthogonal matrix
V	orthogonal matrix
w	weights
W	matrix of weights
y	spatial location

Greek symbols

	model parameters vector
	experimental measurement
	vector of experimental measurements
C_p	density-specific heat product
	standard deviation
	sensitivity matrix: validation experiments
	sensitivity matrix: target application

Subscripts and Superscripts

cv	cross validation
d	decision variable
f	validation experiment model
g	target application model
n	number of validation measurements
m	number of decision variables
p	number of singular values retained
q	number of non-zero singular values
r	number of flux measurements
s	number of important model parameters
	experimental measurement

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1. Introduction

Model validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model (AIAA [1], ASME [2]). In this context, a model is a mathematical and/or computational representation of one or more physical processes. In engineering and science, the assessment of model validity is through comparisons of model predictions to experimental observations. A general literature review on model validation is provided by Oberkampf and Trucano [3] and Oberkampf et al. [4]. One of the benefits of mathematical and computational models is the ability to use these models to predict behavior at conditions for which one does not possess experimental results, based on successful comparisons between model predictions and experimental observations at other related conditions. This process is often referred to as the interpolation or extrapolation of the model from the conditions for which the model was tested.

To many researchers, interpolation in model validation is the application of a model to conditions bounded by supporting validation experiments. The acquisition of sufficient bounding experimental data is often not practical and extrapolation is required for one or more of the model parameters, independent variables, or boundary conditions. Model extrapolation in validation has different meanings to different investigators. Model extrapolation may be 1) the extrapolation of a model outside the range of model parameters/variables tested, 2) the extrapolation of a model to conditions not tested (i.e., different geometries or boundary conditions), or in the most extreme case, 3) the extrapolation of a model to a different physical phenomena for which the model acts as a surrogate (for example, the use of a diffusion model for the spread of a disease).

A search of the SciSearch Plus scientific article databases (ISI [5]) for the phrase *model extrapolation* yields few hits. Because engineering/scientific models are generally developed for the purpose of providing insight for conditions other than those tested, extrapolation is a normal part of predictive modeling and this observation is not surprising. The technical areas for which there were the most hits for model extrapolation were in the environmental and medical fields.

Extrapolation is an important aspect in environmental risk assessment and health fields. This includes the extrapolation over different physical scales (from patch scale to landscape scale; Landis [6], Munns [7]), across different temporal scales (Munns [7], Kalberlah et al. [8]), and biological extrapolation (across levels of biological organization – Munns [7]; between animals and human- Bernillon and Boise [9], Kalberlah et al. [8], Vermeire et al. [10]).

The ability of validation experiments/model prediction comparisons evaluated at one set of conditions to address the validity of a model at other conditions has received less attention and raises three questions. 1) Do the comparisons of experimental data and model predictions performed at one set of conditions adequately test a model for use at a different set of conditions? 2) Can one develop metrics that properly weight the differences between experimental data and model predictions from one or more sets of conditions to represent how a model behaves at a different set of conditions? 3) Can one develop methodology that allows one to relate observed differences between experiment data and model predictions from one set of conditions to predict what the differences may be at another set of conditions? These are three distinct questions. The present paper uses the predictive models to addresses question 1, but can be easily extended to address question 2. The present paper does not address question 3.

Question 2 was addressed by Hills and Trucano [11] and questions 1 and 2 were addressed by Hills and Leslie [12] for cases where the data were obtained from one set of conditions (i.e., the validation experiments), with the intent of applying the model to another anticipated set of conditions (i.e. the target application). Their methodology was based on first order sensitivity analysis of the models used to predict the validation measurements and a first order sensitivity analysis for the target or anticipated application model. In both cases, the sensitivity analysis was performed relative to model parameters representing physics or boundary conditions (thermal conductivity, specific heat, parameters in equations of state, boundary temperatures, etc.). Specifically, they used the sensitivity analysis to develop validation metrics that weighted the differences between model predictions and the experimental data from the validation experiments in a manner that was relevant to the anticipated target application prediction variable. In Hills and Trucano [11], the weights were chosen so that linear combinations of the differences that are not sensitive to the model parameters (hence, the corresponding physics)

were given zero weight. Hills and Leslie [12] developed an approach that more thoroughly accounts for the relationship between a suite of differences between validation experimental measurements and the associated model predictions, and the application prediction variable than that of the method presented by Hills and Trucano [11]. The approach of Hills and Leslie is sufficiently general such that different levels of uncertainty in the appropriate values of model parameters for the models of the experiments, and for the model of the target application, can be accommodated. This approach addresses the first two questions by allowing one to assess (to first order) whether the validation experiments can adequately represents the sensitivity of model predictions of the target application to associated model parameters, as well as to provide an application specific metric. This approach also allows for prediction variables to be different quantities than those measured through the validation experiments. While this approach is conceptually more complex than the first, it requires much of the same information and is not more difficult to implement. Both of these approaches use the models as a basis for the assessment. If the model for the application is not valid, the results for the application oriented validation metric will not be valid. Thus, this approach represents a 'best estimate', based on the knowledge incorporated in the models, for the weights.

Formal methods for the extrapolation of differences observed between the model predictions and experimental observations (question 3), to corresponding differences in the prediction at the conditions of the target application have received less attention and represent a very difficult problem. These differences may be simply due to statistical sampling uncertainties due to model or experimental uncertainties, or due to model form error (e.g., because of wrong or incomplete physics incorporated in the model). A typical approach to address these issues is to calibrate the model using the observed differences between the experimental results and the model predictions, before using the resulting model for prediction. This calibration is done using either the model parameters directly (i.e., properties or tuning parameters), or through the addition of a model corrective terms which includes tuning parameters. A danger with the former approach is that if the model does not adequately represent the physics, extrapolating calibrated results far from the conditions of the validation experiments will also not adequately represent the physics and will give unreliable results. In the second case, extrapolating a model correction term to conditions far from the conditions of the experiment is also likely to fail since one does now

know the functional form of the correction model to use, if one does not possess a physical understanding of why the model produced the differences observed in the first place. Examples of additive correction approaches include those based on Bayesian analysis and Bayesian networks (Hanson and Hemez [13] and Mahadevan et. al. [14]).

The focus of this paper is 1) to formalize the ideas presented by Hills and Trucano [11] and Hills and Leslie [12] to assess the ability of models of the validation experiments to represent behavior of the model of the target application (question 1), 2) to extend the methodology to include both model parameters and independent variables relevant to the application (the previous work only considered model parameters), 3) to extend the methodology to second order dependency in the model parameters so as to capture cross coupling effects, 4) to provide an alternative solution technique for evaluating the weights used in the method, 5) to investigate the trade-off between the ability to resolve the application and the uncertainty in the results due to identified uncertainties in the validation experiments and corresponding models, 6) and to provide numerical examples based on a non-linear one-dimensional transient heat conduction equation. In contrast to Hills and Trucano [11] and Hills and Leslie [12], the present work does not demonstrate the use of the resulting weights to define a validation metric at the application level, based on experimental results from the validation experimental level. Such an extension of the present methodology is very straight forward, as one simply substitutes the weights obtained here for those obtained in Hills and Leslie [12]. One of the most significant benefits of the present methodology is that it allows the assessment of the suitability of the validation experiments to test a model that will be used for a target application, given that the model is approximately correct. This assessment does not require actually experimental data as the assessment is based on only models for the actual or potential validation experiments and models for the anticipated application. This result can be used as part of the experimental design process for the validation experiments to insure that the experiments do tests all of the “modeled physics” for the target application. The method does not address how (and if) differences between model predictions for the validation experiments and the corresponding experimental data be interpolated or extrapolated to corrected predictions of the application (question 3), as this issue is well beyond the scope of this work.

The examples presented were chosen to be tutorial in nature and are thus very simple. Application of the earlier approaches to shock physics is developed in Hills and Trucano [11]. While not demonstrated here, the methodology was developed for applications in CFD, heat transfer, and shock physics (i.e., hypersonic impact, Hills and Trucano [15]). The methodology is very general and can be applied to other areas in engineering and science.

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2. Theory

Multivariate validation metrics, such as those presented by Hills [15], can be used as an indicator of agreement between model predictions and experimental results when test conditions are the same as for the anticipated application. These metrics assess differences between model prediction and experimental observation, accounting for the uncertainties in the measurements and the model parameters. Because engineering models are generally developed to predict and not simply reproduce existing experimental data, a natural questions is – how should one relate the results from a suite of validation experimental measurements to reflect the conditions of the anticipated application, when such conditions are different? A very important question that must be asked in the design of a model validation program is whether a suite of validation experiments represents the anticipated application in some appropriate fashion. The suite of experiments may range over different conditions (i.e., different material properties, initial and boundary conditions), or over different subsets of physics for the anticipated application.

The goal of the present work is to develop methodology to assess how well experiments performed at the validation experiment conditions resolve a prediction or decision variable for an anticipated application in some sense. This relationship is developed from a model validation point of view which allows the result to be also used to define target application weighted metrics. In developing such metrics for model validation, one generally wishes to weight most heavily those measurements that best represent the anticipated application. For example, validation measurements that are taken at conditions closer to the anticipated application conditions are given more weight. To assess how well the conditions associated with planned validation experiments represent the conditions of a target application, the models for both the validation measures and for the prediction or decision variable for the target application are used. These models are used because they represent our best knowledge of the systems of interest in a predictive sense. Specifically, if the model for a target application is sensitive to a particular model parameter or independent variable, those validation measurement models that are also sensitive to this parameter/variable should receive more weight. These last two statements suggest a mechanism for weighting validation models representing the experimental results.

Specifically, data weights are chosen such that the sensitivities of the model predictions for the validation measurements to important parameters and independent variables are the same as those for the anticipated application. If the experimental conditions are similar to those for the application, we expect the behavior of the models for the measurement at the experimental conditions to be closer to those for the application.

In the present context, we use the models for the validation experiments and the model for the anticipated application to approximate the sensitivities to the important parameters and independent variables. This approach is equivalent to taking a linear combination of the models for each measurement, such that the combination best represents the behavior of the target application model with respect to the important model parameters and variables in some neighborhood of the application conditions. This linear combination of validation experiment models will be referred to as the reconstructed model of the application decision or prediction variables. One can think of the individual models for the behavior of the predicted measurements as forming a non-independent set (somewhat analogous to a basis) for the reconstructed model of the application decision or prediction variables. The models in this set may not be independent as several models may represent the predictions associated with repeated measurements at the same experimental conditions. Such repeated models are retained in the set as they have the effect of reducing variance in the reconstructed application model decision variables. An important feature of this construction is if an application model is a function of an important parameter/variable that none of the validation experimental models in the set are, no linear combination of the validation experiment models can represent the sensitivity of the application to this parameter/variable. In such a case, one can say that the validation experiments do not cover the important parameter/variable space of the anticipated application.

Denote the model or models for the application by

$$\mathbf{d}=\mathbf{G}(\mathbf{x}, \quad) \tag{1}$$

where **d** is a vector of decision variables, **G** is a vector of the corresponding models for the application, is a vector of model parameters (e.g., thermal conductivity, specific heat), and **x** is the vector of independent variables (e.g., time and position). The parameters and independent variables include values for which it is important to capture the model dependence for the

application. A decision variable for the target application is a predicted quantity critical to the success of the target application, i.e., a variable used to decide whether the application prediction is successful at meeting its design goal. Examples include temperature in a temperature sensitive critical component, or maximum stress observed throughout a component. A decision variable for an application may or may not correspond directly to quantities measured in validation experiments.

A similar expression for the models of the validation measurements is:

$$=\mathbf{F}(\mathbf{x}, \quad , \quad _{\mathbf{f}}) \tag{2}$$

where represents the prediction vector of validation model outputs simulating measurements from a suite of experiments. These models may represent measurements from suites of experiments that use different experimental apparatus to test the model for different physics, or similar models evaluated at different values for the independent variables and the model parameters, or the same models for repeated measurements at the same conditions. **F** represents a vector of models for the various validation experimental data, each evaluated at the conditions of the data. represents the vector of model parameters important to the anticipated application (Eq. (1)) as discussed in the previous paragraph. The vector $_{\mathbf{f}}$ represents those arguments in **F** whose effects are significant for the validation models, but not for the anticipated target application. **x** is the vector of independent variables. If one or more of the models represented by the vector **F** are not a function of the same arguments, then these arguments should appear as dummy variables in **x**, **,** $_{\mathbf{f}}$ so that the total number of elements in each vector is the same model to model. The sensitivity of these models to the dummy arguments will be zero. While elements in **x**, **,** and $_{\mathbf{f}}$ must represent the same arguments, the numerical values for these arguments need not be the same from function to function in **F** or **G**. Note that if **G** is a function of an argument that is not a non-dummy variable in at least one of the components of **F**, then one simply cannot resolve the sensitivity of **G** to this argument using models representing the suite of the validation experiments. In this case, we can say that the validation experiments do not span the modeled physics of the application.

As stated earlier, the approach of the present analysis is to develop weights on the models for the validation experimental data to best represent the model for the decision variable of the target

application in some sense. This weighted combination of models will be used to assess several features related to the ability of the validation models (i.e., experiments) to represent the anticipated target application. The basic assumption in choosing the weights in the present analysis is to choose these weights such that the changes in the weighted combination of the validation model predicted measurements, $_i$, are equivalent to changes in the predicted decision variables, d_j, relative to the target application model arguments. These changes are due to changes in the model parameters $\boldsymbol{\alpha}$ and independent variables $\mathbf{x}$ about the nominal values of these parameters and independent variables for each simulated experimental measurement and for each modeled decision variable. Specifically, the weights w are chosen for element j of $\mathbf{G}$ such that

$$\Delta d_j \cong \sum_{i=1}^{n} w_{ji}\, \Delta\gamma_i;\ j = 1,\ldots,m \tag{3}$$

where m is the number of decision variables in the vector $\mathbf{d}$ and n is the number of measurement predictions across all suites of experiments in vector . Expanding Eq. (3) in a Taylor's series of the parameters, $\boldsymbol{\alpha}$, and of $\mathbf{G}$ and $\mathbf{F}$ (i.e., Eqs. (1) and (2)) and requiring that Eq. (3) be satisfied up to second order leads to

$$\frac{\partial G_j}{\partial \alpha_k} \cong \sum_{i=1}^{n} w_{ji}\, \frac{\partial F_i}{\partial \alpha_k};\ j = 1,\ldots,m;\ k = 1,\ldots,\mathrm{s} \tag{4}$$

$$\frac{\partial^2 G_j}{\partial \alpha_k \alpha_l} \cong \sum_{i=1}^{n} w_{ji}\, \frac{\partial^2 F_i}{\partial \alpha_k \alpha_l};\ j = 1,\ldots,m;\ k = 1,\ldots,s;\ l = 1,\ldots,s \tag{5}$$

where s is the number of parameters in . Note that one is requiring equivalence up to second order for only the parameters that are deemed important for the target application. Note also that different sets of weights are defined for each decision variable j. We also require equivalence in sensitivity to the independent variables as follows: Define the sensitivity matrix as:

$$\boldsymbol{\Phi} = \left[\boldsymbol{\Phi}_{\mathbf{x}} \quad \boldsymbol{\Phi}_{\boldsymbol{\alpha}}\right] \tag{6}$$

where

$$\mathbf{\Phi_x} = \begin{bmatrix} \frac{\partial F_1}{\partial y} & \frac{\partial^2 F_1}{\partial y^2} & \frac{\partial F_1}{\partial t} \\ \frac{\partial F_2}{\partial y} & \frac{\partial^2 F_2}{\partial y^2} & \frac{\partial F_2}{\partial t} \\ \vdots & \vdots & \vdots \\ \frac{\partial F_n}{\partial y} & \frac{\partial^2 F_n}{\partial y^2} & \frac{\partial F_n}{\partial t} \end{bmatrix} \tag{6a}$$

$$\mathbf{\Phi}_\alpha = \begin{bmatrix} \frac{\partial F_1}{\partial \alpha_1} & \frac{\partial F_1}{\partial \alpha_2} & \cdots & \frac{\partial F_1}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 F_1}{\partial \alpha_1^2} & \frac{\partial^2 F_1}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 F_1}{\partial \alpha_s^2} \\ \frac{\partial F_2}{\partial \alpha_1} & \frac{\partial F_2}{\partial \alpha_2} & \cdots & \frac{\partial F_2}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 F_2}{\partial \alpha_1^2} & \frac{\partial^2 F_2}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 F_2}{\partial \alpha_s^2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial F_n}{\partial \alpha_1} & \frac{\partial F_n}{\partial \alpha_2} & \cdots & \frac{\partial F_n}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 F_n}{\partial \alpha_1^2} & \frac{\partial^2 F_n}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 F_n}{\partial \alpha_s^2} \end{bmatrix} \tag{6b}$$

Eq. (6a) accounts for independent variables. A complete set of first and second order derivatives are not included in Eq. (6a). Only the derivatives in (6a) that correspond to derivatives up to the order of those in the equation or equations governing the application are used. For the case presented here, only first derivatives in time, *t*, and first and second derivations in space, *y*, are used, corresponding to these terms in the model for one-dimensional, non-linear, heat conduction presented in a later section. The corresponding equivalence requirements are

$$\frac{\partial \mathbf{G}}{\partial y} = \mathbf{W}\frac{\partial \mathbf{F}}{\partial y}, \quad \frac{\partial^2 \mathbf{G}}{\partial y^2} = \mathbf{W}\frac{\partial^2 \mathbf{F}}{\partial y^2}, \quad \text{and} \quad \frac{\partial \mathbf{G}}{\partial t} = \mathbf{W}\frac{\partial \mathbf{F}}{\partial t} \tag{7}$$

where **W** is the matrix representation of the weights in Eqs. (3)-(5). Define the sensitivity matrix as follows.

$$\mathbf{\Psi} = \begin{bmatrix} \mathbf{\Psi_x} & \mathbf{\Psi_\alpha} \end{bmatrix} \tag{8}$$

where

$$\mathbf{\Psi_x} = \begin{bmatrix} \frac{\partial G_1}{\partial y} & \frac{\partial^2 G_1}{\partial y^2} & \frac{\partial G_1}{\partial t} \\ \frac{\partial G_2}{\partial y} & \frac{\partial^2 G_2}{\partial y^2} & \frac{\partial G_2}{\partial t} \\ \vdots & \vdots & \vdots \\ \frac{\partial G_m}{\partial y} & \frac{\partial^2 G_m}{\partial y^2} & \frac{\partial G_m}{\partial t} \end{bmatrix} \tag{8a}$$

$$\Psi_\alpha = \begin{bmatrix} \frac{\partial G_1}{\partial \alpha_1} & \frac{\partial G_1}{\partial \alpha_2} & \cdots & \frac{\partial G_1}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 G_1}{\partial \alpha_1^2} & \frac{\partial^2 G_1}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 G_1}{\partial \alpha_s^2} \\ \frac{\partial G_2}{\partial \alpha_1} & \frac{\partial G_2}{\partial \alpha_2} & \cdots & \frac{\partial G_2}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 G_2}{\partial \alpha_1^2} & \frac{\partial^2 G_2}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 G_2}{\partial \alpha_s^2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial G_m}{\partial \alpha_1} & \frac{\partial G_m}{\partial \alpha_2} & \cdots & \frac{\partial G_m}{\partial \alpha_s} & \frac{1}{2}\frac{\partial^2 G_m}{\partial \alpha_1^2} & \frac{\partial^2 G_m}{\partial \alpha_1 \partial \alpha_2} & \cdots & \frac{1}{2}\frac{\partial^2 G_m}{\partial \alpha_s^2} \end{bmatrix} \tag{8b}$$

The second derivative terms in $_\alpha$ and $_\alpha$ are multiplied by ½ to be consistent with the corresponding terms in the Taylor series expansion. For example, the truncated, second order Taylor series expansion of **G** about (**x,** **)** (without cross derivative terms for x and higher order derivatives for time as described previously) is given by

$$\mathbf{G}(\mathbf{x} + \Delta\mathbf{x}, \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}) \cong \mathbf{G}(\mathbf{x}, \boldsymbol{\alpha}) + \mathbf{\Psi a} \tag{9}$$

where

$$\mathbf{a} = \begin{bmatrix} \mathbf{a_x} \\ \mathbf{a_\alpha} \end{bmatrix} \tag{10}$$

$$\mathbf{a_x} = \begin{bmatrix} \Delta y & (\Delta y)^2 & \Delta t \end{bmatrix}^T \tag{10a}$$

$$\mathbf{a}_\alpha = \begin{bmatrix} \Delta\alpha_1 & \Delta\alpha_2 & \ldots & \Delta\alpha_s & (\Delta\alpha_1)^2 & \Delta\alpha_1\Delta\alpha_2 & \cdots & (\Delta\alpha_s)^2 \end{bmatrix}^T \tag{10b}$$

Note that the coupling between and **x** is also ignored.

The equations associated with the sensitivity equivalence requirements (Eq. 7) can be represented as a single matrix equation as follows:

$$\mathbf{\Psi} \cong \mathbf{W\Phi} \tag{11}$$

where w_{ji} are the elements of **W**. While Eq. (11) can be used to define the weights, care must be taken in evaluating **W** as and can be, and typically are, rank deficient. Dependencies between columns may exist due to arguments appearing in naturally occurring dimensionless groups associated with the governing equations or due to the governing equations themselves. For example, a linear one-dimension heat conduction model will result in the second and third columns in each of Eqs. (6a) and (8a) being dependent due to the governing equation. One generally wishes to use as many measurement points as possible to define **W** so that the variance of the results is reduced. Since the number of measurements predictions often exceeds the number of independent columns of or , (11) can also be over determined. Singular Value Decomposition (SVD) is used to address these issues. The SVD decomposition of is

$$\mathbf{\Phi} = \mathbf{USV}^{\mathrm{T}} \tag{12}$$

where **U** and **V** are orthogonal matrices, and **S** is a diagonal matrix comprised of singular values. Eq. (12) can be approximated as

$$\mathbf{\Phi}_p \cong \mathbf{U}_p \mathbf{S}_p \mathbf{V}_p^{\mathrm{T}} \tag{13}$$

where $\mathbf{S}_p$ is a *pxp* diagonal matrix comprised of all or a subset of the *p* largest non-zero singular values, and $\mathbf{U}_p$ and $\mathbf{V}_p$ are orthogonal matrices containing the corresponding eigenvectors. Substitution of the reduced system, $_p$, from Eq. (13) into Eq. (11), and post-multiplying both sides by a pseudoinverse of $_p$, denoted by $_p^+$, yields

$$\mathbf{\Psi\Phi}_p^+ \cong \mathbf{W\Phi}_p \mathbf{\Phi}_p^+ \tag{14}$$

where

$$\mathbf{\Phi}_p^+ = \mathbf{V}_p \mathbf{S}_p^{-1} \mathbf{U}_p^+ \tag{15}$$

As discussed by Jackson [16], the product $_p \; _p^+$ in Eq. (14) may only approximate the identity matrix. This matrix is related to the "resolving" matrix of Jackson (note that the transpose of Eq. (11) gives the usual matrix form $^{\mathrm{T}} \mathbf{W}^{\mathrm{T}} \approx {}^{\mathrm{T}}$ where the rows of **W** are the unknowns – the form considered by Jackson). For the case where has fewer independent rows than columns, $_p \; _p^+$ does give an identity matrix, and in this case, the target application decision variables can be fully resolved. However, stability of the resulting **W** cannot be guaranteed (see Jackson) and the sensitivity of the reconstructed decision variable to parameter uncertainty may be very large. If

has more independent rows than columns, the $_p \quad _p^+$ product will only approximate the identity matrix and the target application decision variable will not be fully resolved. In this case, one obtains the normal least-squares solution, and the sensitivity of the resulting least squares approximation for the decision variable to uncertainty in the model parameters may be less. Take $_p \quad _p^+$ to be approximately an identity matrix. In this case, Eq. (14) gives an approximation for **W**.

$$\mathbf{W} \approx \mathbf{\Psi\Phi}_p^{\ +} \tag{16}$$

If the inverse of exists, Eq. (16) can be written as

$$\mathbf{W} = \mathbf{\Psi\Phi}^{-1} \tag{17}$$

The approximation sign in Eq. (16) will be dropped and Eq. (16) will be used as the definition of **W**. The impact of this approximation will later be evaluated through direct comparison of the decision variable model behavior to the reconstructed decision variable model behavior, rather than through the use of the resolving matrix as discussed by Jackson. Use of SVD and the pseudoinverse is an important aspect of the current work. The key feature of the process is that it allows for the trade-off between uncertainty in the reconstructed decision variable, and ability to resolve the target application using the validation experiments to be characterized. This trade-off is based on the selection of the number of the largest non-zero singular values, *q*, and the corresponding eigenvectors used in the evaluation of Eq. (15).

Eqs. (16) or (17) define the weights to be applied to the models for each of the validation measurement points such that the behavior of perturbations in the reconstructed model predictions due to perturbations in the parameters and independent variables **x** about the experimental conditions represented by the validation measurements, is approximately equal (or equal in the case of Eq. (17)) to the behavior of perturbations of the target application model decision variable due to perturbations in the parameters and independent variables **x** about the target application conditions. The accuracy of this reconstructed representation in some neighborhood of and **x** can be evaluated by direct comparison between the reconstructed model prediction for the decision variables and the predicted decision variable produced by the model for the original target application as follows (see Eqs. (3) through (10)):

$$e_j = \left(G_j(\mathbf{x},\boldsymbol{\alpha}) - G_j(\mathbf{x}+\Delta\mathbf{x},\boldsymbol{\alpha}+\Delta\boldsymbol{\alpha})\right) - \sum_{\mathrm{i}=1}^{\mathrm{n}} w_{ji}\ \left(F_i(\mathbf{x},\boldsymbol{\alpha},\boldsymbol{\alpha}_\mathbf{f}) - F_i(\mathbf{x}+\Delta\mathbf{x},\boldsymbol{\alpha}+\Delta\boldsymbol{\alpha},\boldsymbol{\alpha}_\mathbf{f})\right); \quad j = 1,\cdots,m \tag{18}$$

As discussed later, a Box Behnken experimental design [17] will be used to define and **x.** The incremental size of will be based on the uncertainty in these parameters and the incremental size in **x** will be based on the finite difference grid size in space and time. The vectors **x** and $_{\mathbf{f}}$ are evaluated at their expected or nominal values.

Note that the weights are determined with F_i and G_i evaluated at the mean or nominal parameter values with the uncertainties in these parameters not considered. In contrast, the evaluation of the uncertainty in the reconstructed decision variables does require that the uncertainties in these parameters be included. Here a first order analysis is used to evaluate the uncertainty in the reconstructed decision variable due to the uncertainty in the parameters. Changes in the predicted measurements and in the predicted decision variables can be related to changes in the parameters as follows:

$$\Delta\boldsymbol{\gamma} \approx \nabla_{\boldsymbol{\alpha}}\mathbf{F}\,\Delta\boldsymbol{\alpha} + \nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\,\Delta\boldsymbol{\alpha}_{\mathbf{f}} \tag{19}$$

$$\Delta\mathbf{d} \approx \nabla_{\boldsymbol{\alpha}}\mathbf{G}\,\Delta\boldsymbol{\alpha} + \nabla_{\boldsymbol{\alpha}}\mathbf{G}\,\Delta\boldsymbol{\alpha}' \tag{20}$$

where $\Delta\boldsymbol{\alpha}'$ corresponds to changes in the model parameters associated with **G**. The uncertainties in the model parameters for the application **G** are often larger than those for the models of the validation experiments **F**, requiring the inclusion of this additional term in Eq. (20). The requirement that Eq. (11) be true leads to the following approximation to first order. Since Eq. (11) must be true column by column, and assuming no uncertainties in the values for the independent variables, one can write

$$\nabla_{\boldsymbol{\alpha}}\mathbf{G}\,\Delta\boldsymbol{\alpha} \approx \mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\,\Delta\boldsymbol{\alpha} + \mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\,\Delta\boldsymbol{\alpha}_{\mathbf{f}} \tag{21}$$

Using (21) in (20) leads to

$$\Delta\mathbf{d} \approx \mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\,\Delta\boldsymbol{\alpha} + \mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\,\Delta\boldsymbol{\alpha}_{\mathbf{f}} + \nabla_{\boldsymbol{\alpha}}\mathbf{G}\,\Delta\boldsymbol{\alpha}' \tag{22}$$

If the uncertainties in $\boldsymbol{\alpha}$ are independent of those in $\boldsymbol{\alpha}_{\mathbf{f}}$, and the uncertainties in $\boldsymbol{\alpha}_{\mathbf{f}}$ are independent of those in $\boldsymbol{\alpha}'$, the covariance of **d** can be approximated as follows:

$$\mathrm{cov}(\mathbf{d}) \approx \left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)\mathrm{cov}(\boldsymbol{\alpha})\left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)^{\mathrm{T}} + \left(\mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\right)\mathrm{cov}(\boldsymbol{\alpha}_{\mathbf{f}})\left(\mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\right)^{\mathrm{T}} + \left(\nabla_{\boldsymbol{\alpha}}\mathbf{G}\right)\mathrm{cov}(\boldsymbol{\alpha}')\left(\nabla_{\boldsymbol{\alpha}}\mathbf{G}\right)^{\mathrm{T}} \tag{23}$$

Denote the contribution due to uncertainties in the parameters in **F** to be

$$\mathrm{cov}_{\mathbf{F}}(\mathbf{d}) \approx \left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)\mathrm{cov}(\boldsymbol{\alpha})\left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)^{\mathrm{T}} + \left(\mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\right)\mathrm{cov}(\boldsymbol{\alpha}_{\mathbf{f}})\left(\mathbf{W}\nabla_{\boldsymbol{\alpha}_{\mathbf{f}}}\mathbf{F}\right)^{\mathrm{T}} \tag{24}$$

Eq. (23) can be now be written as

$$\mathrm{cov}(\mathbf{d}) \approx \mathrm{cov}_{\mathbf{F}}(\boldsymbol{\alpha}) + \left(\nabla_{\boldsymbol{\alpha}}\mathbf{G}\right)\mathrm{cov}(\boldsymbol{\alpha}')\left(\nabla_{\boldsymbol{\alpha}}\mathbf{G}\right)^{\mathrm{T}} \tag{25}$$

Eqs. (24) and (25) define the uncertainty in the reconstructed decision variable vector, given the uncertainty in the model parameters for the validation experiments and the uncertainty in the model parameters for the target application. Note that the last term in Eq. (25) represents the uncertainty in the target application model prediction of the decision variable. Thus, the uncertainty in the reconstructed variable will always be greater than the uncertainty in the target application model due to the added uncertainties in the validation model parameters. If a parameter has negligible uncertainty, the corresponding row and column in the covariance matrix is set to zero.

3. Examples

Several examples are presented to demonstrate important features of the methodology. The first example is for steady-state, one-dimensional, linear, heat conduction, which leads to a very simple analytical solution. The remaining examples are based on non-linear, transient, heat conduction, which requires the use of numerical solutions. In each case, the models for the validation experimental measurements and target application decision variables are given.

3.1 Linear Steady Heat Conduction

For the first example case, take the models for the validation experiment and the target application to be

Validation Experiment Model	Application Model	
$d^2T/dx^2=0$	$d^2T/dx^2=0$	(26a,b)
$T(0)=T_0=\ _1$	$T(0)=T_0=\ _1$	(27a,b)
$T(1)=T_1=\ _2$	$T(1)=T_1=\ _2$	(27c,d)
	$d=-k\ dT(1)/dx$	(28)
$_1=T(0.25)$		(29)
$_2=T(0.75)$		(30)

Note that the validation experiment and the target application have the same geometry and material properties. Internal temperature measurements from the validation experiment are used to assess the ability to extrapolate to surface heat flux for the target application. Characterize the uncertainty in the parameters for the validation experiment model by the standard deviation . Assume that parameter uncertainties are uncorrelated. The covariance matrix for the validation model parameters is thus (**I** identity matrix)

$$\mathrm{cov}(\boldsymbol{\alpha}) = \sigma_\alpha^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \sigma_\alpha^2 \mathbf{I} \tag{31}$$

Assume that there are no other sources of uncertainty considered. For this case, the parameter vectors are

$$= [T_1 \quad T_2]^T, \qquad {}_{\mathbf{f}} = \mathbf{0} \tag{32}$$

The analytical solutions to this idealized problem and the corresponding uncertainty analysis is presented in Section 4.

3.2 Non-linear transient heat conduction

To illustrate the methodology for a more complex problem, a series of examples or cases are presented demonstrating the important features of the methodology based on the nonlinear, one-dimensional transient heat conduction equation. In contrast to the previous example (as will be shown later), the validation experiments are not be able to fully resolve the target application and the trade-off between resolution and uncertainty will be considered. Specifically, these examples are used to investigate the capability to resolve the application model for T (temperature) and $q=-k \quad T/ \quad y$ (flux) predictions at the boundary with validation experiments. For Case 1, the validation experiment measurements are temperatures at various spatial and temporal locations. The reconstructed decision variable for the application is boundary temperature. In Case 2, the same validation temperature measurements are used. The model decision variable for Case 2 is flux at the boundary. Case 2 was chosen to test the ability of the methodology to reconstruct a decision variable that is physically different from the measurements. Case 3 uses the same validation temperature measurements as Case 2, with two flux measurements added. The Case 3 reconstructed decision variable is flux at the boundary. Case 3 was included to assess the improvements in evaluating the time dependence of a decision variable when one can measure that variable at a few discrete times. The following models for the validation experimental measurements and target application decision variables are used.

Validation Experiment Model	Application Model	
$C_p \quad T/ \quad t = \quad / \quad y(k(T) \quad T/ \quad y)$ (33a,b)	$C_p \quad T/ \quad t = \quad / \quad y(k(T) \quad T/ \quad y)$	
$k(T)=k_o(1+k_tT)$	$k(T)=k_o(1+k_tT)$	(34a,b)
$T(y,0)=0$	$T(y,0)=0$	(35a,b)
$T(0,t)=T_1$	$T(0,t)=T_1$	(36a,b)
$T(1,t)=T_2$	$T(1,t)=T_2$	(37a,b)

Case 1:

$$d_j = T(1, t_j),\ j=1, \ldots, m \tag{38}$$

$$_j = T(0.25, t_j),\ j=1, \ldots, n/2 \tag{39}$$

$$_j = T(0.75, t_j),\ j=n/2+1, \ldots, n \tag{40}$$

Case 2:

$$d_j = -k \quad T(1,t_j)/ \quad y,\ j=1, \ldots, m \tag{41}$$

$$_j = T(0.25, t_j),\ j=1, \ldots, n/2 \tag{42}$$

$$_j = T(0.75, t_j),\ j=n/2+1, \ldots, n \tag{43}$$

Case 3:

$$d_j = -k \quad T(1,t_j)/ \quad y),\ j=1, \ldots, m \tag{44}$$

$$_j = T(0.25, t_j),\ j=1, \ldots, (n-r)/2 \tag{45}$$

$$_j = T(0.75, t_j),\ j=(n-r)/2+1, \ldots, n-r \tag{46}$$

$$_j = -k \quad T(1,t_j)/ \quad y,\ j=n-r \qquad +1,\ldots n$$

(47)

where n is the total number of measurements and where r is the number of flux measurements. For the cases considered below, n will be 10 or 12 and r 0 or 2. The decision variable will be evaluated at m=10 times for the three cases. Thermal conductivity is assumed linear in temperature (k_t a constant). For the present cases, assume that the dependencies in parameters T_1, T_2, C_p, k_o, and k_t, and the independent variables y and t are important to the application. Also assume that the uncertainty corresponding to the additional model parameters $_{\mathbf{f}}$ are not significant (and hence not important) for these examples. The components in the argument vectors are thus

$$= [T_1 \quad T_2 \quad C_p \quad k_o \quad k_t\ ]^T, \quad _{\mathbf{f}} = 0, \text{ and } \mathbf{x} = [y\ t]^T \tag{48}$$

Table 1 lists the nominal parameter values used for these examples. Figure 1 illustrates the time history for the temperature at the measurement locations, y = 0.25, 0.75; and the corresponding flux history at y = 1.0. For illustrative purposes, assume that the uncertainties for these parameters are independent with the statistics listed in Table 1. Note that the uncertainties in the boundary temperatures for the validation experiments were assumed negligible relative to those in the thermal properties. In contrast, it is assumed that there is significant uncertainty in these boundary temperatures for the application as the conditions for such applications are typically

not controlled or known as well as they are for more carefully controlled validation experiments. As stated earlier, the independent variables *y* and *t* are assumed to possess no uncertainty.

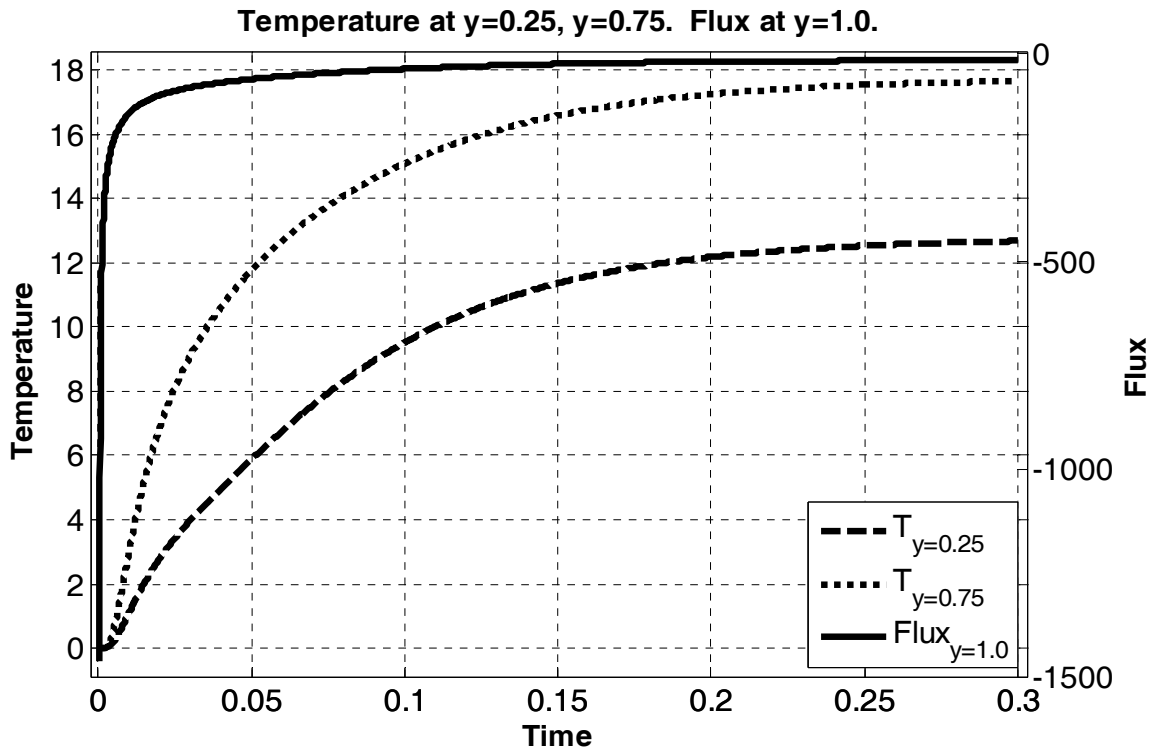

Figure 1. Temperature and Flux Histories

3.3 Code verification

Eqs. (33)-(47) are solved using the second order Crank-Nicholson finite difference algorithm. A two-step process was used to verify the solution, as presented in the Appendix. First, the method of manufactured solutions (Knupp and Salari [18]) was used to verify that the solution converges to a known solution to the nonlinear problem. Application of the algorithm to the verification problem resulted in a maximum difference between the nodal values and the corresponding analytical solution of $O(10^{-3})$, using 41 spatial nodes and t=.0000625. Second, analysis using the Richardson Extrapolation technique (Roache [19]) confirmed that the code converges with approximated second order accuracy, as is appropriate for the Crank-Nicholson method when applied to a nonlinear problem.

Table 1. Model Parameters and Measurement Uncertainty

Parameter/Measurement	Mean Value	Standard Deviation	
		Application Model	Validation Model
T_1	10	2	0
T_2	20	2	0
C_p	1	.1	.05
k_o	1	.05	.05
k_t	.05	.0025	.0025
			.25

3.4 Parameter Setup and Sensitivity Matrix Calculations

Table 2 lists the measurement times and locations and corresponding model predictions using the mean parameter values listed in Table 1. The partial derivatives for the and sensitivity matrices defined by Eqs. (6) and (8) are estimated with central differences, using perturbations of ±0.5% of the mean parameter values. Cross derivatives relative to the model parameters (no cross derivatives with respect to the independent variables) were evaluated using central differences of central differences. The sensitivity matrices contain first and second derivatives for the five important model parameters, plus $T/\ y$, $^2T/\ y^2$, and $T/\ t$. This results in and containing 5 first derivatives with respect to the model parameters, 15 second derivatives, including cross derivatives, and 3 first or second derivatives with respect to the independent variables, for a total of 23 columns. With 10 simulated measurements from the validation experiments for Case 1 (5 times at 2 locations) and 10 measurement prediction times for the target application, and are each 10x23. For Case 2, there are also 10 measurement predictions (5 times at 2 locations). As with Case 1, the Case 2 is 10x23, and is 10x23. For Case 3, is 12x23 (5 times at two locations, plus two flux measurements), and remains 10x23.

The $T/\ y$, $^2T/\ y^2$, and $T/\ t$ terms are estimated for a point through central differences using the nodal values associated with the finite difference approximation of the PDE at that point. The flux measurements, q=-$k\ T/\ y$ at the y=1 boundary used in both the validation measurements and the application model predictions were evaluated from the finite difference solution. The $T/\ y$ term in the flux calculation was evaluated using a quadratic through the three temperature values at the two spatial nodes nearest the boundary and at the boundary node. The resulting quadratic expression was then evaluated at y=1. The sensitivity matrix requires second derivatives of flux. With q=-$k\ T/\ y$, k= $k(T)$=$k_o(1+k_tT)$, y=1, and the quadratic in the form T=a_1+a_2y+a_3y^2, the second derivative term with respect to y in Eq. (8a) is

$$\frac{\partial^2 G}{\partial y^2} = -6k_o k_t \left(a_2 a_3 + 2a_3^2\right) \tag{49}$$

Table 2. Measurements

Case 1 and Case 2		
Time	y	T (i.e. γ)
0.10	0.25	9.51
0.25	0.25	12.53
0.50	0.25	12.78
0.75	0.25	12.79
1.00	0.25	12.79
0.10	0.75	15.08
0.25	0.75	17.54
0.50	0.75	17.75
0.75	0.75	17.75
1.00	0.75	17.75
Case 3: Same Measurements as above, plus Fluxes:		
0.10	1.00	-38.75
0.75	1.00	-17.50
Other Fluxes used for Cross Validation		
0.25	1.00	-19.25
1.00	1.00	-17.50

The $T/\ y$, $^2T/\ y^2$, and $T/\ t$ terms are estimated for a point through central differences using the nodal values associated with the finite difference approximation of the PDE at that point. The flux measurements, q=-k $T/\ y$ at the y=1 boundary used in both the validation measurements and the application model predictions were evaluated from the finite difference solution. The $T/\ y$ term in the flux calculation was evaluated using a quadratic through the three temperature values at the two spatial nodes nearest the boundary and at the boundary node. The resulting quadratic expression was then evaluated at y=1. The sensitivity matrix requires second derivatives of flux. With q=-k $T/\ y$, k= $k(T)$=$k_o(1+k_tT)$, y=1, and the quadratic in the form T=a_1+a_2y+a_3y^2, the second derivative term with respect to y in Eq. (8a) is

$$\frac{\partial^2 G}{\partial y^2} = -6k_o k_t \left(a_2 a_3 + 2a_3^2\right) \tag{37}$$

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4. Results

The results are divided into three sections. The first describes the results obtained from the idealized, one-dimensional, steady, heat conduction problem presented in Section 3.1. The remaining sections address the non-linear, transient heat conduction problem presented in Section 3.2. Specifically, Section 4.2 describes the use of cross validation to verify the methodology by focusing on simulated data from a single experiment. This approach allows one to evaluate whether the methodology has been implemented correctly. Section 4.3 illustrates the methodology when applied to the various cases described in 3.2.

4.1 Steady Heat Conduction

The solutions of Eqs. (26) and (27) are given by

Experiment	Application	
$T = \quad_1(1-x) + \quad_2 x$	$T = \quad_1(1-x) + \quad_2 x$	(50a,b)

The measurements and decision variables are thus given by

$$_1 = 0.75 \quad_1 + 0.25 \quad_2 \qquad d = k\,(\quad_1 - \quad_2) \tag{51a,b}$$

$$_2 = 0.75 \quad_1 + 0.25 \quad_2 \tag{52c}$$

Performing a second order sensitivity analysis as discussed in Section 3 yields

$$\mathbf{\Phi} = \begin{bmatrix} \dfrac{\partial \gamma_1}{\partial \alpha_1} & \dfrac{\partial \gamma_1}{\partial \alpha_2} \\ \dfrac{\partial \gamma_2}{\partial \alpha_1} & \dfrac{\partial \gamma_2}{\partial \alpha_2} \end{bmatrix} = \begin{bmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{bmatrix} \qquad \mathbf{\Psi} = \begin{bmatrix} \dfrac{\partial d}{\partial \alpha_1} & \dfrac{\partial d}{\partial \alpha_2} \end{bmatrix} = \begin{bmatrix} k & -k \end{bmatrix} \tag{53}$$

Because the models are linear in the parameters, the second derivatives are zero and have been dropped from the matrices. For this full rank case, Eq. (17) can be used directly leading to

$$\mathbf{W} \cong \mathbf{\Psi\Phi}^{-1} = \begin{bmatrix} 2k & -2k \end{bmatrix} \tag{54}$$

Because the columns of are independent, $^{-1}$ exists, and the experiment can resolve the decision variable of the target application, Using these results of Eq. (54) in Eq. (3) gives

$$\Delta \mathbf{d} = \mathbf{W}\Delta\boldsymbol{\gamma} = -k\,\frac{\Delta\gamma_2 - \Delta\gamma_1}{0.5} = -k\,\frac{\Delta T(0.75) - \Delta T(0.25)}{0.5} \tag{55}$$

Note that Eq. (55) provides the first order finite difference approximation to the flux. Because the present problem is steady, the flux in the interior is equal to the flux at the surface and one

should expect to obtain the corresponding finite difference approximation to flux if the present methodology is appropriate. Given these weights, the uncertainty in the reconstructed decision variable is given by Eq. (24). Note that the only source of uncertainty considered is due to the validation model parameters (i.e., cov($\boldsymbol{\alpha}_\mathbf{f}$) = **0**). Also, note that $\nabla_\alpha \mathbf{F}$ is the same as for this simplified example.

$$\mathrm{cov}_{\mathbf{F}}(\mathbf{d}) \approx \left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)\mathrm{cov}(\boldsymbol{\alpha})\left(\mathbf{W}\nabla_{\boldsymbol{\alpha}}\mathbf{F}\right)^{\mathrm{T}} = 2k^2\sigma_\alpha^2 \tag{56}$$

The variance in the reconstructed target application decision variable is twice the conductivity-squared times the variance of the validation model parameters.

What do these results suggest? First, the sensitivity of the target decision variable to the model parameters can be represented by a linear combination of first order models for the sensitivities of the predicted validation measurements. A weighting of the validation experiment measurement perturbations can be defined to represent the perturbations of the target application decision variable. In fact, the weights correspond to the finite difference approximation of flux, which is appropriate for the present case. The variance in the reconstructed decision variable is $2k^2$ times the variance of the model parameters. If the acceptable level of uncertainty in the decision variable for the actual target application is, say k^2, then the validation experiment must be designed so that the corresponding variance in the model parameters is less than 0.5, i.e.;

$$2k^2\sigma_\alpha^2 < k^2 \Rightarrow \sigma_\alpha^2 < 0.5 \tag{57}$$

4.2 Cross Validation Applied to One Experiment

Prior to evaluating the use of validation measurement models and weights to assess application model results, a cross-validation exercise was used to verify the weighting methodology for the nonlinear cases. This is done by using the methodology to predict behavior at one measurement location based on the remaining locations. Because the measurements are from a single simulated experiment, the predicted measurement for the decision variable at the selected measurement location and time should be approximately reproduced, when the remaining observed validation measurements are used with the weights developed by the methodology. The procedure is to generate of a vector of predicted validation measurements,

$$=\mathbf{F}(\mathbf{x}, \quad , \quad _{f}) \tag{2}$$

and then select one of the measurement locations and time, say that for measurement k, and using the remaining measurements to represent behavior for the kth measurement.

$$_{k}= d_{cv} =G(\quad , y_k)_{cv} \tag{58}$$

where the subscript *cv* indicates cross validation. The remaining predicted validation measurements are

$$_{cv} = [\quad _1,\ldots, \quad _{k-1}, \quad _{k+1},\ldots, \quad _j]^T = \mathbf{F}(\mathbf{x}, \quad , \quad _f)_{cv} \tag{59}$$

Simulated measurements are generated (listed in Table 2) using the nominal values of the parameters listed in Table 1. The previous defined procedure is used to evaluate the weights and the error associated with representing behavior at one location/time using model behavior at the remaining times. The cross-validation difference, e_{cv}, which is the difference between the decision variable d and the reconstructed decision variable (denoted d_{cv}) is defined as

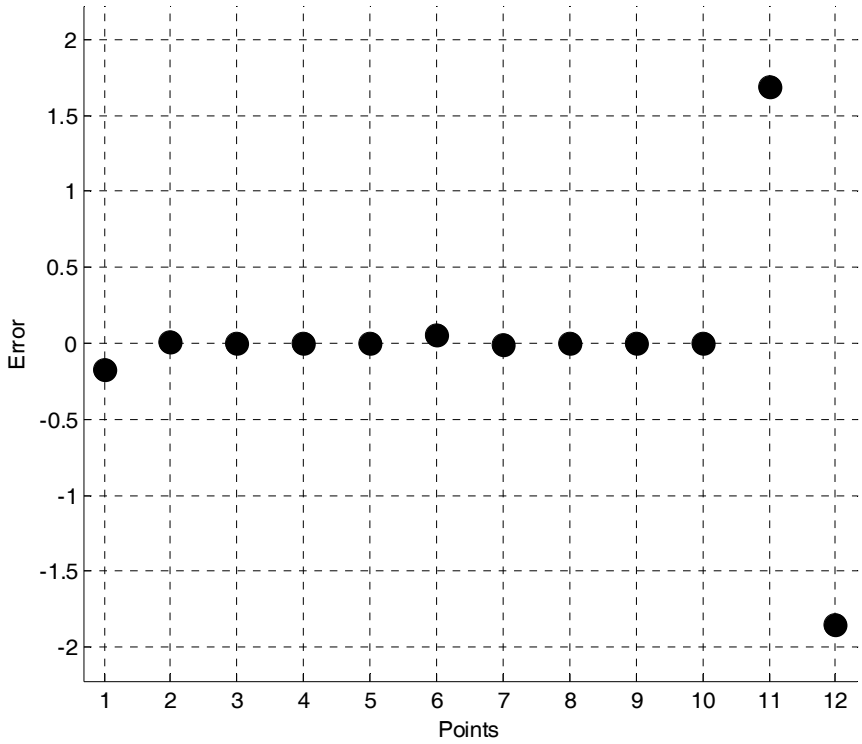
$$\text{Error} = \mathbf{e}_{cv} / \gamma_{max} = \left(\mathbf{G}(\mathbf{x},\boldsymbol{\alpha})_{cv} - \mathbf{W}_{cv}\,\mathbf{F}(\mathbf{x},\boldsymbol{\alpha},\boldsymbol{\alpha}_f)_{cv}\right)/\gamma_{max} \tag{60}$$

The quantity γ_{max} is a normalization constant with the value 20.0 for the case of a reconstructed temperature and -38.75 for the reconstructed flux (see Table 2). Each of these values corresponds to the maximum specified temperature for the boundaries, or measured flux, respectively. Figure 2 shows representative results. Refer to point 1 for illustration. Point 1 represents the normalized error in the reconstructed value for the temperature, T=9.51, at y=0.25, and t=0.10 (see Table 2). The results shown for Points 2 through 10 are reconstructed temperatures for the nodes and times shown. Points 11 and 12 are reconstructed fluxes at y=1, at times 0.10 and 0.75, respectively. The cross validation process progresses as follows:

1. Create a vector from the predicted measurement (i.e., results from Table 2), $=\mathbf{F}(\mathbf{x}, \quad , \quad _f)$ (Eq. (2)) and corresponding $\quad _n$ (Eq. (6)). $\quad _n$ has n rows, one row per measurement (n=12 for this case).
2. Take point 1 out of from step 1. Treat point 1 as $d=G(\mathbf{x}, \quad)$ (Eq. (1)), where d is the reconstructed value corresponding to measurement location/time 1.
3. will contain all rows of $\quad _n$, except for row 1. will correspond to row 1 of $\quad _n$.
4. Evaluate a weight matrix, $\mathbf{W}_{cv}$, using Eq. (16).
5. Evaluate how well the reconstructed difference is estimated for point 1, using Eq. (60). The Eq. (53) error, e_{cv} scaled by $\quad _{max,}$, is -0.1717 (see Figure 2).

6. Repeat steps 2 through 5 for the other measurement locations and times.

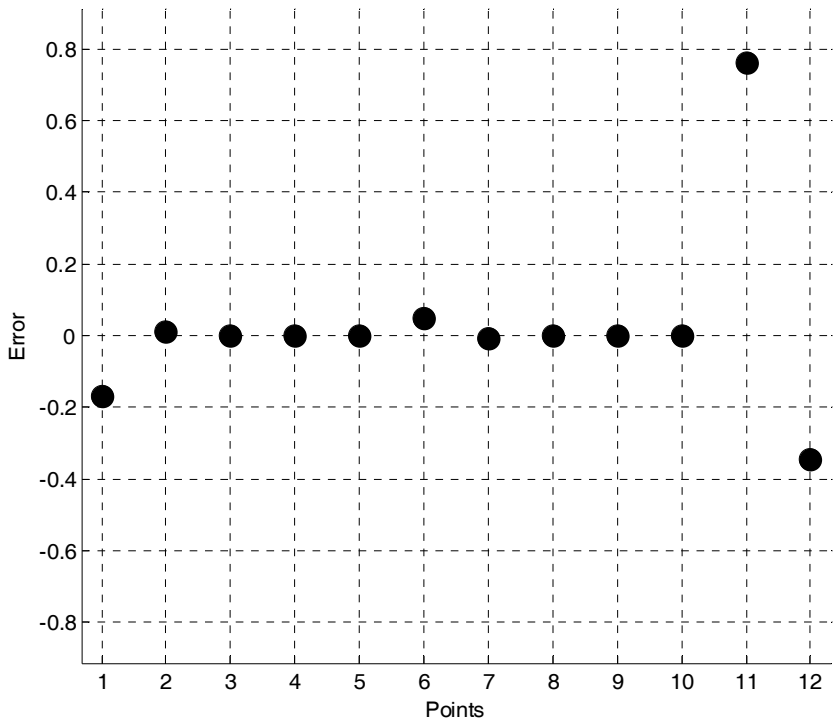
The case shown has ten simulated temperature measurements and two simulated flux measurements (i.e. based on Case 3). The first flux measurement is at t=0.1, during transient behavior. The second flux measurement is at t=.75, toward steady state. The cross validation results in Figure 2 indicate the accuracy with which the methodology can reconstruct the conditions at the various measurement locations and time, using experimental/prediction differences at the remaining measurement locations. The example problem involves a fast transition to a long period of steady state behavior. The largest deviations in Figure 2 are for the flux predictions. The first flux prediction involves a situation where transient flux condition at t=0.1 is predicted by multiple temperatures measured over a time frame spanning transient to steady state and a single flux measurement at steady state. The second flux prediction involves the same temperature measurements, but now the steady state flux is predicted using a transient flux condition as the only other flux involved. The maximum relative error for this case is about -1.80 at point 12. Figure 3 shows results for a case using the flux measurements at t=.1 and t=.25 (both times prior to steady state). For this case, the maximum relative error is less than .8. Figure 4 shows results for a case using the flux measurements at t=0.75 and t=1.0 (both times during steady state). The maximum relative error is 0.15, and occurs not for the two flux predictions but for the temperature predictions at points 1 and 6. These are the temperatures at t=.1 and y=[.25, .75] shown in Table 2. The largest errors for temperature predictions occur when steady state fluxes are in the measurements described in Step 1 above. The largest errors for flux predictions occur when the measurements include a steady state flux predicting a transient flux, and vice versa. Overall, the cross validation results show that the methodology predicts the steady state conditions better than the early transient behavior. The ability to predict normalized flux also appears to be less than that to predict temperature, unless near steady state fluxes are used to predict near steady state fluxes.



Measurements

Point	Time	y	Temp
1	0.10	0.25	9.5
2	0.25	0.25	12.5
3	0.50	0.25	12.8
4	0.75	0.25	12.8
5	1.00	0.25	12.8
6	0.10	0.75	15.1
7	0.25	0.75	17.5
8	0.50	0.75	17.7
9	0.75	0.75	17.7
10	1.00	0.75	17.7
			Flux
11	0.10	1.00	-38.8
12	0.75	1.00	-17.5

Figure 2. Cross Validation 1. Case 3, 2nd Order Sensitivities, 1 transient flux, 1 steady state flux. p=11



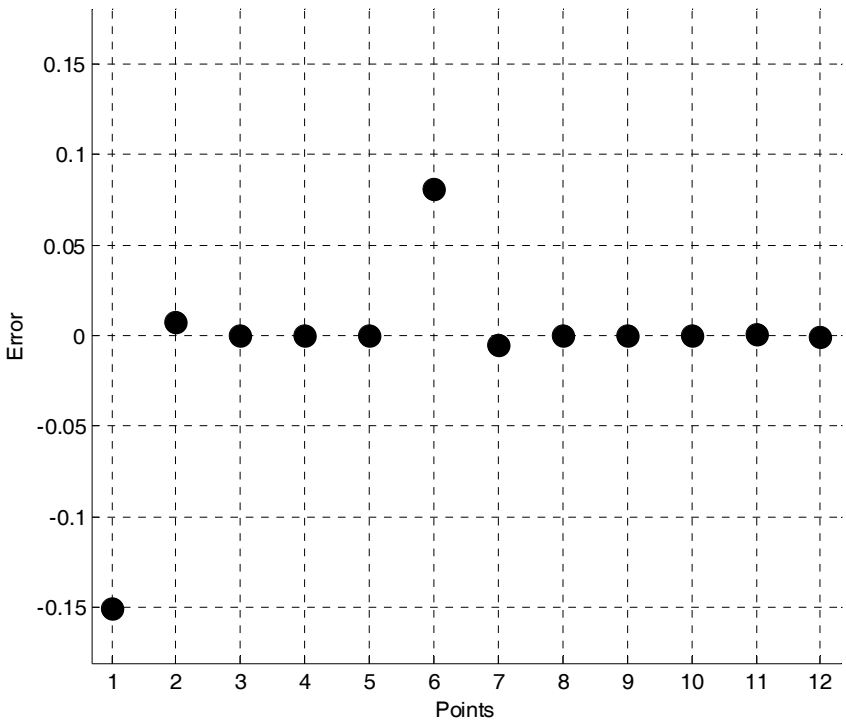
Measurements

Point	Time	y	Temp
1	0.10	0.25	9.5
2	0.25	0.25	12.5
3	0.50	0.25	12.8
4	0.75	0.25	12.8
5	1.00	0.25	12.8
6	0.10	0.75	15.1
7	0.25	0.75	17.5
8	0.50	0.75	17.7
9	0.75	0.75	17.7
10	1.00	0.75	17.7
			Flux
11	0.10	1.00	-38.8
12	0.25	1.00	-19.3

Figure 3. Cross Validation 2. Case 3, 2nd Order Sensitivities, transient fluxes. *p*=11

4.3 Resolution and Accuracy for Multiple Experiments

One of the objectives of the current work is to investigate the use of second order sensitivity matrices to increase the ability to resolve the decision variable. To form a bases for comparison, a first order sensitivity approach was used. In the case of a first order sensitivity matrix, there are 7 first order terms for each measurement prediction: 5 terms for each of the parameters $_i$, and two terms for the independent variables *y* and *t*. Here, each of Cases 1, 2, and 3 are considered utilizing four (i.e., the four largest) singular values to a complete set of seven for the sensitivity matrix. The weights as a function of measurement time for Case 3 for the first order approach (i.e., no second derivatives were included in and) using all seven singular values are listed in Table 3 for the case of flux measurements at t = 0.1, 0.75.



Measurements

Point	Time	y	Temp
1	0.10	0.25	9.5
2	0.25	0.25	12.5
3	0.50	0.25	12.8
4	0.75	0.25	12.8
5	1.00	0.25	12.8
6	0.10	0.75	15.1
7	0.25	0.75	17.5
8	0.50	0.75	17.7
9	0.75	0.75	17.7
10	1.00	0.75	17.7
			Flux
11	0.75	1.00	-17.5
12	1.00	1.00	-17.5

Figure 4. Cross Validation 3. Case 3, 2nd Order Sensitivities, steady state fluxes, *p*=11

Equation (18) is used to assess the quality of the reconstructed target application decision variable over an argument space in the neighborhood around the expected or nominal values of and **x**. Specifically, a Box-Behnken experimental design [17], as implemented by the MatLab [20] routine 'bbdesign', is used to produce the test points for Eq. (18). For the parameters, , the Box-Behnken experimental design points were scaled the standard deviations listed in Table 1. For independent variables, **x**=[y t], the design points were taken to be the neighboring nodal points based on the finite difference grid (over time and space). The upper plot in Figure 5 shows the normalized errors, e_j, for the Case 3 presented in Tables 2 and 3. The errors are normalized by the maximum absolute value for flux (i.e, $\gamma_{max} = q_{max}$=38.75). Case 1 results are normalized by the maximum temperature in the system (i.e., $\gamma_{max} = T_{max}$=20).

Table 3. Case 3 Weights. *p*=7, First Order Sensitivity Matrices

	t_g	t_f				
		0.100	0.250	0.500	0.750	1.000
		Weights for temperature Measurements				
y=0.25	0.1250	0.3579	5.0149	-1.9008	-2.2060	-2.2125
	0.2500	-0.1489	4.0456	-1.2102	-1.4436	-1.4486
	0.3750	-0.0612	0.8635	-0.2368	-0.2862	-0.2873
	0.5000	-0.0120	0.1725	-0.0497	-0.0601	-0.0603
	0.6250	-0.0017	0.0212	-0.0056	-0.0074	-0.0074
	0.7500	0.0002	-0.0027	0.0011	0.0007	0.0007
	0.8750	0.0004	-0.0060	0.0020	0.0018	0.0018
	1.0000	0.0005	-0.0065	0.0022	0.0020	0.0020
	10.0000	0.0005	-0.0065	0.0022	0.0020	0.0020
	100.0000	0.0005	-0.0065	0.0022	0.0020	0.0020
y=0.75	0.1250	0.4149	4.5682	-1.1782	-1.4315	-1.4368
	0.2500	-0.1073	3.4499	-0.9158	-1.1095	-1.1136
	0.3750	-0.0525	0.7252	-0.1940	-0.2351	-0.2360
	0.5000	-0.0085	0.1521	-0.0394	-0.0481	-0.0483
	0.6250	-0.0017	0.0234	-0.0060	-0.0076	-0.0076
	0.7500	-0.0003	0.0033	-0.0007	-0.0012	-0.0012
	0.8750	-0.0001	0.0005	-0.0000	-0.0003	-0.0003
	1.0000	-0.0000	0.0001	0.0001	-0.0002	-0.0002
	10.0000	-0.0000	0.0001	0.0001	-0.0001	-0.0001
	100.0000	-0.0000	0.0001	0.0001	-0.0001	-0.0001
y=1.0		Weights for flux Measurements				
	0.1250	0.4651			0.7876	
	0.2500	0.0368			1.0186	
	0.3750	0.0077			0.9944	
	0.5000	-0.0009			1.0033	
	0.6250	-0.0000			1.0003	
	0.7500	0.0000			1.0000	
	0.8750	0.0000			1.0000	
	1.0000	0.0000			1.0000	
	10.0000	0.0000			1.0000	
	100.0000	0.0000			1.0000	

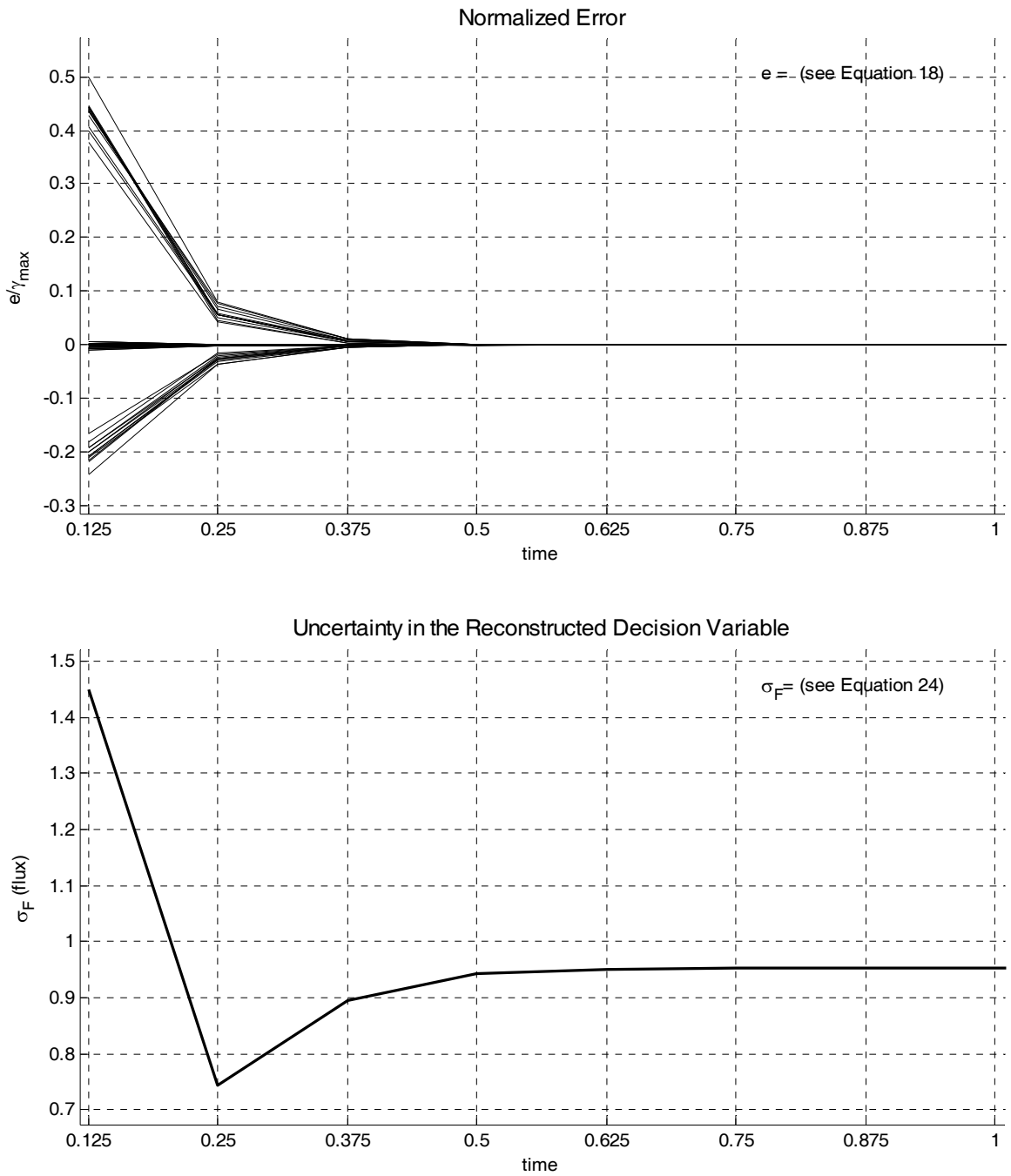


Figure 5. Case 3 Results. First Order Sensitivities, *p*=7

Standard deviations of the reconstructed decision variable as a function of time are evaluated using Eqs. (24) and (25). The standard deviation for each measurement time is given by the square root of the diagonal elements in the corresponding covariance matrices of Eqs. (24) and (25). The resulting standard deviations for Case 3 for the weights as defined in Table 3, are listed in Table 4. The second column is the contribution due to uncertainty in the validation parameters , Eq. (24). The third column is the contribution due to uncertainty in the target application model parameters ' (last term on RHS of Eq. (25)), and the last column lists the total uncertainty. In contrast, Figure 5 (lower plot) results reflect only Eq. (24) to evaluate the standard deviation of the decision variable as reconstructed by the models for the validation measurements. It is important to note that the standard deviations of the target application models parameters ' are not used to develop the weights **W** or to study the trade-off between accuracy and resolution of the reconstructed decision variables. These uncertainties are used only if one wishes to assess the significance of target application model parameter uncertainty relative to the effects of parameter uncertainty for the validation experimental models. Note that the total uncertainty in the reconstructed decision variable is greatest at early times and decreases toward steady state. The major contribution to the total uncertainty is the uncertainty due to the model parameters associated with the target application rather than validation experiment model parameter uncertainty. At early prediction time, this uncertainty is due to uncertainty in the target application thermal diffusivity and the boundary temperatures. At late time, the uncertainty approaches steady state with impact of the uncertainty associated with the target application thermal diffusivity becoming less. The contribution to total uncertainty due to uncertainty in validation parameters for this case is significantly less than for the target application. Refer to Table 1 for comparisons between the validation experiment and the application prediction values used for standard deviations for the boundary temperatures and the density-specific heat product. The minimum uncertainty due to validation parameters (F column in Table 4) occurs at t = 0.25. This suggests that at this time, the effect of the surface flux at y=1 at the internal temperature measurement locations is significant to maximize the ability to resolve this flux with a minimum sensitivity to parameter uncertainty. Note that the ability to represent the target application surface flux improves as the time of interest approaches steady state. The ability to resolve the target application decision variable over the Box-Behnken design space (upper plot of Figure 5) increases rapidly as steady state is approached. This is not

surprising considering that the information contained in the earlier internal temperatures should be reflected in the reconstructed decision variable at later times.

Table 4. **Uncertainty in the Reconstructed Decision Variable.** Case 3. *p*=7. First Order Sensitivity Matrices

t	F	,	d
0.1250	1.4510	5.9175	6.0928
0.2500	0.7447	5.0769	5.1313
0.3750	0.8945	5.0743	5.1525
0.5000	0.9424	5.0866	5.1732
0.6250	0.9504	5.0890	5.1770
0.7500	0.9517	5.0894	5.1776
0.8750	0.9519	5.0894	5.1777
1.0000	0.9519	5.0894	5.1777
10.0000	0.9519	5.0894	5.1777
100.0000	0.9519	5.0894	5.1777

Trade-off exists in the ability to resolve the target application behavior using the models for a set of validation experimental measurements. Generally, as one attempts to better resolve the application decision variables using more singular values, the results are increasingly sensitive to uncertainty in the model parameters. Figure 6 illustrates this effect. The plots in the left column of Figure 6 illustrate the trade-off between uncertainty in the reconstructed decision variable for a single time, *t*=0.375, when only the first order terms are retained in and . The numbers in the circles represent the number of singular values (i.e., *p* largest singular values) retained in the evaluation of Eq. (15). The second column of Figure 6 reflects the results obtained when second order terms are utilized in and . For Case 1, with only the first order terms used, the trade-off suggests that the best result is obtained with *p*=5. This value of *p* results in the lowest maximum error in the reconstructed decision variable over the Box-Behnken design points, while maintaining a minimal sensitivity to uncertainty. Figure 7 (upper plot) shows the results obtained for this case, as a function of *t*, for each of the design points of the Box-Behnken

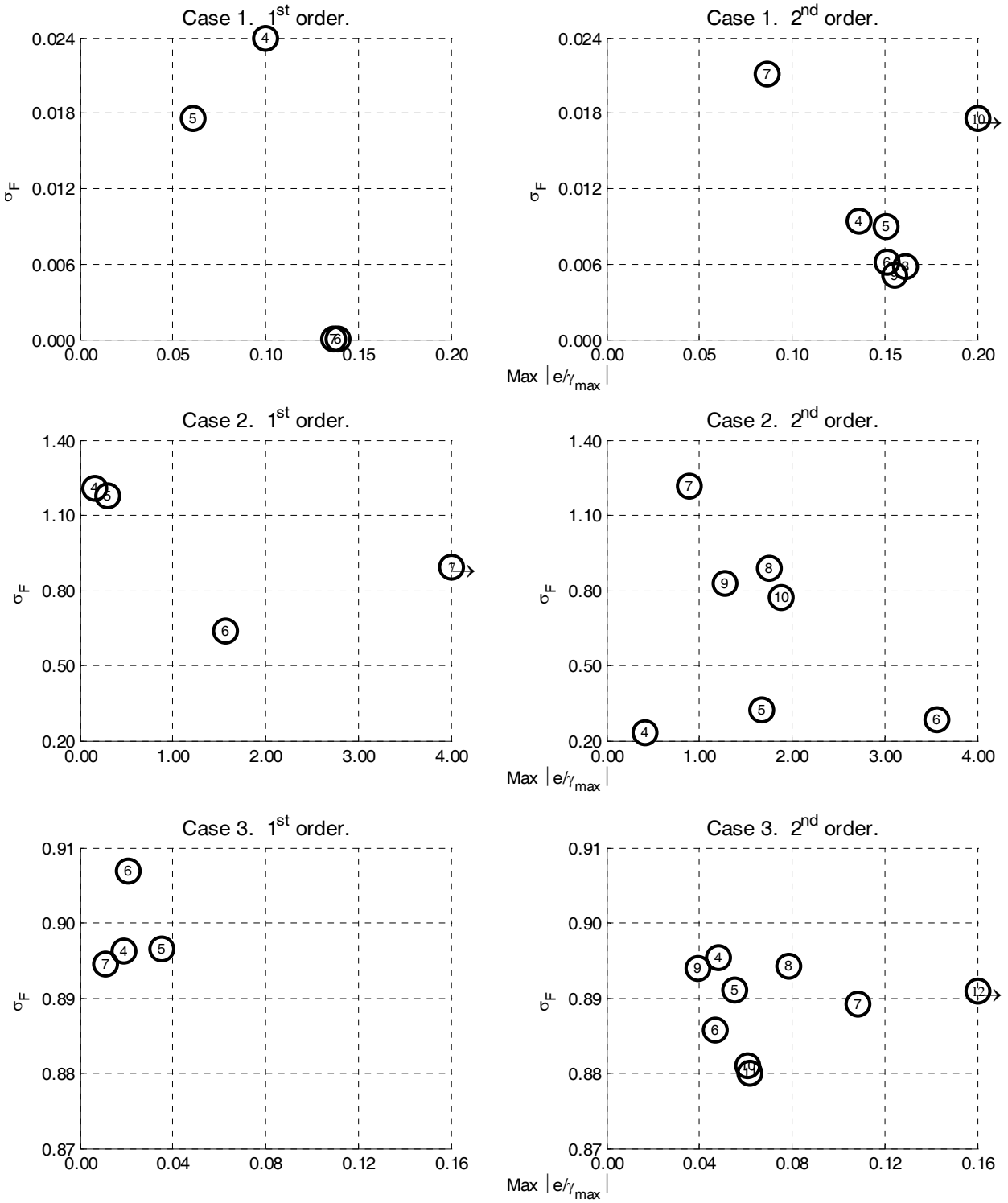


Figure 6. σ_F vs. Error at *t*=0.375 for Reconstructed Decision Variable. *p* shown in markers

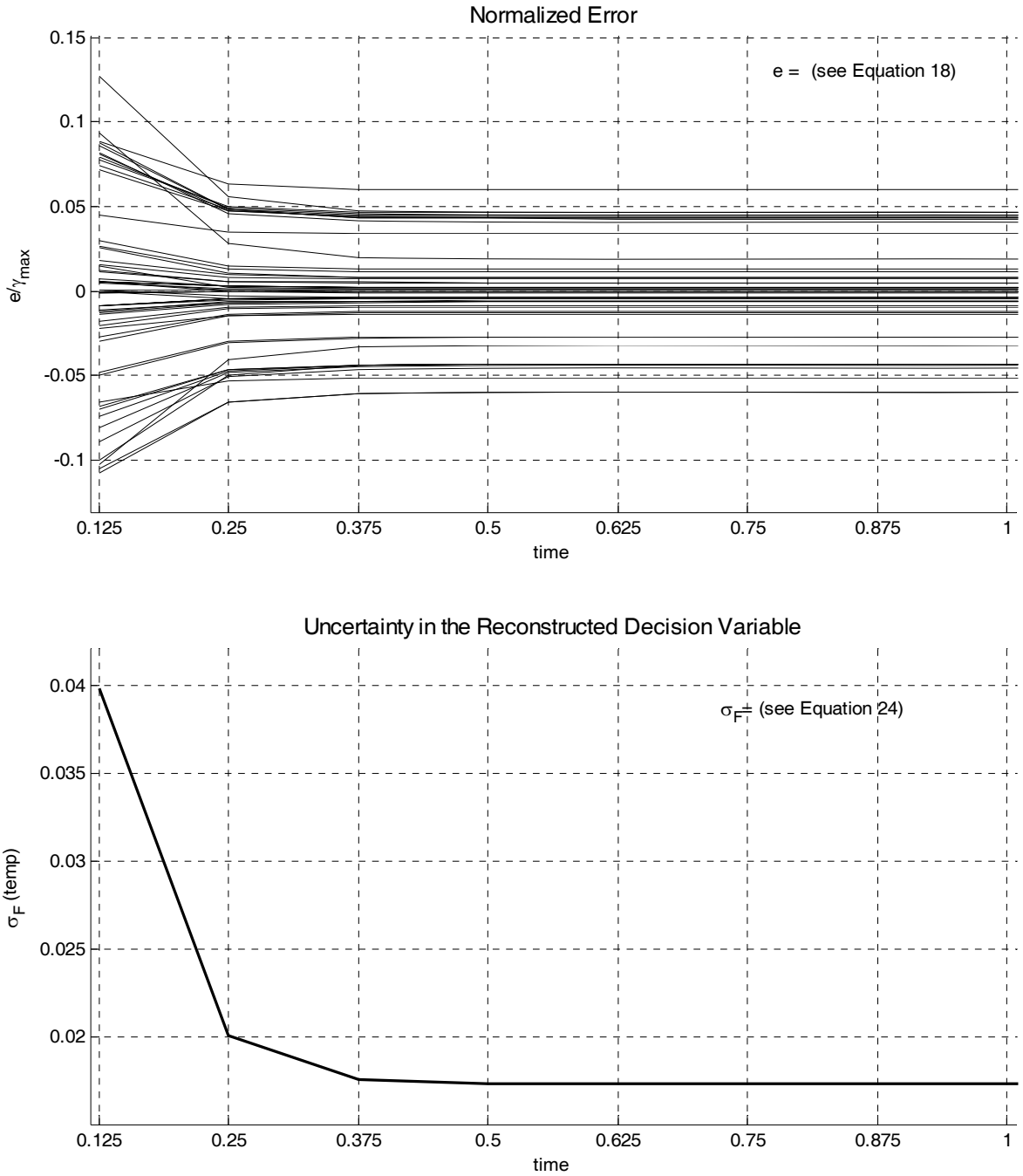


Figure 7. Case 1 Results. First Order Sensitivities, *p*=5

design. Note that the normalized error does not go to zero for large time. On the other hand, the uncertainty in the reconstructed decision variable at larger times is considerably smaller than it was for Case 3 (see Figure 5, lower plot).

Using second order derivatives for Case 1 (Figure 6, top-right plot) does not result in improved ability to resolve the decision variable. For this case, nothing is gained by using second order derivatives in and . The Case 2 results (Figure 6, middle plots) indicate that the second order method can provide reduced sensitivity for uncertainty when the largest 4 singular values are retained. This comes at the expense of a minor degradation in the ability to resolve the decision variable as indicated by the larger ratio of normalized error. Comparison of the results for Cases 1 and 2 indicate that the ability to resolve surface flux (Case 2) using internal temperature measurements is less than the ability to resolve surface temperature using these measurement times and locations. It is interesting to note that this is the only case where the decision variable is different from all of the quantities measured during the validation experiments. Case 3 reflects the impact of the addition of two surface flux measurements to the set of validation measurements. Note that we are simultaneously incorporating two types of measurements, temperature and flux. Comparison of the Case 2 and Case 3 results, as illustrated in Figure 6, shows a significant improvement in the ability to resolve surface flux at a time different from the surface flux measurements, with generally less sensitivity to uncertainty in the model parameters. The p=7 results for first order derivatives and p = 9 case for second order derivatives appear optimum for the t=0.375 reconstructed flux for Case 3. The corresponding time histories are illustrated in Figures 5 and 8. Note that the inclusion of the second order sensitivities increased the maximum normalized error for time less than 0.5 (upper figures), without a significant change in the uncertainty of the reconstructed decision variable (lower figures).

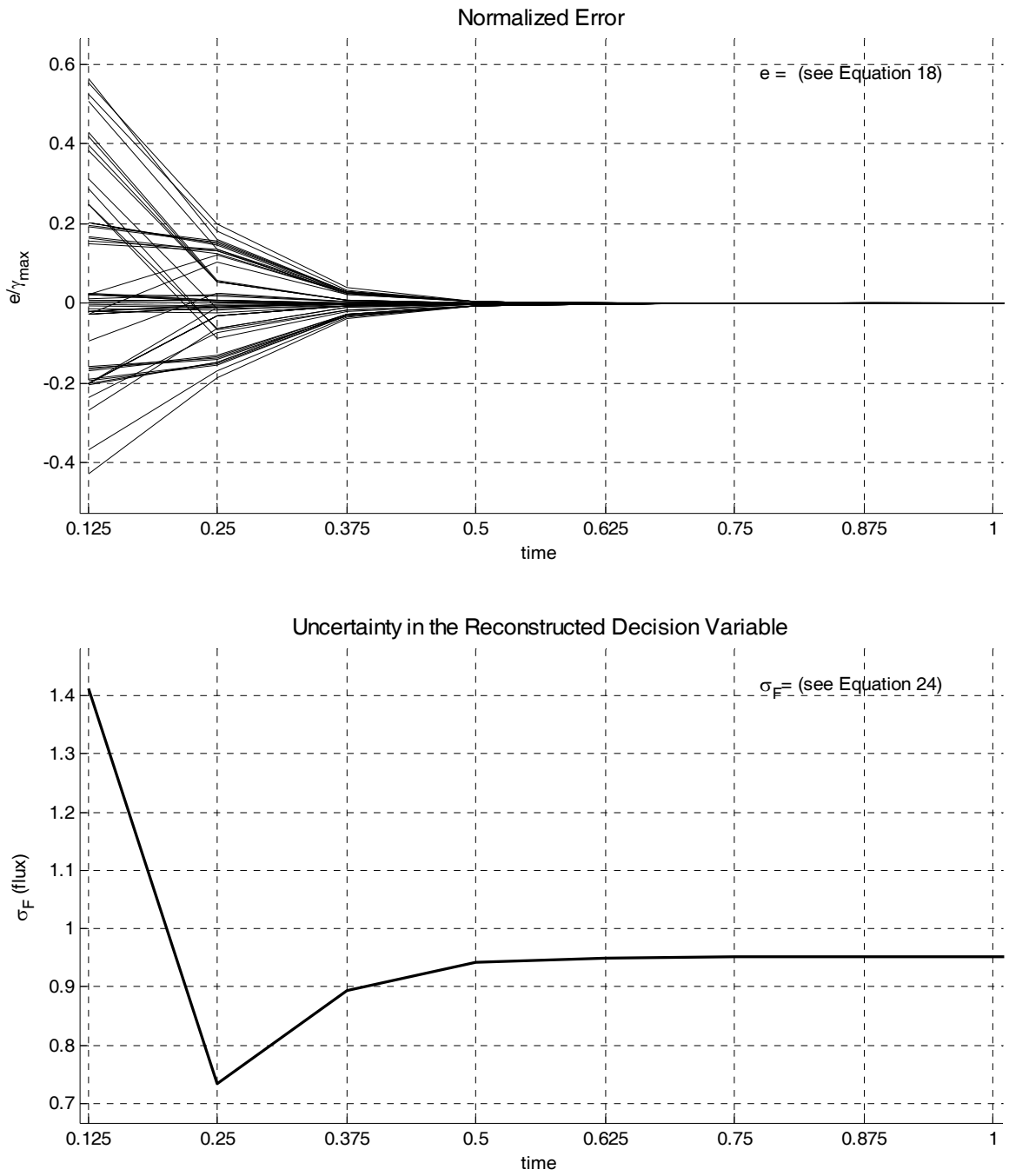


Figure 8. Case 3 Results 2. Second Order Sensitivities, *p*=9

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5. Summary and Discussion

The availability of experimental data to test a model at the anticipated target application conditions is very desirable from a model validation point of view. Unfortunately, such data is not always available, and methodology is required to relate information gained from data obtained under different conditions or for different variables to the conditions and variables for the target application. The key benefit of the present methodology is its ability to assess whether a set of validation experiments can "represent" a target application. As the results illustrate, the ability to resolve the target application depends directly on the level of uncertainty in the model parameters used to model the experiments as well as the uncertainty in the model parameters for the target application. The present methodology provides a means to quantify the trade-off that exists between the ability to resolve the target application decision variables, and the impact that model parameter uncertainty has on this ability.

Specifically, the methodology develops weights that are applied to model predictions for the validation data to represent the model predictions at the target application conditions. First, a sensitivity analysis is used to develop a reconstructed target application decision variable for the validation experiments, and then the tradeoff between resolution and accuracy is investigated. This effort shows that, at least for the cases considered, inclusion of second order sensitivities generally do not produce better results. In the case of a model more non-linear in the parameters, or the case of increased uncertainty in the validation experimental parameters (i.e., the Box-Behnken design [17] would utilize parameter values farther from the nominal values for this case), one may obtain an improvement in the ability to resolve the design variables using second order analysis. However, this increased ability to resolve the design variables may result in an increase in sensitivity to the model parameter uncertainties. In general, if one finds that the reconstructed model is too sensitive to uncertainties in the parameters for the validation and target application models, then one should acquire more data to reduce the standard deviation of the reconstructed decision variable, redesign validation experiments to have less uncertainty, or acquire data from experiments closer to the target application conditions and measurement type. It should be noted that the resulting trade-offs between resolution and accuracy are very system

specific. The choice of the number of singular values to retain is also system specific and must be done after the trade-offs have been characterized.

The weights developed here can be used to evaluate whether validation prediction/experimental differences are consistent, weighted for the target application, using a validation metric as discussed in Hills and Leslie [12]. Caution must be exercised since the methodology is based on an existing model for the target application, tested at conditions different from the target application conditions. A more rigorous test would be to test the target application model at the target application conditions, but this is not always possible.

The example problems presented were based on a sensitivity analysis about the nominal values for the parameters used in the models to simulate validation measurements and about the anticipated values for the parameters for the target application. If data from validation experiments are available, then one can consider using these data to calibrate the model parameters to provide a better representation of the conditions of the individual experiments. This may improve the ability of the reconstructed decision variable model to represent the decision variable. While this approach has some value for use in assessing the coverage of the target application model by the validation experiments, it should not be used if the purpose is to develop target application relevant metrics that use the observed differences between the data from the validation experiments and the model predictions of this data. The data used for validation metrics must be independent of the data used to calibrate models for the metrics to be viable. Otherwise, there is a danger that one is evaluating how well a model can be made to 'fit' the data, rather than how well the model can predict the data.

Full system models for a complex multi-physics target applications can contain tens to hundreds of model arguments and these models often are computational expensive. For the approach presented here to be useful, one should use judgment, coupled with targeted sensitivity analysis, to evaluate which model arguments have the most significant effect on the model predictions and include only those sensitivities in the sensitivity matrices used here. Once the sensitivity matrices are evaluated, the tradeoff between the resolution and accuracy, through the retention of a subset of the singular values, does not require further model runs and is not computational

expensive. Another approach that can be used is to evaluate the target application model at points sampled from a space filling experimental design (such as Latin Hypercube Monte Carlo sampling). The validation experimental models can also be evaluated at these points and a concept analogous to that provided here can be used to evaluate the weights. In this case, the rows of the matrices will not be sensitivities, but model predictions at the various sampling points about the nominal values for the model parameters and arguments. The weights can be developed from these matrices and the resolution/accuracy analysis performed using these weights. This approach has the disadvantage that it may not capture the important behavior of the models (especially if a limited number of samples are used) but has the advantage that the weights are developed using predictions at the design points rather than first and second derivatives at the nominal points. As a result, this approach may better represent off nominal value behavior of the models. A case where this may be so is when the estimated standard deviations in the model parameters for the validation experimental models are sufficiently large such that a first or second order Taylor series cannot capture the behavior. The second author has used, but not reported, this sampling approach with some success.

Finally, we wish to emphasize that the purpose of the reconstructed model for the decision variables is to assess how well this reconstruction can represent the target application behavior. This reconstruction should not be used as a substitution for the target application model for prediction.

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6. References

[1] AIAA (1998), Guide for the Verification and Validation of Computational Fluid Dynamics Simulations, American Institute of Aeronautics and Astronautics, AIAA-G-077-1998, Reston, VA.

[2] ASME (2006), Guide for Verification and Validation in Computational Solid Mechanics, The American Society of Mechanical Engineers, ASME V&V 10-2006, New York, NY.

[3] Oberkampf, W. L., and T. G. Trucano (2002), Verification and Validation in Computational Fluid Dynamics, Progress in Aerospace Sciences, Vol. 38(3), pp. 209-272.

[4] Oberkampf, W. L., T. G. Trucano, and C. Hirsch (2004), Verification, Validation, and Predictive Capability in Computational Engineering and Physics, Applied Mechanics Reviews, Vol. 57(3), pp. 345-384.

[5] ISI (2008), SciSearch Plus, www.isinet.com, Philadelphia

[6] Landis, W.G. (2002), Uncertainty in the Extrapolation from Individual Effects to Impacts upon Landscapes, Human and Ecological Risk Assessment, Vol. 8(1), pp. 193-204, January.

[7] Munns, W.R. (2002), Axes of Extrapolation in Risk Assessment, Human and Ecological Risk Assessment, Vol. 8(1), pp. 19-29, January.

[8] Kalberlah, R., U. Fost, and K. Schneider (2002), Time Extrapolation and Interspecies Extrapolation for Locally Acting Substances in Case of Limited Toxicological Data, Annals of Occupational Hygiene, Vol. 46(2), pp. 175-185, March.

[9] Bernillon P., and F.Y. Boise (2000), Statistical Issues in Toxicokinetic Modeling: A Bayesian Perspective, Environmental Health Perspectives, Vol. 108(5), 883-893, October.

[10] Vermeire T, T. Jager, G. Janssen, P. Bos, and M. Pieters (2001), A Probabilistic Human Health Risk Assessment for Environmental Exposure to Dibutylphthalate, Human and Ecological Risk Assessment, Vol. 7(6), pp. 1663-1679, November.

[11] Hills, R. G. and T. G. Trucano (2001), Statistical validation of Engineering and Scientific Models with Application to CTH, SAND2001-0312, Sandia National Laboratories, Albuquerque.

[12] Hills, R. G., and I. H. Leslie (2003), Statistical Validation of Engineering and Scientific Models: Validation Experiments to Application, SAND2003-0706, Sandia National Laboratories, Albuquerque.

[13] Hanson, K. M., and F. M. Hemez (2001), A Framework for Assessing Confidence in Computational Predictions, Experimental Techniques, Vol. 25, pp. 50-55.

[14] Mahadevan, S., R. Zhang, N. Smith (2001), Bayesian Networks for System Reliability Reassessment, Structural Safety, Vol. 23. 231-251.

[15] Hills, R. G. (2006), Model Validation: Model Parameter and Measurement Uncertainty, Journal of Heat Transfer, Vol. 128, pp. 339-351.

[16] Jackson, D. D. (1977), Interpretation of Inaccurate, Insufficient and Inconsistent Data, Geophys. J. R. Astr. Soc., Vol. 23, pp.97-109.

[17] Box G. E. P., D. W. Behnken (1960), Some new 3 level designs for the study of quantitative variables, Technometrics, Vol. 2, pp. 455-475.

[18] Knupp, P., and K. Salari (2003), Verification of Computer Codes in Computational Science and Engineering, Chapman & Hall/CRC, Boca Raton, FL.

[19] Roache, P. J. (1998), Verification and Validation in Computational Science and Engineering, Hermosa Publishers, Albuquerque, NM.

[20] Matlab® Mathematics (2004), Version 7, The MathWorks, Inc., Natick, MA.

Appendix. Code Verification

Because the thermal diffusivity, *k*, is a function of *T*, Eqs. (33 a, b) are nonlinear in temperature. These equations are solved using the second order Crank-Nicholson finite difference algorithm. To verify the solution, both code verification and solution verification is used. We begin by applying the method of manufactured solutions, as presented by Knupp and Salari [18]. In the present application, the manufactured solution chosen is as follows:

$$T_{\text{manufactured}} = T_m = 1-(4y-1)^2 \mathrm{e}^{[(-k_o t)/(\rho C_p)]} \tag{61}$$

With this known analytical solution for temperature, Eq. (33) becomes

$$\begin{aligned}\rho C_p \partial T/\partial t - \partial/\partial y[k(T)\partial T/\partial y] = {} & k_o(4y-1)^2 \mathrm{e}^{[(-k_o t)/\rho C_p)]} \\ & - k_o k_t[(8-32y)\mathrm{e}^{[(-k_o t)/(\rho C_p)]}]^2 \\ & - (k_o + k_o k_t T)(-32)\mathrm{e}^{[(-k_o t)/(\rho C_p)]} = g(y,t)\end{aligned} \tag{62}$$

and Eqs. (35), (36), and (37) become

$$T_m(y,0) = 1-(4y-1)^2 \tag{63}$$

$$T_m(0,t) = 1-\mathrm{e}^{(-k_o t)/(\rho C_p)} \tag{64}$$

$$T_m(1,t) = 1-9\mathrm{e}^{(-k_o t)/(\rho C_p)} \tag{65}$$

Using the model parameters shown in Table 1, the Crank-Nicholson algorithm is applied to Eqs. (62) through (65) and the results are compared to the manufactured solution given by Eq. (61). In this case, the maximum difference between any nodal value and the corresponding analytical value is $O(10^{-3})$ using 41 spatial nodes and a time step of .0000625.

Analysis using the Richardson Extrapolation as presented by Roache [19] confirms that the code has second order convergence, as intended. Roache [19] defines a convergence rate, *o*, as follows:

$$o = \frac{1}{\ln(r)} \ln\left(\frac{u_2 - u_1}{u_3 - u_2}\right) \tag{66}$$

where u_1, u_2, u_3 are solutions at some common points for grid resolutions h_1, h_2, h_3. The "r" in the ln(r) term is the ratio of grid refinement between successive grids. Comparing results at common spatial points between cases with 21, 41, and 81 spatial nodes corresponds to r=2. With time steps of 0.00025, 0.0000625, and 0.000015625, respectively, the result for o as a function of time and space is shown in Figure A1. Note that the method demonstrated second order convergence at all locations and time, except at time zero at the boundary conditions, where a step change in temperature occurs.

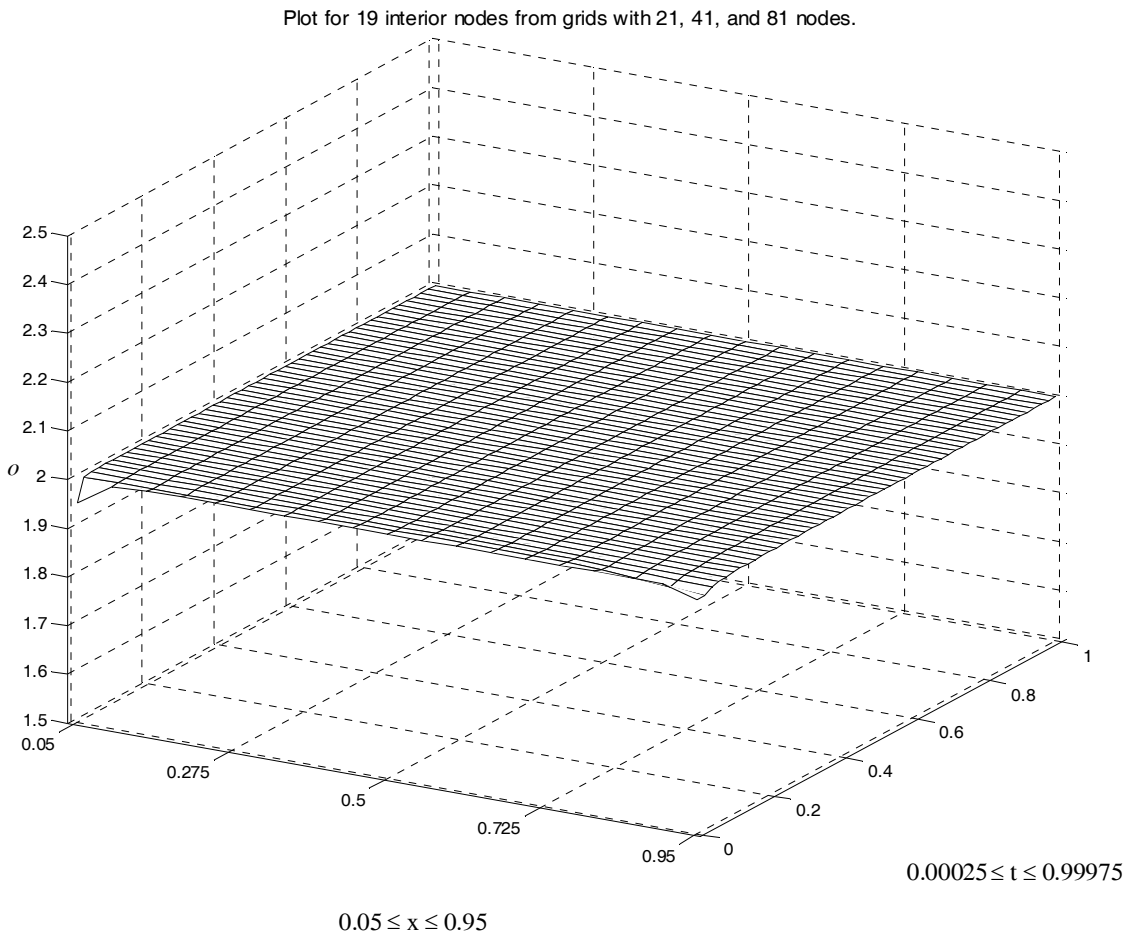

Figure A1. Richardson Extrapolation Observed Order of Convergence.

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