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SURROGATE MODEL DEVELOPMENT AND VALIDATION FOR RELIABILITY ANALYSIS OF REACTOR PRESSURE VESSELS

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ABSTRACT

In nuclear light water reactors, the reactor core is contained within a thick walled steel reactor pressure vessel (RPV). Over time, material embrittlement caused by exposure to neutron flux makes the RPV increasingly susceptible to fracture under transient conditions. Because of parameter uncertainties, probabilistic methods are widely used in assessing RPV integrity.

For efficient probabilistic analysis, techniques to rapidly evaluate the stress intensity factor for given flaw geometry and stress conditions are essential. The stress intensity factor influence coefficient (SIFIC) technique is widely used for this purpose, but is limited to axis-aligned flaw geometries. To consider a wider range of flaw geometries, surrogate models to compute stress intensity factors are explored.

Four surrogate modeling techniques are applied here to compute SIFICs from a set of training data, including two different response surface polynomials, a model utilizing ordinary kriging and another using interpolation. Errors in the SIFICs are assessed for all of these techniques. These techniques are benchmarked against a benchmark solution by computing the time history of the stress intensity factor for an axis-aligned, semi-elliptical surface breaking flaw in an RPV subjected to a transient loading history. All of these techniques compare well with the benchmark solution.

Keywords: reactor pressure vessel, fracture, surrogate model

NOMENCLATURE

FAVOR – Fracture Analysis of Vessels Oak Ridge
INL – Idaho National Laboratory
K_I – Mode I stress intensity factor
ORNL – Oak Ridge National Laboratory
PTS – Pressurized Thermal Shock
PWR – Pressurized Water Reactor
RPV – Reactor Pressure Vessel
RSM – Response Surface Methodology
SIFIC – Stress Intensity Factor Influence Coefficient
a – Flaw depth
(a/t) – Relative flaw depth to wall thickness
C_j – Stress Coefficients
K_j – Stress intensity factor influence coefficient (SIFIC)
L – Flaw length
(L/a) – Flaw aspect ratio
t – RPV wall thickness
t_{clad} – Cladding thickness
φ – Angular position along flaw front

PART 1: INTRODUCTION

In nuclear light water reactors, the reactor core and coolant are contained within a large, thick walled steel vessel known as a reactor pressure vessel (RPV). These structures typically consist of two primary materials—the base material and a very thin layer of cladding. The base material is low alloy ferritic steel, with a thickness of approximately 15-22 centimeters. The cladding is a thin layer of austenitic stainless steel, typically with a thickness of less than 0.635 cm, which lines the inner surface of the vessel to protect against corrosion [1]. Given the tremendous size of these structures, RPVs can contain a relatively high number of internal and surface-breaking defects introduced in the manufacturing process [2]. These flaws are typically of little concern in the early stages of a reactor's operating life as the vessel’s constituent materials have sufficiently high fracture toughness. However, as the reactor operates, the neutrons emitted from the reactor core bombard the RPV steel. Over many years of operation, high levels of irradiation begin to change the material's behavior from ductile to brittle. [3]

Over time, material aging and embrittlement, make the vessel increasingly susceptible to brittle fracture initiating at preexisting flaws. The issue of assessing the damage tolerance of these vessels then arises when attempting to determine the safe life of these structures. Damage tolerant systems, especially critical systems such as RPVs, begin to require extra attention during long term operation. Inspections can help to characterize flaws, but by themselves provide little insight into how an RPV with a given flaw population may react to a transient event. As such, simulation based studies of the fracture response of RPVs under transient conditions that would be experienced both during normal operation and abnormal conditions are essential in assessing the risk associated with the continued operation of the nuclear reactors. [2]

There are a number of scenarios that can cause an RPV to experience non-normal operating conditions. Therefore, RPVs must be able to withstand many types of thermal-hydraulic loading scenarios, many of which are drastically different from their normal operating conditions. One such transient event of concern is a Pressurized Thermal Shock (PTS) event [4]. PTS events could occur in an accident scenario in which the vessel is rapidly cooled introducing a strong thermal gradient in the vessel, while the internal pressure is high. The presence of a large mechanical stress induced by a high internal pressure combined with a sudden high thermal stress can result in a high stress intensity factor at the tip of an existing flaw. The coolant may also sufficiently decrease the temperature at the flaw location to bring it into a brittle behavior regime. The combination of the high stress intensity and the reduced fracture toughness may be sufficient to initiate crack growth.

PART 2: BACKGROUND

To study the fracture response of a given flaw, it is possible to create a detailed 3D finite element model of the region of the flaw and compute fracture parameters. This is commonly done to evaluate specific flaws. However, the large amount of uncertainty associated with the flaw population (number of flaws, sizes, shapes, orientations etc.) [5] necessitates a probabilistic approach to address the inherent randomness within these studies. Single flaw evaluations can require several minutes of computing time for a single time step, and a full scale transient finite element analysis of a 3D RPV could potentially take days of computation time. Thus, a method for the precise and rapid evaluation of the stress intensity factor of general flaw types and geometries would be incredibly valuable to use as a surrogate for the finite element model. An efficient surrogate model would be incredibly useful in this application because probabilistic assessment methods such as Monte Carlo simulations generally require on the order of millions of model evaluations to reach a useful result.

2.1: FAVOR

Fracture Analysis of Vessels – Oak Ridge (FAVOR) is a program created to perform deterministic and probabilistic risk-informed analyses of the structural integrity of an RPV when subjected to a range of thermal-hydraulic events. [6] FAVOR’s analysis is focused solely on the beltline region of the RPV--the large unobstructed cylindrical wall of the RPV directly in-line with the fuel. This region of the RPV experiences the highest level of irradiation and is therefore the section most susceptible to embrittlement, and also generally contains the highest population of flaws.

FAVOR employs a library of SIFIC solutions derived from 3D finite element simulations for assessing fracture for axis aligned flaws, where cracks are normal to the axial and longitudinal axes for Mode *I* fracture loading. However, there is interest in having a more general capability to assess fracture at flaws of arbitrary geometry, which may not necessarily be aligned with the RPV axes, and in being able to use those to assess the entire system's response. Furthermore, the ability to evaluate a wider range of aspect ratios would increase the potential of the existing model.

2.2: Grizzly

Grizzly is a finite element based simulation tool that is currently under development at Idaho National Laboratory (INL) as part of the US Department of Energy's Light Water Reactor Sustainability program to provide improved safety assessments of structures and components in nuclear power plants subject to age-related degradation [7]. Grizzly is based on INL’s MOOSE simulation framework, which provides a very general capability for tightly coupled multiphysics simulations in a parallel computing environment. Grizzly is being developed to leverage the capabilities of MOOSE to model aging processes in a variety of nuclear power plant systems, components, and structures, and to assess the capability of these components for safe performance. Grizzly’s tightly coupled multiphysics simulation capability is particularly useful for this application, as it can simultaneously solve for both thermal and mechanical effects within the RPV wall.

The RPV was chosen as an initial application for Grizzly because of its safety significance and the extreme difficulty involved in RPV replacement or repair. Grizzly is being used to model phenomena of interest at a wide range of length scales, including the global thermo-mechanical response of the RPV, engineering fracture mechanics, and microstructure evolution.

For engineering fracture assessments, Grizzly has capabilities for solid and fracture mechanics in one, two and three dimensional analyses, and can compute embrittlement using an embrittlement trend curve. Grizzly can simulate the global response of an RPV during any process where time dependent temperature and pressure boundary conditions are specified. Further details regarding the development and formulation of the methodology can be found in [7]. While Grizzly can currently be used for deterministic fracture mechanics analysis of specific flaws, it will ultimately be extended to allow its efficient use for probabilistic fracture mechanics. The development of efficient and accurate surrogate models to stand in for finite element fracture mechanics models, as documented here, is in support of that goal.

PART 3: APPROACH

Although FAVOR was developed for probabilistic analyses, its deterministic capability provides a useful measure for benchmarking the work of this study. For a purely deterministic analysis of a surface breaking flaw, FAVOR runs a one-dimensional finite element analysis on the un-cracked structure for the given material properties, RPV geometry and thermo-mechanical boundary conditions. The stress intensity factors for mode I loading (axial and circumferential flaws in this instance) with the presence of cladding are obtained using the equation:

$$K_I = K_{I_{base}} + K_{I_{clad}} \tag{1}$$

As shown in Equation (1), the total stress intensity factor solution is found by independently calculating the stress intensity for the base material and the cladding. The respective K_I values are calculated using the principle of linear superposition proposed by Buckner [8] shown in equations 2 and 3.

$$K_{I_{base}} = \sum_{j=0}^{3} C_j K_j \sqrt{\pi a} \tag{2}$$

$$K_{I_{clad}} = \sum_{j=0}^{1} C_j K_j \sqrt{\pi a} \tag{3}$$

In Equations (2,3), C_j are the coefficients of the following polynomial, which describes the stress in the direction normal to the flaw as a function of distance from the inner wetted surface of the RPV.

$$\sigma(a') = C_0 + C_1\left(\frac{a'}{a}\right) + C_1\left(\frac{a'}{a}\right)^2 + C_1\left(\frac{a'}{a}\right)^3 \tag{4}$$

Where a' in this equation is some distance between the value of zero and a, such that the values used in the equation are normalized from zero to one. In this approach, the stress intensity factor influence coefficients (SIFICs), K_j values, are computed from a local 3D finite element model of the material in the vicinity of the defect. Pressure loads are applied directly to the surface of the flaw in these models. This procedure makes it unnecessary to directly model the full structure, including the crack. The results were then assembled into a library of discrete SIFIC values assembled with respect to flaw and RPV geometry characteristics. This data is available in appendix B of the FAVOR theory manual [6].

A separate global model of the thermo-mechanical RPV response is used to compute the stress profile through the thickness, and a least-squares fit [6] is employed to obtain the coefficients to the polynomial in Equation 4. Because FAVOR is applied to the beltline region of the RPV, a 1D model is sufficient to model the response of an infinite cylinder. Higher dimensionality models could also be employed for other geometries.

The global finite element model outputs the normal stresses in the RPV wall at radial positions a' where a used in equations (2,3) is the depth of the flaw being analyzed, but a in equation 4 is measured from the interface of the base and cladding, therefore it is the total flaw depth with the cladding thickness subtracted.

It is important to emphasize the fact that the stress coefficients as well as the SIFICs used in the base and cladding materials will not be the same. The process described above is the method utilized to find the stress coefficients in the base material.

To find the coefficients used for the cladding, the coefficients for two lines are required. The first is a line fit using a linear least squares method (a truncated equation (4) at the linear term) fit to the integration point values within the cladding. The second is a linear extrapolation through the cladding using stress values obtained from the first two integration points in the base metal. The stress coefficients used in equation (3) are the result of subtracting the extrapolated coefficients from the actual cladding coefficients.

3.1: Determining K_I in FAVOR

FAVOR utilizes a database of stress intensity factor influence coefficients (SIFICs) together with Equations 2 and 3 to compute the time history of the stress intensity factor at a given flaw during a transient. These solutions were developed at Oak Ridge National Laboratory (ORNL) using ABAQUS finite element models. The SIFIC values are reported for both axial and circumferentially oriented flaws for relative flaw depths up to 30% of the thickness of the RPV wall. The study conducted in [9] indicates that there is very little difference between the SIFICs for axial and circumferential flaws with a relative depth of (a/t) < .5.

The library of SIFIC solutions used in FAVOR was created for a range of the following input parameters: flaw aspect ratio (L/a), relative flaw depth(a/t), and the angle along the flaw front (φ), shown in Figure 1.

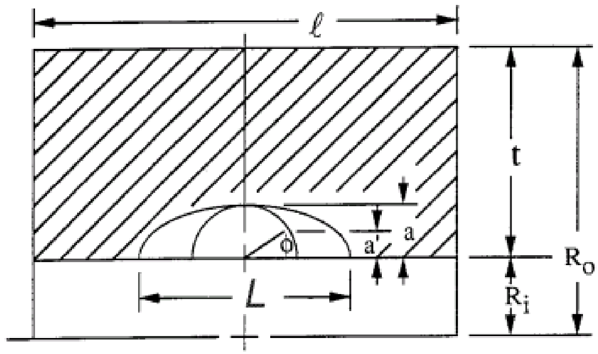

Figure 1: FAVOR's flaw geometry definitions [6]

The SIFIC values are provided for the following finite set of crack aspect ratios: (L/a) = 2, 6, 10, and 999 (infinite), relative flaw depths: (a/t) = .01, .0184, .05, .075, .1, .2, and .3, and 9 angular positions along the crack front φ = 0 – 90, (increments are not constant). Additionally, for analysis of the cladding, SIFICs are tabulated with an additional parameter, the cladding's thickness (t_{clad}), using two finite values: .156 and .25 inches (.396 and .635 cm respectively).

Currently, for surface breaking flaws, FAVOR can consider aspect ratios of 2, 6, 10, and infinite. Also, although the SIFICs are parameterized with respect to angular position along the crack front, only the results from φ = 90 are reported in FAVOR's deterministic evalutation. Therefore, the only continuously variable parameter taken into account by FAVOR is the variation of the relative crack depth. To obtain SIFIC values for varying (a/t) and cladding thickness values, FAVOR uses an interpolation scheme based upon the cubic stress polynomial used for the stress coefficients.

3.2: Proposed Methodology

For the previously described method of obtaining a stress intensity solution, there are two major components. The first is the evaluation of a global finite element model for the thermo-mechanical response of the RPV. From this model the stress coefficients for both the base and cladding materials can be obtained. The second step is determining the proper SIFIC values for the flaw geometry of interest, and using those to compute the stress intensity factor.

The proposed methodology follows that same basic process, but employs surrogate models to compute SIFICs. The global response of the RPV is computed using the Grizzly code. Once the spatial distribution of the stresses has been computed, four different methods for finding the appropriate SIFICs are applied and compared. All of these methods use FAVOR's existing SIFIC data in the current demonstration.

3.2.1: Global RPV Model

Grizzly is employed here to model the global response of the RPV subjected to a representative pressurized thermal shock transient. Grizzly has been successfully applied to model the response of the full vessel modeled in 3D or 2D axisymmetry, which demonstrates its flexibility for considering flaws beyond the RPV beltline. For cases where it is only necessary to consider the RPV beltline, a 2D axisymmetric model of a single strip of elements can also be used, which requires minimal computational resources. The Grizzly model uses the inputs specific to the materials and time dependent boundary conditions simulating the PTS event, and outputs the normal stresses and positions in the RPV wall at each integration point.

3.2.2: Determination of Stress Coefficients

To measure the RPV's thermo-mechanical response to the PTS event described above, a 2D axisymmetric finite element model consisting of a strip of elements to represent the beltline response was created for evaluation using Grizzly. Equations (2-3) require the stress coefficients, which are obtained from the global finite element model. For a cubic least squares regression, four data points are required, however, additional points would ensure a more accurate and robust distribution of the stress profile. Therefore it was required to create a mesh such that the crack length of interest spanned a minimum of four integration points in the base material as well as two integration points in the cladding for the linear least square fit. For this study, a mesh convergence study was performed to determine convergence of the stress results. For the demonstration case shown, the converged mesh contained two quadratic elements in the cladding and 62 quadratic elements in the base metal. This mesh was sufficient for flaws with a depth of .05 times the wall thickness or greater, but for smaller flaws a more refined base mesh would be ideal.

3.2.3: Determination of SIFIC Values

From Equations 2 and 3 it is shown that the SIFICs (K_j values) are required to compute the stress intensity factor for a given flaw. The FAVOR Theory and Implementation Manual includes a large database of these values, each corresponding to a particular crack and RPV geometry. To evaluate arbitrary crack depths, FAVOR uses an interpolation scheme to find a solution when (a/t) falls between data. However, it does not interpolate between flaw aspect ratios, angular positions along the crack front, or cladding thicknesses.

The primary interest of this study is to develop an automated and general capability to evaluate a wider variety of flaw geometries. Off-axis flaws have not yet been considered, but additional parameters such as flaw orientation angles will be required as inputs to models used to represent such geometries. Interpolation schemes can become complex at higher dimensions and require a large population of data, so it would be valuable to explore other potential surrogate modeling techniques. To verify the potential use of surrogate models for higher dimensional analysis, it must first be determined that these additional techniques provide comparable results in the 1D case to the interpolation scheme utilized in current practice.

PART 4: SURROGATE MODELING

To compute the stress intensity factor using Equations 2 and 3 requires the selection of the appropriate SIFIC values based upon the given flaw's characteristics. As mentioned previously, FAVOR computes solutions for flaws with a discrete set of aspect ratios and cladding thickness, but uses an interpolation scheme to allow solutions for any flaw depth. It would be useful to extend this capability to allow solutions for any aspect ratio or cladding thickness as well as flaw depth and angular position. This capability would enable the analysis of a wider array of crack geometries.

When moving into a highly multi-dimensional space, where there are more input parameters, interpolation can become increasingly complex and difficult due to the large number of data points needed to populate the design space and the limitations in the structure of the approach. This work aims to explore the capabilities of several alternatives to interpolation to determine their predictive capabilities in predicting SIFIC values given the discrete data points provided in the tables.

This demonstration will explore the utilization of three methodologies: linear interpolation, Response Surface Methodology (RSM) and Gaussian Process Modeling, also known as Kriging. All of the models were calibrated using FAVOR's library of SIFIC data, and will produce approximations of SIFICs when given input variables specified in section 3.1.

As opposed to the methodology utilized by FAVOR, none of the methods utilized in this work require any of the input flaw parameters to be discrete values that correspond exactly to the tabular data, but must instead only be contained within the range of the supplied parameters.

4.1: Interpolation

The first method utilized to compute SIFIC values is multi-dimensional linear interpolation. For the SIFICs corresponding to the base material, the SIFIC value is dependent upon the flaw aspect ratio, relative flaw depth, and the angular position along the front of the flaw. Similarly, the SIFICs used in the cladding are output as a function of the same three parameters, as well as the cladding thickness, for which FAVOR provides two discrete values.

In the given application, this approach is limited in that data points are required to be relatively close together to adequately capture the trends of the data in the undiscovered region of the design space. With future plans to implement this method in the analysis of off-axis flaws, significant computational effort would be required to gather sufficient data points for an accurate representation.

4.2: Response Surface

An additional surrogate modeling method considered was response surface methodology (RSM) [10]. RSM allows the designer to determine the form of a closed-form expression of the parameters *a priori*, and then calibrates the model's parameters using a least-squares approach. In this work, this method was implemented twice to explore two different polynomial forms, as shown in the following equations (5-6). The two equations are representative of a cubic model without any interaction terms (Equation (5)) and a quadratic model with first-order interaction terms (Equation (6)). It is important to note that for this demonstration, the polynomial forms were not selected in a mathematically rigorous manner, but instead, general forms were selected for demonstration of the approach. For the given SIFIC data, a response surface was created for each of the six SIFICs (4 in the base material, 2 in the cladding), and for each of the forms shown—resulting in a total of 12 equations. For the sake of analysis, each of the two forms of the response surface model shown in Equations. (5-6) were considered as different models.

$$K_j = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_i x_i^2 + \sum_{i=1}^{n} \beta_i x_i^3 \tag{5}$$

$$K_j = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_i x_i^2 + \sum_{i<j}^{n} \sum^{n} \beta_{ij} x_i x_j \tag{6}$$

In Equations (5-6), the number of design variables modeled differs between the cladding and the base material. For the base material, $n = 3, x_i = [\varphi,\ ar,\ at]$ representing the angular position along the flaw front, flaw aspect ratio and relative flaw depth, respectively. For the cladding, $n = 4, x_i = [\varphi,\ ar,\ at,\ t_{clad}]$, where the added parameter is the cladding thickness. The β coefficients for each of the six SIFIC models are found independently of one another and vary between each of the six polynomials. Furthermore, a different polynomial form can be selected for each of the 6 SIFICs required for the analysis in order to get a more accurate solution. However, for simplicity they were kept the same in this demonstration.

To create each of the response surfaces used, the SIFIC dataset was partitioned to avoid issues with numerical noise and improve the accuracy of the meta-model. The partition primarily separated the larger flaw data from the smaller flaws, and maintained enough data for adequate model calibration. Additionally, no continuity conditions were enforced at the boundaries for each of the partitioned datasets.

4.3: Kriging

The final method utilized to determine SIFIC values was ordinary kriging. Unlike RSM, ordinary kriging does not result in a closed form representation of each of the SIFICs, but instead produces a probabilistic representation of the value to be estimated, which for this demonstration was the SIFIC values. This method stands out due to its ability to represent the level of uncertainty that exists in the model's prediction of values not provided in the data. Although the output from the kriging model is probabilistic, for the purpose of this comparative demonstration, only the mean output of the probabilistic representation was considered, and was treated as a purely deterministic value. Future studies will utilize the probabilistic representation to further refine reliability predictions

For each of the outputs of interest (four SIFICs for the base, and two for the clad) a separate kriging model was developed. For each of the six cases, a semivariogram was constructed using the SIFIC data provided. The semivariogram is used to describe the degree of spatial dependence in a random field of data. It can take on many forms, but for this demonstration only the following four curve forms were considered: spherical, exponential, Gaussian, and power. Each type of the four curves were fit to each of the 6 the semivariograms using a least-squares methodology. The form with the lowest R-squared value for each individual curve was selected. It was found in this study that all six of the semivariograms were fit most accurately using the Gaussian curve.

PART 5: RESULTS

Fracture response of the RPV was computed using two analysis toolsets. The first set of analyses described here was performed to determine the validity of the proposed surrogate modeling techniques given FAVOR's existing SIFIC data. After conducting those analyses, a deterministic analysis of the same flaw subjected to the same transient was performed using FAVOR to benchmark the proposed surrogate modeling techniques.

5.1: Surrogate Model Comparison

Given a set of data, both interpolation and kriging will always reproduce the exact output for data points that were used in the calibration of the model, while a response surface might not necessarily do so. To allow for a comparative study to be performed given the limitations of the FAVOR interpolation scheme, the following procedure was utilized in order to compare each of the four surrogate modeling techniques.

For each of the four meta-models (interpolation, kriging, and two response surfaces), one data point was randomly selected to be withheld from the dataset. The four surrogates were then created, and used to predict the withheld input. The corresponding SIFIC output for each of the four surrogates was then compared to the actual value provided by FAVOR. This process was then repeated a number of times--100 times for the base metal SIFICs and 200 times for the cladding SIFICs. A rough convergence study was conducted in order to determine the number of appropriate samples. As the existing datasets are relatively small for the base and cladding SIFICs (189 and 378 respectively) 100 and 200 respective samples proved to be adequate.

After finding the predicted SIFIC for each of the surrogate models, the absolute difference between the actual and predicted value for each of the four surrogates was found and converted to a percentage error. The tables below represent the mean error percentage for each of the surrogate types, as well as the standard deviation of the corresponding 100 or 200 error percentage values.

	Mean Error Percentage Value					
Model	K0	K1	K2	K3	K0_cl	K1_cl
Interp.	1.69	5.60	8.60	24.01	14.42	11.88
Cubic RS	3.23	3.58	5.23	8.01	23.22	20.88
Quad RS	1.45	2.13	3.76	6.51	92.60	55.77
Kriging	2.17	10.62	10.92	40.10	48.31	28.86
	Standard Deviation of Error Percentage					
Model	K0	K1	K2	K3	K0_cl	K1_cl
Interp.	2.23	8.21	10.73	51.72	40.25	18.11
Cubic RS	4.45	4.79	7.22	11.07	59.30	19.13
Quad RS	1.19	2.12	4.25	7.11	558.57	269.63
Kriging	3.00	36.63	17.53	96.06	268.21	62.68

Table 1: Raw error percentages and std. deviations

The results in Table 1 show that for each of the modeling techniques, it becomes more difficult to accurately predict the values of the SIFIC as the order of said value increases. Additionally, the cladding coefficients in general were more difficult to accurately predict than those for the base metal. An acceptable level of error for each of the models would be less than roughly ten percent, which means many of these are far too large to implement. This is, however, an issue that can be addressed in a number of ways.

Upon analyzing the outputs, most values were consistent with the actual FAVOR SIFIC values. The prevailing issue with these meta-models is their inability to extrapolate outside of the design space. As such, if the randomly selected point to be excluded and analyzed happens to fall near the edges of the supplied data, the metamodel is forced to extrapolate, and the resulting output can be wildly inaccurate. The small percentage of extreme values then drives up the mean error percentage shown in Table 1. In future studies to generate the SIFICs for 3D flaw orientations, a wide range of parameter values will need to be sampled to ensure that the metamodels will not be required to extrapolate beyond the bounds of the model.

In order to combat the issue of extrapolated data in the above data set, the extrapolated values were removed from each of the surrogate models to represent their predictive abilities in a fully realized design space. Table 2 shows the results of the same study with the extrapolated values removed.

	Mean Error Percentage Value					
Model	K0	K1	K2	K3	K0_cl	K1_cl
Interp.	0.78	2.19	4.21	6.67	4.26	4.33
Cubic RS	1.43	1.64	2.38	3.94	13.98	13.49
Quad RS	1.01	1.29	1.92	3.61	13.14	13.61
Kriging	0.96	2.14	3.30	7.90	8.04	12.08
	Standard Deviation of Error Percentage					
Model	K0	K1	K2	K3	K0_cl	K1_cl
Interp.	0.77	2.64	5.06	6.97	10.83	10.85
Cubic RS	1.18	1.34	1.86	2.62	7.61	8.48
Quad RS	0.63	0.82	1.62	2.69	7.11	8.02
Kriging	0.97	2.59	5.09	11.23	9.45	10.94

Table 2: Adjusted error percentages and std. deviations

As shown in Table 2, after the extrapolated values are removed from the dataset, each of the models show a fairly significant increase in overall accuracy. The interpolation method appears to represent the cladding coefficients somewhat more effectively than the other methods. This result is due to the fact that only two discrete values of the cladding thickness were provided in the table. As such, given the method of randomly selecting a point to exclude from the model calibration set, the excluded point always occurred at one of the two discrete values, meaning that no interpolation was required between cladding thickness values. Table 2 shows that all of the methods are relatively equal in their ability to represent the base coefficients.

5.2: FAVOR Comparison

For this analysis, both FAVOR and Grizzly were used to simulate the PTS event shown in Figure 3.

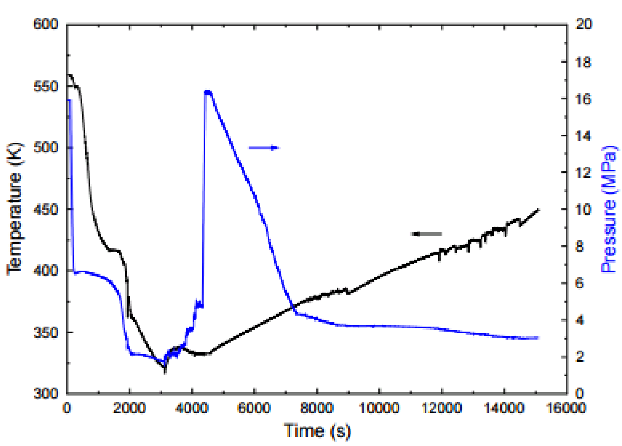

Figure 3: PTS pressure and temperature history [11]

This particular transient simulates the event during which a pressure release valve is stuck open resulting in a depressurization and significant decrease in temperature followed by a rapid re-pressurization and slow temperature increase once the valve is closed [11]. Both models were evaluated using the same RPV dimensions and temperature-dependent material properties. The results from [11] show that Grizzly can be used successfully to determine the global response of an RPV for a PTS event, therefore a direct comparison of the finite element outputs between each of the models is not shown directly in this work.

Using FAVOR's FAVLOAD module, and separately, the Grizzly code, the global RPV response to the PTS event was found. The results from FAVLOAD were then used in FAVOR's FAVPFM module where deterministic analyses can be performed to find the stress intensity factor as a function of time for flaws of a prescribed depth. Similarly, the resulting stresses found from the Grizzly code were utilized in conjunction with the four surrogate modeling techniques described previously to find four separate solutions, each of which was compared directly to the FAVPFM output. Although only one flaw sample is shown Figures 4-5, the results shown are representative of the many cases evaluated during the course of the comparison. Figure 5 is simply a closer view of Figure 4 in order to better show the modeling differences.

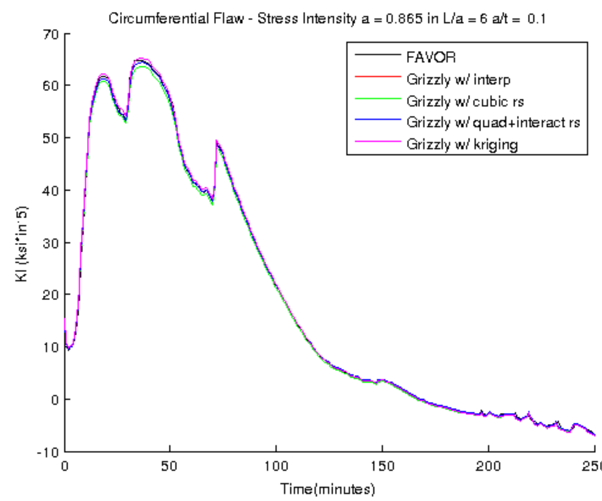

Figure 4: FAVOR Grizzly/surrogate model comparison

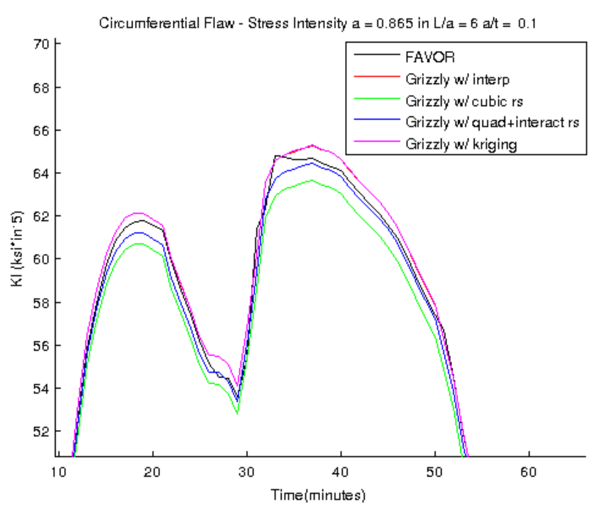

Figure 5: FAVOR Grizzly/surrogate model comparison (zoomed in on early response)

PART 6: SUMMARY

The goal of this study was to investigate the capabilities of various surrogate modeling techniques to represent FAVOR's SIFIC data, which are required for rapid, accurate deterministic stress intensity analyses of flaws in the beltline region of an RPV. The methods used in current practice for computing the stress intensity factor are limited in that only the flaw depth can vary as a continuous value, which would be a difficult limitation for the evaluation of 3D off axis flaws. The extension of this capability to off axis flaws will allow for more robust and accurate simulations, however, will also require additional SIFIC data where values will need to be calculated as functions of additional parameters. It is therefore useful to first explore more efficient methods for representing SIFICs. Response surface methodology, linear interpolation and ordinary kriging were the methods analyzed in this demonstration, all of which utilized the database of SIFIC values available in the FAVOR theory manual.

6.1: Results of this study

Each of the techniques was compared in a process where random data points were removed for the construction of the metamodel. The removed value was then used as the model's input and the predicted value was compared to the actual solution. This process was repeated 100 and 200 times for base metal and cladding SIFICs respectively. The results showed that when extrapolated values were considered, the surrogates produced wildly inaccurate results. However, when only interpolated values were utilized, the resulting SIFICs were comparable for all modeling techniques. This result shows that as long as the input falls within the range of values utilized for the creation of the surrogate, the output is sufficient for implementation and utilization in finding the stress intensity factor for a given flaw.

6.2: Future plans for work utilizing this study

The implications of these results suggest that additional data points may be required in order to use these modeling techniques. For the current method utilized in FAVOR, there is very little reason to use the techniques demonstrated in this paper. However, as the eventual goal of this project is to develop a more general capability for evaluating a wider variety of flaw geometries, it is important to explore the possibility of utilizing these surrogate modeling techniques. Such an extension would require a larger database of SIFICs where the values are dependent on additional input parameters. As the dimensionality of interpolation increases, so does the number of required data points for accurate representation. With kriging or RSM, this increased cost may not be as pronounced, allowing a potential savings in simulation time required to populate the SIFIC tables and an increased accuracy in their predictive capabilities. Furthermore, due to the probabilistic output of the kriging approach, the uncertainty (potential error) that exists in the surrogate model's prediction of an unknown flaw geometry's SIFIC values can be determined and could be potentially propagated through the probabilistic analysis.

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