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Ultrasonic Modeling and Simulation for Nuclear Nondestructive Evaluation

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Ultrasonic Modeling and Simulation for Nuclear Nondestructive Evaluation

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ABSTRACT

The guidance and conclusions provided in this report are the result of a multi-year effort to understand the potential role of modeling and simulation in improving the efficiency and efficacy of ultrasonic inspections of nuclear power plant components. Conclusions are coalesced from previous work, and strategies and best practices are suggested for successful implementation of modeling and assessment of simulation outcomes. An overview of challenges in modeling and simulation is given, along with strategies for overcoming these challenges. Methods of validation and verification are outlined to help assure that models and simulation outcomes are reliable. Specific direction for implementing the models is provided as well as guidance for assessing the outcomes. In addition, key takeaways and lessons learned for different modeling scenarios are listed. The guidance and conclusions summarized in this report are intended to form the technical framework for development of a nondestructive evaluation modeling and simulation best practices document that will support standardization of modeling practices across the commercial nuclear power industry.

FOREWORD

The use of modeling and simulation software to accurately predict the quality of an ultrasonic examination has been a goal of many researchers for decades. Starting in the mid 2000s, commercial modeling and simulation software packages became available to the public with some simple ultrasonic modeling software bundled into versions of commonly used ultrasonic data collection software. These software tools provided the Nuclear Regulatory Commission (NRC) and the nuclear industry with the ability to make images of ultrasonic fields in components and simulate the responses from hypothetical flaws. In the 2010s, as these software packages evolved and became more mature, it appeared as if simulations of ultrasonic examinations would be relatively simple and commonly used by the nuclear industry to evaluate examinations and the NRC for regulatory purposes.

There was one issue, however, in that the ultrasonic simulation results were often at odds with experimental results. Work conducted by the Pacific Northwest National Laboratory (PNNL) under the sponsorship of the NRC has attempted to understand the causes of models failing to replicate actual ultrasonic fields and flaw responses. In 2018 (ML19010A072), PNNL's research showed that one major issue when modeling ultrasonic examinations is that physical ultrasonic transducers with nearly identical specifications showed significant variability in the ultrasonic fields produced in steel. The idea that some transducers are better than others is not novel, but any computer model of an inspection will be using an "ideal" transducer, while actual examinations are performed with real transducers. Further, modeling welds and complex microstructures is made more complicated by the fact that these microstructures vary significantly from component to component and even from one part of a component to another part of the same component. These and other issues present serious challenges to the proposed uses of ultrasonic modeling for use in proposed alternatives and other licensing actions.

The use of ultrasonic modeling and simulation is further complicated by the complexity of the software packages available for modeling. Multiple people can attempt to model the same problem and come up with different results. Any model sent to the NRC requires extensive information as to how the modeling was done to enable the NRC to conduct confirmatory modeling to verify that the models were performed correctly.

Through the methodical assessment of modeling and simulation software tools conducted at PNNL, the NRC staff has gained a much better understanding of the appropriate uses and limitations of ultrasonic modeling. This NUREG/CR will be a useful resource in defining the role of ultrasonic modeling and simulation in the future and understanding the limits of the models and what information is needed to verify the accuracy of the simulations.

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EXECUTIVE SUMMARY

The Pacific Northwest National Laboratory (PNNL) conducted confirmatory research for the U.S. Nuclear Regulatory Commission (NRC) to evaluate commercially available nondestructive examination (NDE) modeling and simulation software used in the nuclear industry. Increases in computing power and advances in knowledge related to NDE have made it practicable in recent years to simulate NDE methods to help in the design of qualification and inspection methods and to aid in analysis of inspection results.

The U.S. nuclear industry is increasingly relying on beam simulations (sound field simulations) to demonstrate the effectiveness of ultrasonic inspection techniques. In commercial nuclear NDE, inspection scenarios can be modeled to inform examination procedures, assess beam coverage, predict flaw detection, guide probe and mockup design, and ultimately save time, money, and resources.

In those cases where the required 100 percent examination volume coverage cannot be obtained due to access limitations or component geometry, nuclear power plant licensees have begun to use beam simulation models to illustrate that adequate sound field coverage has been achieved within the reduced inspection volume. Results of these simulations often indicate that the flaws should be detectable in these reduced inspection volumes, but the simulations cannot be guaranteed to represent reality. In addition, industry representatives have indicated the desire to determine if simulations can be used in lieu of examinations of physical mockups to reduce the time and cost associated with procedure and personnel qualifications. Other applications of modeling and simulation include examination coverage prediction, new probe design and assessment, and mockup design.

The report provides validation and verification steps that are critical to any modeling and simulation application. Best practices that are required for using computational models to simulate the ultrasonic testing scenarios being conducted on nuclear power plant components and interpreting the results are defined. Guidance is provided as to how ultrasonic models, sound maps, and simulated flaw responses should be carried out and interpreted when applied to a variety of materials and various degradation mechanisms.

ABBREVIATIONS AND ACRONYMS

CAD	Computer-Aided Design
CASS	Cast Austenitic Stainless Steel
DMW	Dissimilar Metal Weld
EBSD	Electron Backscatter Diffraction
ECNDT	European Conference on Non-Destructive Testing
FEM	Finite Element Modeling
IUS	International Ultrasonics Symposium
NDE	Nondestructive Examination
NRC	U.S. Nuclear Regulatory Commission
NRR	Nuclear Reactor Regulation
PA	Phased Array
PNNL	Pacific Northwest National Laboratory
SME	Subject Matter Experts
UV	UltraVision

1.0 INTRODUCTION

1.1 Background and Objectives

For the past several years, the Pacific Northwest National Laboratory (PNNL) has been conducting confirmatory research for the U.S. Nuclear Regulatory Commission (NRC) to evaluate nondestructive examination (NDE) modeling and simulation[1] used in the nuclear industry. The goal of this research is to define best practices required for using and interpreting computational models to simulate ultrasonic testing scenarios being conducted on nuclear power plant components. In commercial nuclear NDE, inspection models can be used to inform examination procedures, assess beam coverage, predict flaw detection, inform probe and mockup design, and ultimately save time, money, and resources.

In this report, the term “model” is used when referring to the digital representation of a specimen, probe, flaw, etc. or combination thereof. “Model” also describes the mathematical framework used for computation. The term “simulation” is used when referring to the computational execution of a model scenario with a particular set of input parameters. A model provides an imitation or representation of the real-world scenario, whereas a simulation uses the model to predict behavior under user-defined conditions.

Nuclear power plant licensee requests for relief from inservice inspection requirements are submitted for review to the NRC Office of Nuclear Reactor Regulation (NRR). Relief requests may contain modeling and simulation results to help establish the technical basis of the request. This report is intended to provide NRR with the fundamental understanding needed to effectively evaluate such licensee submittals. In addition, industry representatives have indicated the desire to determine if simulations can be used in lieu of examinations of physical mockups to reduce the time and cost associated with inspection qualification. In research applications, modeling and simulation have been used to help design mockups and probes, predict beam coverage, and predict flaw detection probabilities. Detailed examples of modeling and simulation in the nuclear industry are given in Section 4.0.

A model can never be truly representative of the actual specimen to be examined. For example, the microstructural properties of the specimen may vary continuously throughout the material Jacob et al. (2022a). In addition, anisotropic grains can strongly affect the propagation of ultrasound through a specimen causing attenuation, changes in velocity, and scattering of ultrasonic energy. Thus, the model becomes an approximation at best and completely unrepresentative at worst. Reality is too detailed and complex to be fully and completely described in a mathematical model. Models are designed to represent a subset of reality, perhaps simplifying a problem to the most important or interesting points. Models provide accessibility and convenience to understanding simplified problems that can then be built upon to study more complex scenarios. While models can be used to understand data and predict results, they cannot be used to imitate human factors or equipment limitations, replace empirical measurements, or definitively predict beam coverage through materials with complex microstructures or geometries. Models are also not well suited for predicting unanticipated noise sources and spurious signals.

[1] Throughout this report, “model” refers to the mathematical framework, parameter inputs, and material or specimen descriptions. “Simulation” refers to the computed output of a modeled scenario. Beam models are used to simulate ultrasonic beam characteristics, and flaw response models are used to simulate an echo response from an insonified flaw or machined reflector.

PNNL has explored the capabilities of several commercially available modeling platforms, including an assessment of strengths and limitations of each platform in particular and of ultrasonic modeling in general. The guidance and conclusions provided in this report are the result of a multi-year effort to understand the potential role of modeling and simulation in improving the efficiency and efficacy of ultrasonic inspections in nuclear power plants. This report will present a brief overview of PNNL's previous work, but for the sake of conciseness, it will not delve into technical details. Rather, this report will focus on coalescing conclusions from previous work and suggesting strategies and best practices for successful implementation of modeling and assessment of simulation outcomes.

1.2 Summary of Previous Work

To date, PNNL has published five technical reports on ultrasonic modeling and simulation:

1. Validation of Ultrasonic Nondestructive Examination (NDE) Computational Models – Phase 1 (Dib et al. 2017).

2. Ultrasound Modeling and Simulation: Status Update (Dib et al. 2018).

3. Modeling and Simulation of Austenitic Welds and Coarse-grained Specimens: (Jacob et al. 2020).

4. Modeling and Simulation of Austenitic Welds and Coarse-grained Specimens: Part II (Jacob et al. 2022b).

5. Ultrasonic Modeling and Simulation Status Update. Part 1: Flaw Response Simulations using Flaw Profiles Obtained by Destructive Testing, and Part 2: Review of OnScale Simulation Software (Jacob et al. 2022a).

An overarching theme of all these reports is validation and verification, which are critical to gaining confidence in simulation results. An effective validation and verification procedure should include: (1) an assessment of the quality and limitations of the physics the models used; (2) an understanding of input parameter uncertainties; (3) quantitative comparisons of simulation results with empirical results; and (4) parametric studies to evaluate effects of parameter variability. During the validation and verification process, it is important to remember that empirical data are indispensable and provide accumulated evidence to support confidence in the simulation output; however, empirical data cannot prove that the model or the simulation results are correct. Validation and verification will be explored in more depth in section 5.0.

Figure 1.1 shows a roadmap of key topics that have been addressed in the modeling and simulation technical reports listed above. Each step of the roadmap is briefly discussed below with a reference to the relevant report(s) where detailed information can be found.

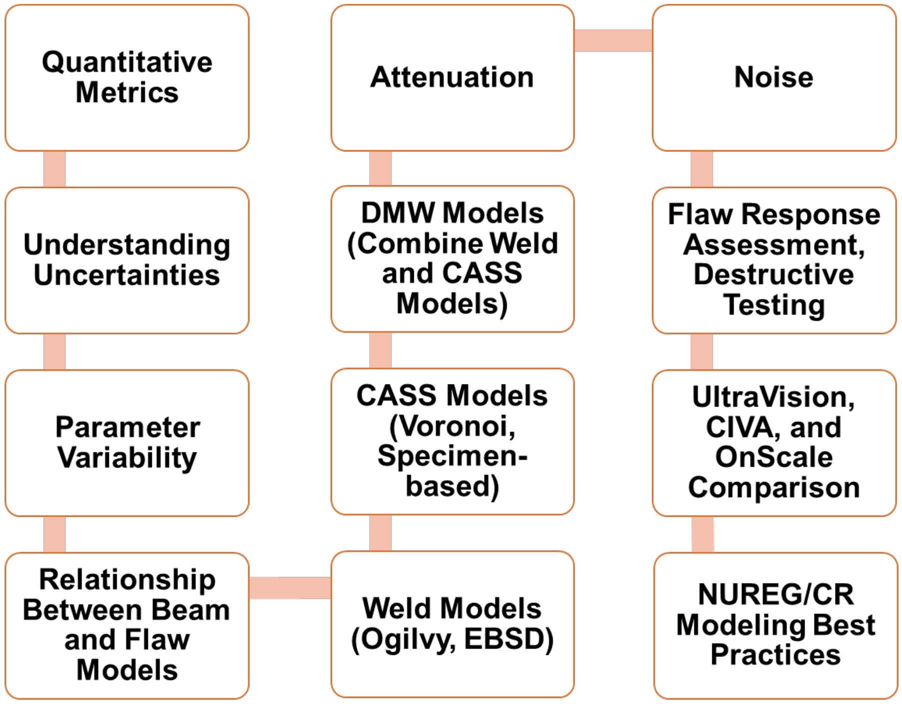

Figure 1.1 Roadmap Illustrating the Topics that have been Covered in the Ultrasonic Modeling and Simulation Work at PNNL

A verification framework should include a set of **quantitative metrics** to compare simulations to empirical data and to compare simulations to one another (Dib et al. 2017; Dib et al. 2018; Jacob et al. 2020). A metric is required to quantify the accuracy of a simulation in comparison to, say, an empirical result or another simulation. A metric cannot identify whether the simulation or the empirical result is correct; it can, however, highlight the difference between them. Simple metrics can be used, such as signal amplitude, or more sophisticated metrics can be developed for specific measurements or situations, such as quantifying beam scatter. The metrics should take into account sources of uncertainties in both observations and predictions.

It is important to **understand uncertainties** in simulation results. In Dib et al. (2017), models in CIVA agreed qualitatively with empirical results; however, quantitative metrics showed large variances in accuracy, and the associated empirical and simulation discrepancies were large. The authors concluded that using models for applications that require quantitative reasoning (such as predicting the detectability of small flaws or model-assisted probability of detection studies) can be unreliable, and errors over 20 dB could occur.

Model **parameter variability** can have strong impacts on simulation outcomes (Dib et al. 2017). It is important to understand the parameters that the simulation is most sensitive to and then acquire precise measurements of those parameters. When measurements are not available, the bounds of parameter variability should be understood, such as possible flaw tilt angles or the minimum and maximum possible values of the sound speed in the material, so that the model can be tested with a range of realistic inputs.

The **relationship between beam simulations and flaw-response simulations** was explored (Dib et al. 2018). Beam simulations are expected to be particularly useful in helping to develop estimates of sound field coverage, assuming that appropriate specimen models and model parameters are used. By predicting insonification of an inspection region, beam simulations may be useful for predicting whether a flaw response would occur in certain scenarios, such as when there are inspection limitations caused by a weld crown. In general, beam simulations should not be relied on as surrogates for flaw-response simulations. Effects of parameters such as microstructure, attenuation, and probe position play an important role in beam and flaw-response simulations. In addition, the properties of the flaw, such as tilt and through-wall depth, are critical parameters that are not captured in beam simulations.

Realistic, multi-grained **weld models** scatter the sound beam in ways that are not duplicated by idealized models (Jacob et al. 2020). Idealized models, such as the Ogilvy model, do not contain microstructural detail and therefore do not duplicate observed scatter or attenuation.

Voronoi regions are an effective and efficient approach to **cast austenitic stainless steel (CASS) models** in cases where an unknown degree of microstructural variability exists (Jacob et al. 2022b; Jacob et al. 2020). Microstructural variability is too complex to be fully represented by a single simulation, no matter how well conceived or carefully executed the simulation is. It is critical to avoid basing examination protocols or coverage calculations on individual simulation results. Rather, complex scenarios require multiple simulations that explore the practical limits of both the inspection scenario and model parameters. Using different parameters and/or specimen models can establish best-case, worst-case, and nominal scenarios.

CASS base material and austenitic weld models can be combined to create **dissimilar metal weld (DMW) models** (Jacob et al. 2022a; Jacob et al. 2022b). In CIVA, Voronoi regions cannot be used in these cases, so a CASS model must be created manually. Advantages and disadvantages of using a DMW model over a simpler model should be evaluated on a case-by-case basis.

Attenuation and **noise** can add realism to a simulation, but they should be used with care and with a basis in empirical results (Jacob et al. 2022a; Jacob et al. 2021). Attenuation is often not necessary at lower frequencies in carbon steel model specimens, while noise can increase simulation times significantly. In coarse-grained models, attenuation from scatter can be simulated by controlling the model specimen parameters. Determining the ideal attenuation and noise parameters is an iterative process.

Flaw-response simulations can be useful for assessing an inspection scenario (Jacob et al. 2022a). However, significant challenges are inherent for predicting ultrasonic testing (UT) inspection reliability, especially through materials with complex microstructure. Care must be taken to address uncertainties in material property specifications, transducer parameters, and flaw geometries. Comparing simulated flaw responses to empirical data is challenging, especially in the absence of a calibration signal from a machined reflector. Flaw-response simulations using actual flaw geometries derived from destructive testing were not predictive of empirical data due to randomness in empirical weld microstructure.

Throughout the project, PNNL evaluated the software packages **UltraVision, CIVA,** and **OnScale** for usability and to assess how well results compare to empirical data (Dib et al. 2017; Dib et al. 2018; Jacob et al. 2022a; Jacob et al. 2022b; Jacob et al. 2020). A brief introduction to these software packages is provided in section 2.0.

1.3 Applications of Modeling and Simulation in Nuclear NDE

Historically, NDE methods and techniques used in nuclear power inservice inspections are well established and have been applied successfully for several decades. Even so, methods have evolved and new technology has become available. Below are some examples with references of the role modeling and simulation have played in NDE:

- Wedge design (Isenberg et al. 1994)
- Understanding sound propagation in welds or coarse-grained materials (Chatillon et al. 2003; EPRI 2018 ; Gueudré et al. 2019; Wan et al. 2017)
- Testing focal laws (Lim et al. 2022; Poguet et al. 2005; Van Pamel et al. 2015)
- Predicting inspection reliability (Liu and Wirdelius 2007; Mahaut et al. 2007)
- Developing advanced inspection techniques (Brizuela et al. 2019; Kim et al. 2016; Nageswaran et al. 2009; Szávai et al. 2016)
- Developing and testing procedures (Carpentier et al. 2010; Dunlap et al. 2020; Jezzine et al. 2018)
- Understanding inspection results (Gardahaut et al. 2013)
- Optimizing inspection parameters (Bannouf et al. 2014; Nowers et al. 2016)
- Improving inspection performance (Nakahata et al. 2016; Zhou et al. 2018)
- Beam coverage predictions for relief requests (EPRI 2017)
- Probe design (Foucher et al. 2018)
- Understanding unexpected observations (Ginzel 2020).

1.4 Report Overview

This report provides a global summary of what PNNL has learned about ultrasonic modeling and simulation to date. Details of the research are not provided, but references are given to specific findings of the research and testing performed.

Section 2.0 provides a brief overview of the three modeling and simulation platforms that PNNL evaluated: UltraVision, CIVA, and OnScale. A comparison is provided of many of the software features used by PNNL. Section 3.0 discusses many of the difficulties and challenges presented by modeling and simulation. It is important to understand sources of uncertainty and the effects of parameter variability. Real-world examples of modeling and simulation in the nuclear industry are presented in section 4.0. Section 5.0 discusses validation and verification steps that are critical to any modeling and simulation application. Two sets of questions, one for the modeler and one for the reviewer, are presented to provide guidance throughout the modeling process, from setting up models to analyzing the results. Section 6.0 explores many of the figure 1.1 roadmap steps by providing detailed lists of key findings, guidance, and open questions with references to specific PNNL reports. Section 7.0 provides a summary and key takeaways from the multi-year assessment, while section 8.0 lists the references cited in this report.

2.0 SOFTWARE PACKAGES ASSESSED

PNNL evaluated three UT modeling and simulation software packages for the NRC: UltraVision, CIVA, and OnScale. Below is a brief overview of each. These packages were selected because of the current interest and utilization within the U.S. nuclear industry. PNNL does not endorse or encourage the use of any particular software package; rather, PNNL encourages using sound modeling and simulation practices and data analysis methods regardless of the platform used.

2.1 UltraVision

UltraVision (UV) is a software package developed by Zetec, Inc. (Snoqualmie, WA, USA)[2]. UV was designed for UT data acquisition and analysis for both field and laboratory applications. UV also has capabilities for beam simulations to assist in designing probes and wedges and simulating sound field coverage. PNNL assessed UV beam simulations in Dib et al. (2017) using conventional, single-element probes. UV can also simulate more complicated scenarios, such as phased-array (PA) probes, and PNNL has used that capability extensively in the past (cf. (Crawford et al. 2014; Diaz et al. 2009; Diaz et al. 2019; Moran et al. 2017). UV simulations are relatively simple and rely on a ray-tracing approach. UV does not have flaw-response simulation capabilities.

2.2 CIVA

CIVA is a modeling and simulation platform that was originally developed by the French Alternative Energies and Atomic Energy Commission and is currently distributed by EXTENDE (Massy, France). CIVA was designed for simulating ultrasonic inspections relevant to the nuclear industry but has since included other NDE methods with applications to a broad range of industries. UT simulation modules in CIVA include beam simulations and flaw-response, or inspection, simulations. CIVA implements a transient pencil-ray approximation (Deschamps 1972); this approach allows most CIVA applications to run relatively quickly on a desktop PC, as compared to finite element modeling (FEM) applications. Because of CIVA's relevance to the nuclear industry, PNNL and others in the U.S. have used CIVA extensively for UT simulations (Connolly et al. 2018; Dib et al. 2017; Dib et al. 2018; Dunlap et al. 2018; Jacob et al. 2022a; Jacob et al. 2022b; Jacob et al. 2020; Le Lostec et al. 2014).

2.3 OnScale Solve

OnScale[3], formerly PZFlex, is a multi-physics simulation platform distributed by OnScale, Inc. (Redwood City, CA, USA). OnScale uses finite element analysis and a cloud-based architecture to allow for massively parallel computing and short simulation times. Because it is an FEM platform, OnScale is flexible enough to simulate virtually any situation, but it requires knowledge of specialized code for developing models. Knowledge of (and access to) MATLAB (The MathWorks, Inc., Natick, MA, USA) is also helpful for developing models and analyzing results. OnScale has also been used in the U.S. nuclear industry (Dunlap et al. 2020; Le Lostec et al. 2014), although to a lesser extent than UV or CIVA. PNNL's experience with OnScale is presented in (Jacob et al. 2022a).

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[2] Zetec was acquired by Eddyfi Technologies (Quebec, Canada) during the preparation of this report.

[3] Note that there are multiple OnScale products. OnScale SOLVE is the online Web interface FEM product. OnScale Lab is the desktop client product with three interfaces, Designer for graphical user interface model creation, Analyst for scripted interface, and PostProcess for visualizing data generated from simulations. In this report, the OnScale products are referred to collectively as OnScale. OnScale was acquired by Ansys, Inc. (Canonsburg, PA, USA) during the preparation of this report.

Table 1 summarizes the UT-specific features of the three modeling platforms based on PNNL's experience as of May 2022. This is not a comprehensive comparison.

Table 2.1 Comparison of UT-Specific Features of UltraVision, CIVA, and OnScale

Modeling Features	UV	CIVA	OnScale
Beam Simulations	✓	✓	✓
Flaw-response simulations (A-scans, B-scans, and C-scans)		✓	✓
3D models	✓	✓	✓
Built-in PA probe definitions	✓	✓	
PA focal law calculator	✓	✓	
Built-in specimen geometries, such as welds and nozzles	✓	✓	
Built-in signal or beam calibration tools	✓	✓	
Built-in noise simulation		✓	
Built-in attenuation simulation		✓	✓
Built-in options for modeling specimen microstructure		✓	
Data analysis tools	✓	✓	✓ most UT analysis is done in the MATLAB toolbox or Python
FEM		✓ with CIVA Athena 2D	✓
Cloud computing			✓
Metamodels/Parametric studies		✓	✓
Interfaces with Python or MATLAB for simulation setup and analysis		✓ available as an add-on for additional cost	✓
Remote access	✓	✓ remote access license available for an additional cost	✓
Full graphical user interface (GUI)	✓	✓	✓ complex models require the Analyst Module and knowledge of SYMB programming

3.0 CHALLENGES IN MODELING AND SIMULATION

Creating models that generate accurate and predictive simulation results is challenging because mathematical approximations must be used to describe physical phenomena, input parameters are often uncertain or unknown, and variations in results require careful interpretation. Weather forecasting provides an excellent analogy for understanding difficulties in modeling. Weather forecasts, for example, are based on dozens or hundreds of measurements, such as wind speed, atmospheric pressure, and humidity. Meteorologists rely on the most accurate and current information available from a variety of sources, such as networks of weather stations, radar, weather balloons, and satellites. They use their understanding of meteorological processes and fundamental physics to develop predictive mathematical models. To create a forecast, meteorologists account for uncertainties by running an ensemble forecast, or generating a group of results by running simulations multiple times with each forecast having slightly different input parameters. Results are assessed for quality, and probabilities are derived based on the ensemble forecast.

The first challenge in modeling is knowing the input parameters. In ultrasonic modeling and simulation for the nuclear industry, there are many parameters that need to be measured, such as the probe center frequency, the probe bandwidth, the wedge properties, the sound velocity in the specimen, and the specimen geometry and thickness. As with weather forecasting, the most accurate available data should be used in the model. A major challenge for weather forecasting is that dynamics of the earth's atmosphere are chaotic, with minute changes in initial conditions potentially leading to large changes in outcomes and forecast uncertainty. Fortunately, nuclear NDE inspections are performed in well-controlled environments on well-behaved systems. However, there are some parameters that cannot be measured, such as grain structures or the shape or depth of a potential flaw. Furthermore, there are parameters that cannot be accounted for in models, such as human factors and variability in equipment performance. All of the variables and parameters are sources of uncertainty.

Another challenge comes from uncertainty in the mathematical assumptions and approximations that form the basis of the models. These sources of uncertainty are inevitable, meaning that exact solutions to complex equations are often not possible. Models are usually not designed to cover all possible scenarios and may "break down" or give unrealistic results. It is the responsibility of the user to understand the model's limitations. Also, different model approximations may emphasize some variables over others, as it is possible for two models with identical input parameters but different mathematical frameworks to produce very different results. Certain models may be optimized to increase efficiency and speed but at the expense of accuracy. For example, the mesh density can have a strong impact on simulation time and accuracy—a finer mesh will give more accurate results but will require a longer computation time. In weather forecasting, a fine mesh can be used to obtain a local forecast for a specific home or address, but the simulation time would be so long that the weather system will have passed long before the results are available. Sources of uncertainty must be balanced with the tolerance for ambiguity.

Next is the challenge of assessing the simulation results and making comparisons with reality, which requires human intervention and experience. Such comparisons are straightforward for weather forecasters—simply wait to see if the forecast was correct. For the nuclear industry, however, comparing simulation results with a true-state requires carefully designed mockups and destructive testing, both of which are time consuming and costly. Destructive testing is not likely to be possible for an inservice component (especially if it is contaminated with radiation) or for a one-of-a-kind mockup. Simulation results can be difficult to validate, but it is extremely important to do so. Validation is needed to refine and adjust model parameters and to assess whether the results are reflective of reality. Important questions to ask include: Are the simulation results realistic? Do the results predict the correct scenario? What do the results mean?

Finally, the uncertainties and challenges lead to questions about the predictability of results. To create an accurate, probabilistic forecast, weather simulations are run many times with different initial conditions. This is often done by running a "control" simulation with the best available data, then by running dozens of additional simulations with realistic perturbations to that data. The results are a range of possible outcomes with four important effects.

1. Varying the input parameters can reveal which input parameters have the strongest impact on simulation outcomes. Care can then be taken to carefully measure those parameters or to perform additional iterations with those parameters.

2. Varying input parameters can reveal relationships between parameters. For example, tweaking parameter "A" may have a small effect and tweaking parameter "Z" may also have a small effect, but changing "A" and "Z" together could have a large effect. These relationships can be unexpected.

3. A range of forecasts, or simulation results, is generated that can be used to determine the most probable outcomes. Inspection simulations may predict a 50% chance that a flaw may be detected, much like an ensemble of weather forecasts may predict a 50% chance of rain.

4. The range of results can help bound the range of possible outcomes by showing the worst and best-case scenarios.

It is important to understand that compromises must often be made when making modeling decisions. For example, model realism may be compromised for model efficiency. Developing a realistic DMW model is difficult and time consuming, and such a model will never be truly representative of the actual specimen due to microstructural randomness in the specimen (Jacob et al. 2022a). A model can be developed that represents a snapshot of the specimen at a particular location, but the specimen microstructural properties vary continuously throughout the material. At other locations in the material, the model becomes an approximation at best and completely unrepresentative at worst. However, by compromising realism for efficiency, a small amount of effort could be put into generating many *representative* specimen models as opposed to putting great effort into developing a few *realistic* models. This would permit more simulations to be run, generating a broader picture of the range of outcomes and allowing for a probabilistic prediction. An example of this approach is using the built-in Voronoi regions in CIVA to represent CASS microstructure. The Voronoi regions have been shown to be an excellent representation of many CASS materials; however, the regions are only available in simple geometries (as of 2021 version of CIVA). Thus, one may choose to compromise the geometric complexity for model functionality by eliminating the weld and focusing on simulating the effects of the CASS microstructure. This approach was taken Jacob et al. (2022a) to explore the effects of CASS on flaw-response simulations.

In summary:

- There may be challenging inspection scenarios that will require modeling and simulation to help inform whether or not the inspection will be successful.
- Understanding the operational limits of the modeling tool is essential prior to running simulations (i.e., knowing where the model breaks down or the results stop making sense).
- Some empirical confirmation may be required. Custom-designed mockups can be valuable for empirical confirmation.
- Multiple simulations should be run—despite inconvenience—by using both conservative and non-conservative inputs. This approach will help bound possible outcomes by creating a range or envelope of simulation results.
- Simulation results do not always provide consistent, realistic, or representative outcomes. Statistical analysis needs to be considered to determine which results are outliers and which results are most probable.
- A thorough analysis of model inputs and outputs will inform any simulation-based decision making.

Simulation results will never be *perfectly* accurate, as approximations and uncertainties always reduce accuracy. However, by working within the constraints of the model and understanding the limitations and challenges of modeling, predictive results can be obtained. Predictive does not mean precise, it simply means that a probability of an outcome can be established that can then be used to guide decision making.

4.0 SIMULATION EXAMPLES

This section contains several examples of real-world applications of modeling and simulation in or related to the nuclear industry. Subsection 4.1 describes how beam simulations were used to help understand how axially-oriented flaws were missed during inspections of North Anna Power Station Unit 1. Subsections 4.2, 4.3, and 4.4 illustrate how beam simulations and flaw-response simulations were used to evaluate licensee requests for relief from examination requirements. Subsection 4.5 describes the use of beam simulations and flaw-response simulations to support mockup design for tests to determine the effects of limited beam coverage scenarios. Subsection 4.6 compares the flaw response from inspection results to simulation results in the case of an oddly shaped flaw found in River Bend Station Unit 1 in the 1980s. Finally, subsection 4.7 summarizes an example of how modeling was used to design a multi-element probe for heat exchange tubing inspections in Korea. Each example summarizes work from a publicly available report or publication.

4.1 North Anna Power Station Unit 1

Beginning in 2012, PNNL conducted a technical assessment of issues that led to several missed detections of axially-oriented flaws in a steam generator primary inlet DMW at North Anna Power Station Unit 1 (Anderson et al. 2014). Two through-wall flaws were discovered during surface machining in preparation for a structural overlay. Additional ultrasonic tests discovered five axial flaws around the weld. PNNL conducted work to determine why the initial field exams missed the flaws, and modeling and simulation played a key role in the assessment.

The field exams were conducted using manual, non-encoded, conventional inspection methods. The probe was a tandem front-rear pitch-catch probe designed for a 30° inspection angle. The required metal path at 30° to reach the inner diameter (ID) was approximately 148 mm (5.83 in.). To assess the appropriateness of the probe, PNNL performed sound field simulations in CIVA and noted that the weld microstructure was not accounted for in the simulations; thus, the simulations were best-case scenarios. Simulation results in figure 4.1 showed that the tandem configuration produced a sound field with a maximum intensity along the metal path at 44 mm (1.73 in.) from the outer diameter. The −6 dB focal zone along the metal path was 83 mm (3.27 in.) long, or only 56% of the entire through-wall metal path, well short of the needed 148 mm (5.83 in.). Simulations also showed that just a small fraction of the sound energy would reach the ID surface, which portends a poor signal-to-noise level for detection of ID surface-connected flaws. Therefore, the simulations suggested the tandem probe was not well suited for detection of ID-connected flaws in this configuration.

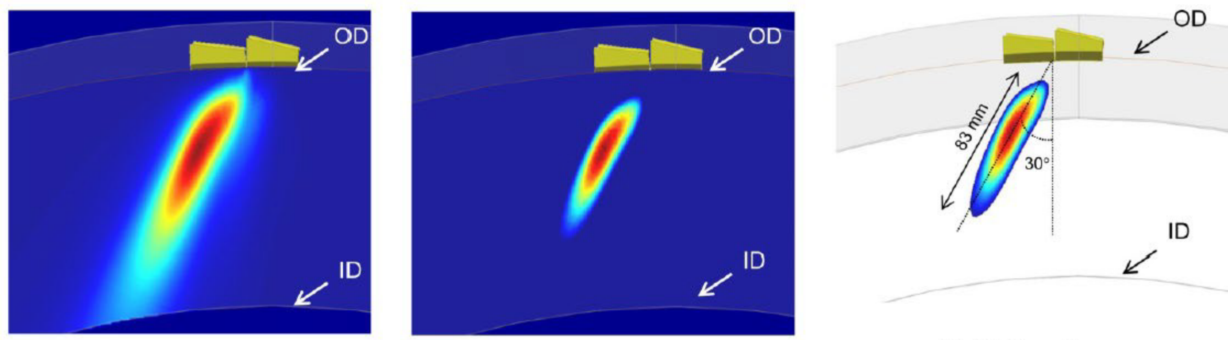

Figure 4.1 Sound Field Simulations of the Tandem Probe

Left: the full sound field. Center: the −6 dB limits of the sound field. Left: the −6 dB limits of the sound field with the refraction angle and specimen geometry more clearly identified. This figure is Figure 5.5 from PNNL-22553.

Additional simulations were performed on three PA probes to assess whether they would be better suited for the inspection scenario. The PA probes were 0.5 MHz, 1.0 MHz, and 2.0 MHz. UltraVision 3.3R4 was used to calculate the focal laws and simulate the sound fields. UltraVision produces a simple image of the probe on the wedge, ray-tracing to show the focal depth and steering desired, and density mapping to show the sound field at each angle. Grating lobes (unwanted energy formed off-axis from the design angle), if present, are also mapped. Such simulations provide a useful first-approximation for sound beam modeling and enables the user to estimate sound field parameters and transducer performance. Focal laws were generated to optimize axial flaw detection. Results showed that the 0.5 MHz probe (figure 4.2) theoretically produces a beam that reaches slightly beyond the specimen ID surface at the −6 dB level. The sound fields of the 1.0 MHz probe at the −6 dB level (figure 4.3) were short of the ID surface by about 15 mm and 25 mm (0.6 in. and 1.0 in.) at refracted angles of 30° and 40° degrees, respectively. Thus, the 1 MHz probe had an approximate shortfall of 10% to 15% of the specimen through-wall, a marked improvement over the 44% shortfall with the tandem probe. The 2.0 MHz probe at the −6 dB level (figure 4.4) also did not extend to the ID surface. At 30° and 40°, the sound beams were short of the ID by about 45 mm and 50 mm (1.8 in. and 2.0 in.), respectively. The simulations indicated that either the 0.5 MHz or 1.0 MHz PA probe should be well suited for the inspection.

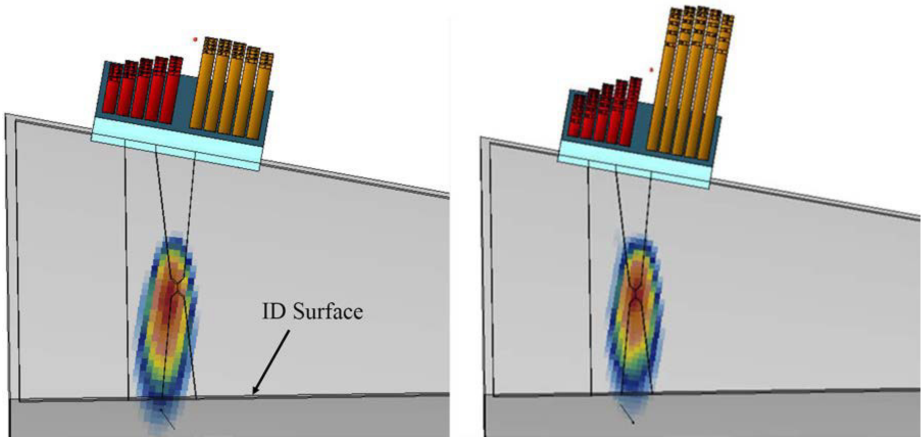

Figure 4.2 Simulated Sound Fields for the 0.5 MHz Probe

The −6 dB extents are shown at 30° (left) and 40° (right). This figure is Figure 6.5 from PNNL-22553.

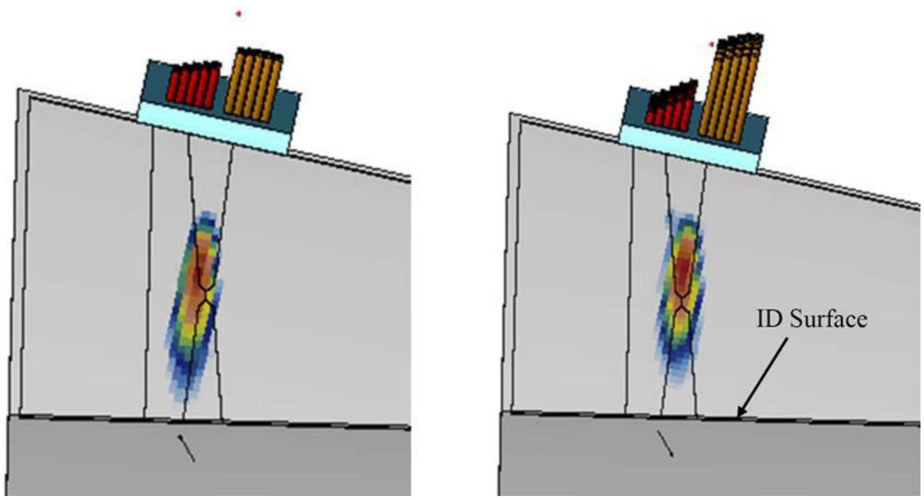

Figure 4.3 Simulated Sound Fields for the 1.0 MHz Probe

The −6 dB extents are shown at 30° (left) and 40° (right). This figure is Figure 6.6 from PNNL-22553.

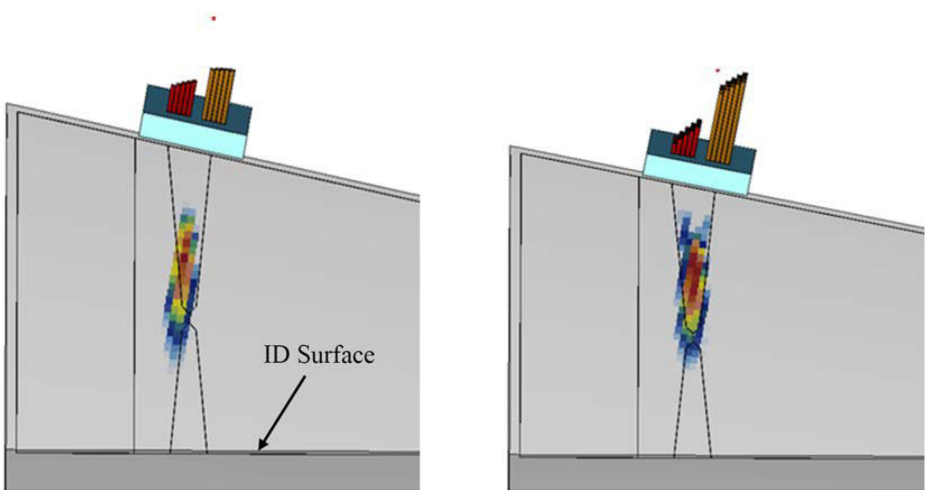

Figure 4.4 Simulated Sound Fields for the 2.0 MHz Probe

The −6 dB extents are shown at 30° (left) and 40° (right). This figure is Figure 6.7 from PNNL-22553.

As concluded in PNNL-22553,

> *The results of probe modeling and beam simulation were critical in providing a theoretical basis for understanding the performance of the transducers to inform confirmatory work in quantifying actual sound field densities and beam propagation characteristics   Initial modeling results indicated the tandem probe configuration, as fabricated, would produce maximum longitudinal mode ultrasonic energy at a refracted angle of approximately 30 degrees. The optimum ID impingement angle in accordance with PDI-UT-10[4] for detecting axial PWSCC [primary water stress corrosion cracks] in dissimilar metal welds is between 55-60 degrees. Theoretical simulations validated by empirical assessments showed that the probes produced an ID impingement angle of about 41 degrees. Additionally, based on the small overall probe aperture, adequate sound field intensities appear to be located at only a shallow distance within the component (along the metal path) which would significantly decrease the effectiveness of inspection for the detection of ID-connected flaws.*

Thus, simulations verified that the tandem probe was not optimal for the required task and could not insonify the inspection volume adequately, which contributed to the missed detections. If modeling and simulation of the probe performance had been performed prior to the inspection, then it is possible that the probe's shortcoming could have been identified and an alternative approach chosen. Additional simulations could also have been used to aid in the design of a new probe or to predict performance of alternative probes.

As noted above, the models used were best-case scenarios because the weld region was treated as isotropic material; sound field scatter and attenuation from the weld microstructure were ignored. Recent work at PNNL has shown that austenitic and dissimilar metal weld models can be used to provide predictive simulation results (Jacob et al. 2022b; Jacob et al. 2020). Implementing such models would likely improve predictions of sound field penetration.

4.2 Arkansas Nuclear One, Unit 2

This example refers to an alternative to examination requirements, or relief request, submitted by a licensee regarding the ultrasonic volumetric coverage requirements of DMWs at Arkansas Nuclear One, Unit 2 (see ML13113A218 (PNNL 2013a)). The alternative applied only to circumferential scans for the detection of axially-oriented flaws. The NRC requested that PNNL evaluate the licensee's proposed alternative with respect to the coverage claims. Modeling and simulation were included in the evaluation based on the PA probe design and geometrical information provided by the licensee.

PNNL noted that the modeling did not account for the microstructure of the austenitic weld, which can cause beam attenuation, redirection, sound field partitioning and scatter. In addition, the potential for inconsistent transducer coupling was not accounted for in the model due to limitations in the modeling software.

Figure 4.5 is an example of the licensee's calculated volumetric coverage for one of the welds (labeled 09-008). The licensee's estimated volumetric coverage was 73.8%, which includes the inner one-third of the ID-clad carbon steel piping but no coverage on the CASS safe-end (on the right in the figure).

[4] PDI-UT-10 is the Performance Demonstration Initiative procedure applicable to pre-service and inservice manual ultrasonic examination of dissimilar metal welds.

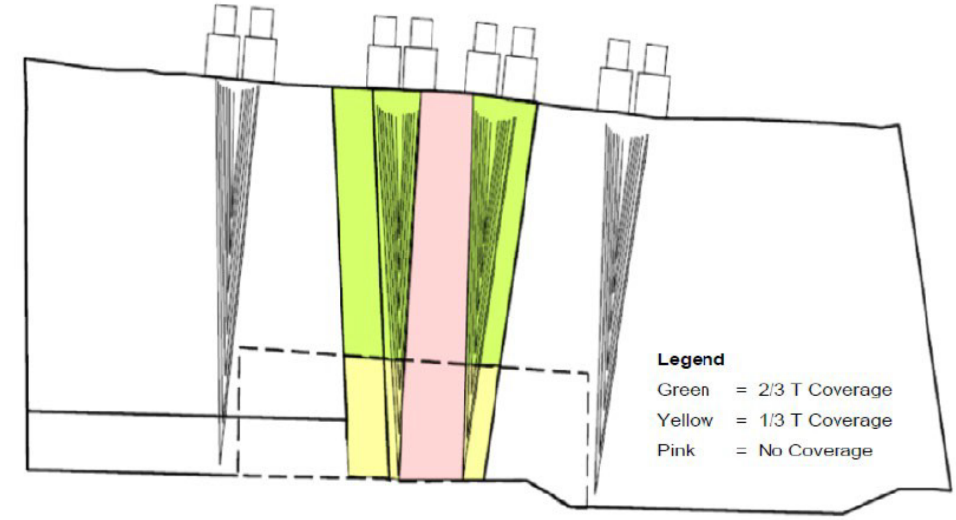

Figure 4.5 Licensee Calculated Volumetric Coverage for Weld 09-008. This is Figure 2 from ML13113A218

Figure 4.6 shows the simulation results obtained by PNNL. Regions where volumetric coverage from a combination of all steered beams is predicted to be above the −6 dB level are shown in green. Note that the PNNL specimen model had flat OD features, resulting in volumetric coverage throughout the center of the weld. Also, the PNNL results are based on theoretical −6 dB limits as opposed to a ray-tracing sketch that only highlighted the sound path. As noted in the report, the licensee's coverage sketch was more conservative than the PNNL model.

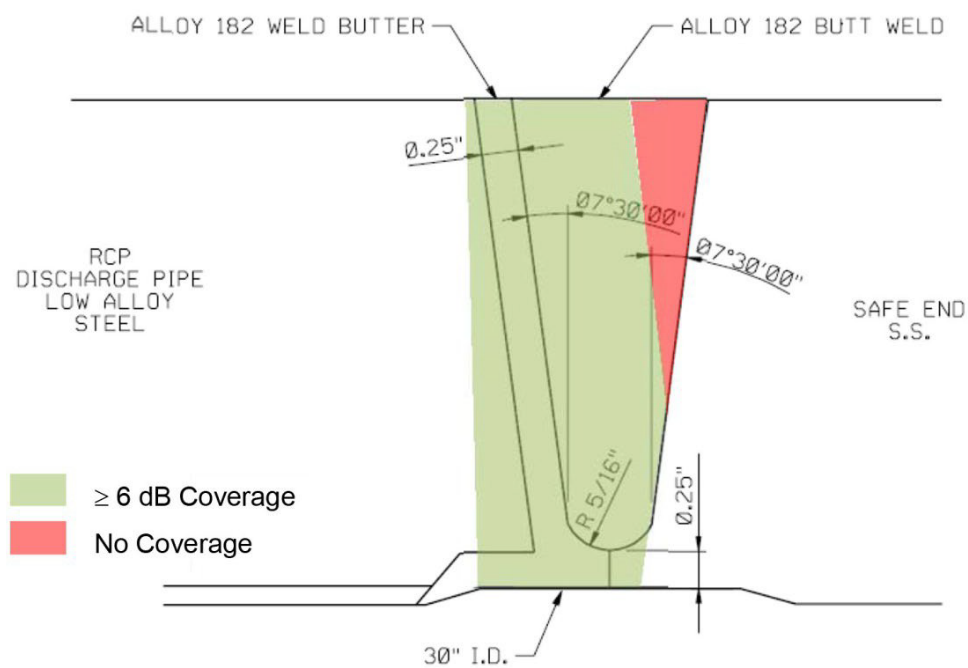

Figure 4.6 PNNL-Modeled Volumetric Coverage at the −6 dB Level. This is Figure 3 from ML13113A218

Additional simulations were done in UltraVision to characterize the sound beams produced by the various PA focal laws. The beams were focused at a constant metal path of 122 mm (4.8 in.), as shown by the arc on the right side of the figure. Results showed that the beams above about 30° were not expected to effectively insonify the region near the weld ID (see figure 4.7). The simulations represented a best-case scenario—the model did not include scatter or attenuation from the austenitic weld—so it is possible that the lower angles will be less effective than the simulations suggest.

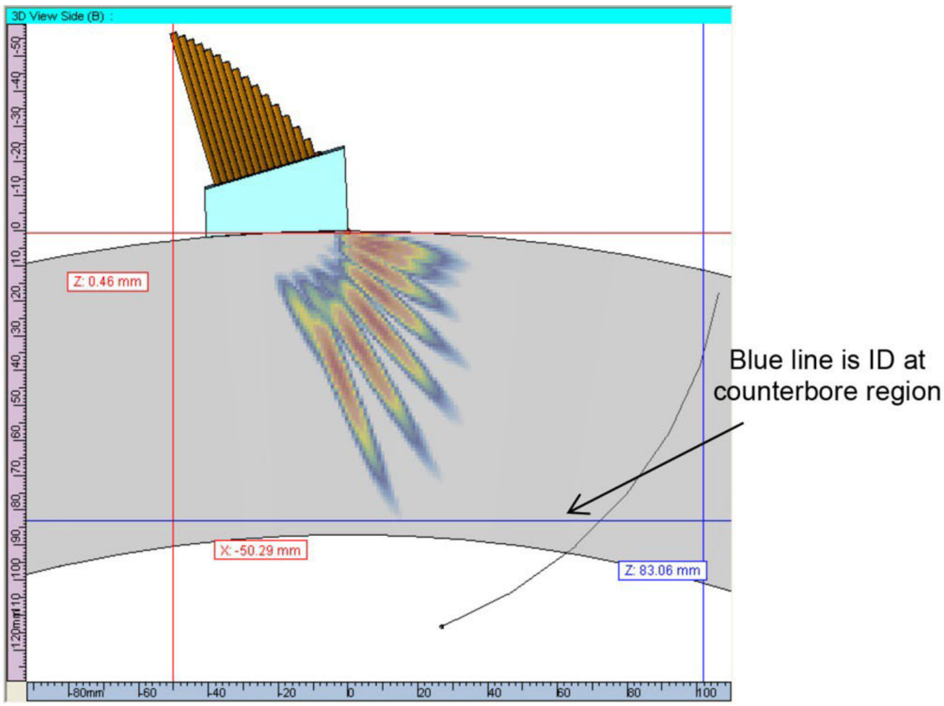

Figure 4.7 Sound Beam Intensity Profiles for the 20° to 80° Beams. This is Figure 4 from ML13113A218.

Simulations predicted that the inspection region would have essentially full coverage, but that coverage would come only at the lowest angles, about 20°-25°. Such low angles are typically not well suited for flaw detection because the echo from the backwall tends to dominate. Therefore, simulations confirmed that flaw detection in this weld using the proposed approach would likely be challenging.

In this example, beam simulations were used to confirm that coverage in the inspection area was not expected to be adequate. Additional simulations could provide insight into whether a different inspection method would be more successful. For example, the focal laws projected the beam to a constant metal path of 122 mm (4.8 in.)—this is referred to as half-path focusing. An alternative to test would be true-depth focusing, where the beam is focused at a constant depth in the part. True-depth focusing is best suited for lower inspection angles, such as up to about 40-45°, but it might improve coverage in the inspection volume. Another option would be to test alternative probes, perhaps with lower frequencies or larger apertures that could penetrate deeper into the part.

As noted above, the PNNL models did not account for the microstructure of the austenitic weld. Weld models developed more recently by PNNL can account for austenitic microstructure and potentially improve simulation accuracy (Jacob et al. 2022b; Jacob et al. 2020). In addition, the models also did not account for inconsistent transducer coupling. This is a limitation in UltraVision, but CIVA can account for inconsistent coupling due to outer surface geometrical features, as long as those features are included in the model.

4.3 Calvert Cliffs Nuclear Power Plant

Similar to the example in section 4.2, a licensee submitted an alternative to the examination coverage requirements for several DMWs at Calvert Cliffs Nuclear Power Plant (see ML13113A233 (PNNL 2013b)). The alternative applied to both circumferential and axial scans. The NRC requested that PNNL evaluate the request using modeling and simulation. PNNL used PA design parameters and component geometries provided by the licensee. Figure 4.8 shows the licensee drawing of the weld and the predicted coverage. They noted that scan limitations could allow a flaw up to 30.5 mm (1.2 in) deep to be undetected in the examination region (shown by the red line in the figure). The licensee estimated that 93% coverage of the required examination volume could be obtained (without taking any credit for the CASS safe-end material).

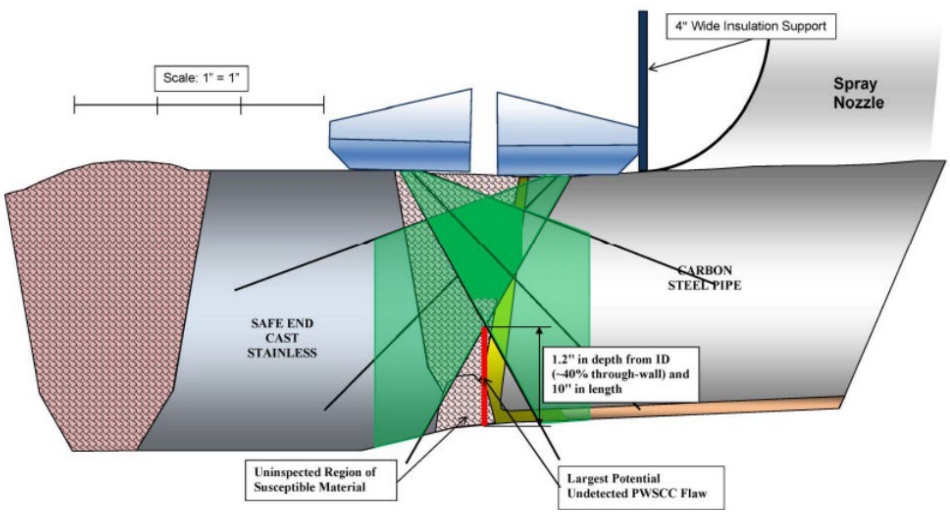

Figure 4.8 Licensee Calculated Volumetric Coverage for Weld 30-RC-21B-10. This is Figure 2 from ML13113A233

PNNL used CIVA to simulate the ultrasonic beam intensities in 10° increments from 0° to 80°. The focal law values, specimen drawing, and probe parameters were supplied by the licensee. The licensee did not take credit for angles below 30°, but simulation results showed that improved volumetric coverage could be obtained if angles as low as 10° were accounted for (see figure 4.9). Results also showed that angles above about 65° would not provide useful sound fields for near-ID detection. The models represented a best-case scenario, as weld microstructure and probe coupling were not accounted for.

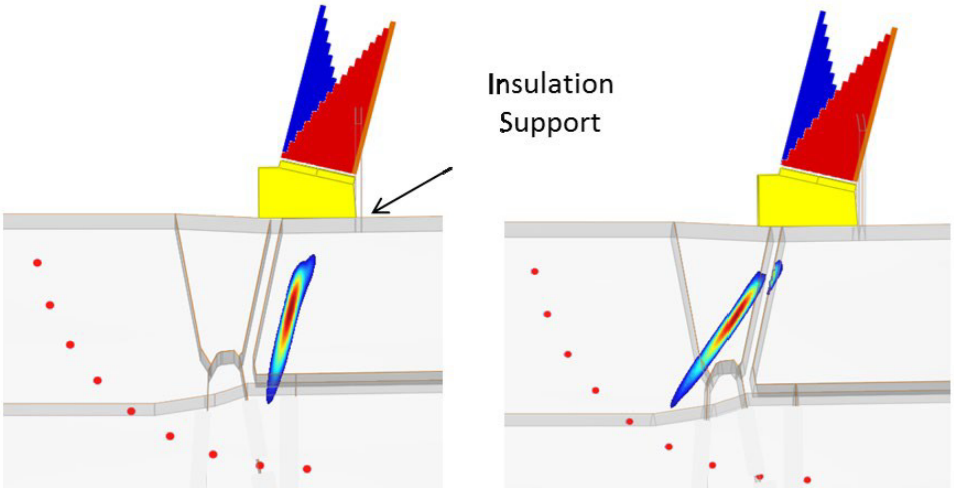

Figure 4.9 The −6 dB Extent of Simulated Beams for 10° (Left) and 30° (Right) . This is Figure 4 from ML13113A233

The licensee postulated that a flaw as deep as 30.5 mm (1.2 in) in the weld could be missed due to the coverage limitations, so PNNL used modeling and simulation to evaluate the detectability of such a flaw. The simulations used a simplified planar flaw with a semi-elliptical profile. The flaw was 254 mm (10 in.) long and 30.5 mm (1.2 in.) deep, as shown in figure 4.10. Sound beam angles were modeled from 0° to 60° in 5° increments.

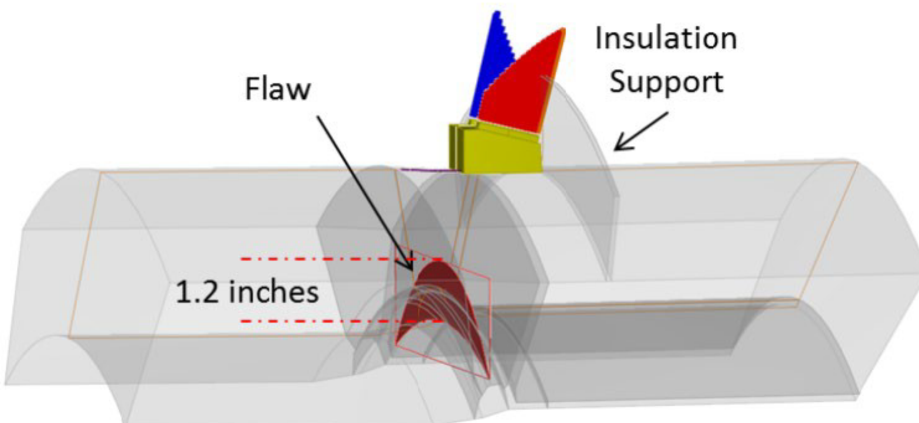

Figure 4.10 The Specimen Model Showing the Planar Flaw and the Scan Limitation Imposed by the Insulation Support. This is adapted from Figure 5 of ML13113A233

The flaw-response simulations showed that corner and tip responses were detected at 30° with the probe in the initial scan position, abutted against the insulation support. As shown in figure 4.11, the corner response was too weak to be able to determine if the flaw was ID connected, but simulations indicated that a lower angle, such as 20°, might improve detection. As the probe was moved toward the weld region, the signal from the flaw disappeared. The simulations suggested that it is imperative to start the scan as far back from the weld centerline as possible to maximize the chances of detecting the flaw.

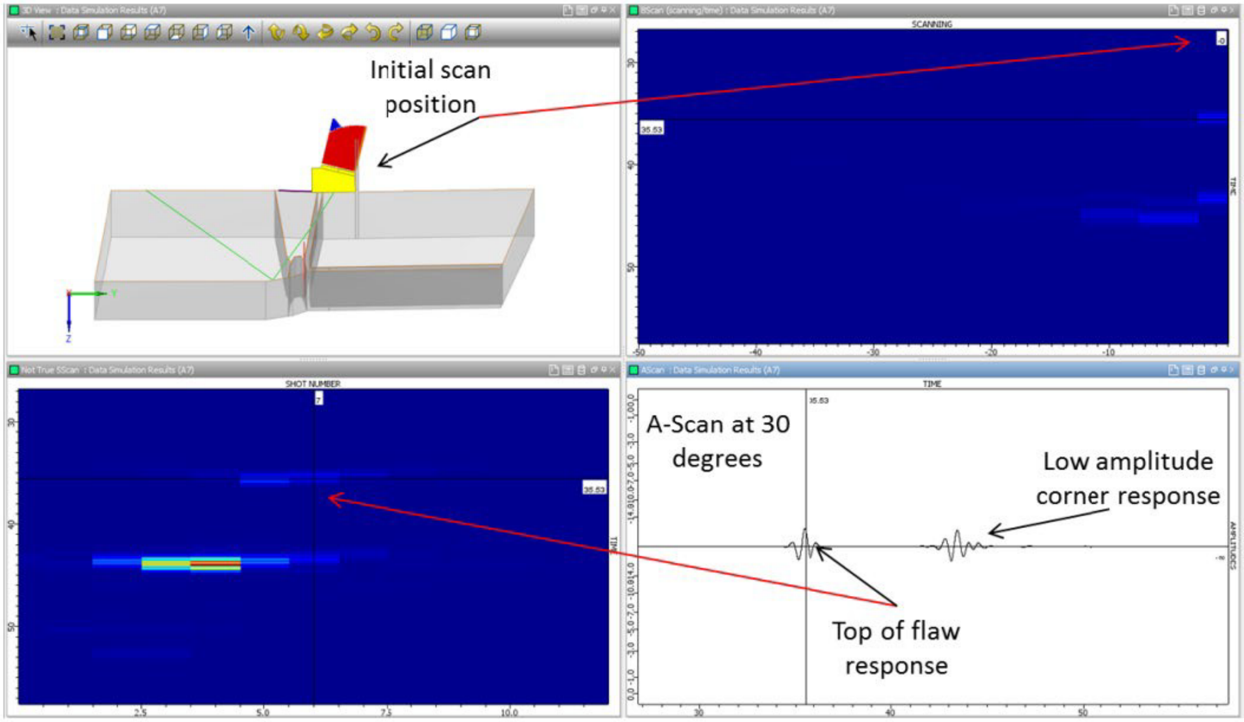

Figure 4.11 Flaw-Response Simulation Results at 30°. This is Figure 7 from ML13113A233

Additional flaw-response simulations were performed to determine if flaw detectability would increase as the flaw depth was increased. A parametric study was performed by increasing the flaw depth in increments of 2.5 mm (0.1 in.). Results showed that the maximum tip signal was obtained from a 35.6 mm (1.4 in.) flaw when using a 30° inspection angle (see figure 4.12). Additional simulations (not shown here) were performed to assess flaw detection at other probe locations on the component.

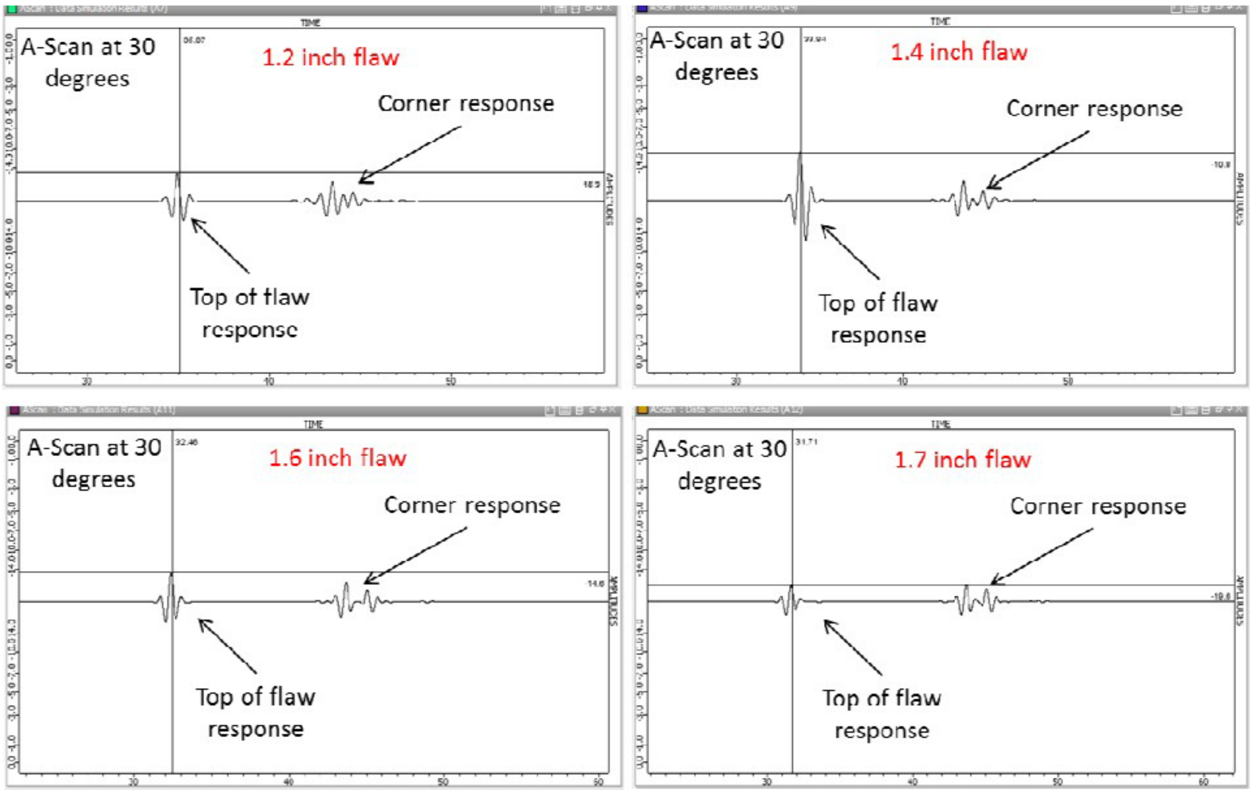

Figure 4.12 Flaw Responses from the Parametric Study of Variable Flaw Height

The probe was at the position shown in Figure 4.10. The tip response peaks when the flaw is 35.6 mm (1.4 in.) deep. This is Figure 9 from ML13113A233.

PNNL concluded in ML13113A233 that the simulations were in agreement with the licensee's coverage predictions at 30°. PNNL also agreed that the minimum detectible flaw depth was 30.5 mm (1.2 in.). However, simulations predicted that a 35.6 mm (1.4 in.) deep flaw would give a maximum response while deeper flaws and shallower flaws would be difficult to detect if a strong corner response was not visible.

The Calvert Cliffs example illustrates the use of both beam simulations and flaw-response simulations in a realistic scenario to predict flaw detectability. Importantly, a parametric study was used to determine the detection limits for flaws of various depths, since individual simulations provide limited information. The insulation support posed a limitation to probe motion, but additional simulations could be used to explore other probe geometries. For example, simulations may indicate whether a fixed-angle probe with a smaller wedge could be used to get farther back from the weld centerline and better insonify the inspection region. Simulations could also predict whether phased-array probes would provide additional coverage.

Simulations showed that it was important for the probe to be as far back from the weld as possible to maximize the chances of detecting a flaw in the weld. The probe size limits how far back the probe can go, but with PA probes it is possible to do electronic scanning where a subset of the elements is used. For example, a 10×5 array probe has 50 elements. The first 25 elements (elements 1-25) could be used for the initial scan. Then the beam can be incremented forward by using elements 6-30 without even moving the probe, and so forth. The advantage of this approach is that a subset of elements at the rear of the probe would effectively move the aperture back further away from the weld and may improve coverage. The disadvantage is that the aperture, and therefore the total intensity of the transmitted sound energy, is reduced. Simulations could be used to investigate whether electronic scanning would be effective at improving coverage.

4.4 St. Lucie Nuclear Power Plant, Unit 1

As with the examples in sections 4.2 and 4.3, PNNL was asked to review a licensee submittal for alternative volumetric examination coverage for DMWs, as described in ML14149A195 (PNNL 2013c). Again, modeling and simulation were performed using parameters and drawings provided by the licensee. Weld RC-124-7-504 is a CS-CASS DMW on a reactor coolant pump outlet nozzle. A spray nozzle caused a physical limitation to probe motion for axial exams of circumferential flaws. At the location of the most restrictive obstruction (i.e., where the spray nozzle extended closest to the weld), the PA probe was determined to have only 40.6 mm (1.6 in.) of motion, and the backward limitation of the probe caused a reduction in coverage. The licensee estimated that the coverage would be about 97.7% of the required volume (not including the CASS material) using inspection angles between 40° and 50°. Figure 4.13 shows the licensee drawing of the coverage limitation.

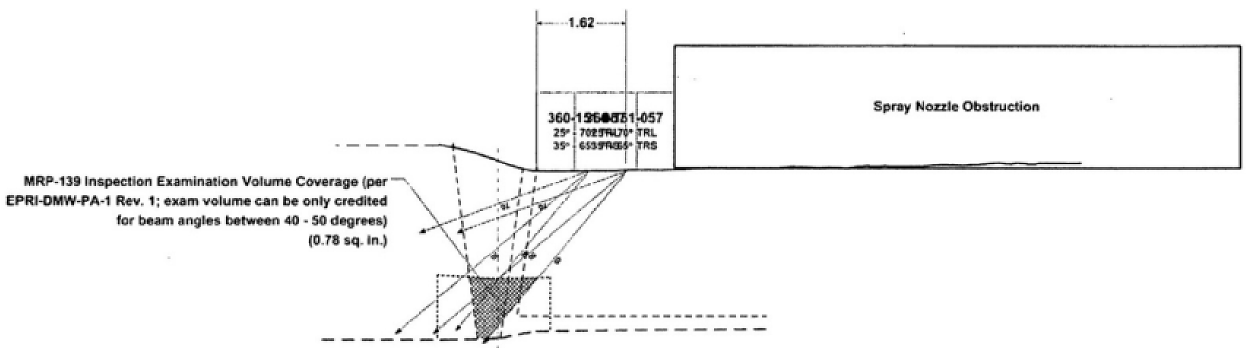

Figure 4.13 Licensee Ray Trace Diagram of Volumetric Coverage for Weld RC-124-7-504. This is Figure 4 from ML14149A195

PNNL used CIVA to simulate the sound field using the focal laws provided by the licensee. The simulations included a range of angles from 25° to 70° in 5° steps using half-path focusing with a metal path of 76.2 mm (3.0 in). Figure 4.14 shows the simulation results at 40° and 50° at the −6 dB and −12 dB extents. The simulations largely confirm the licensee’s coverage descriptions if the −12 dB extent is considered. Simulations also showed that lower inspection angles might improve the volumetric coverage.

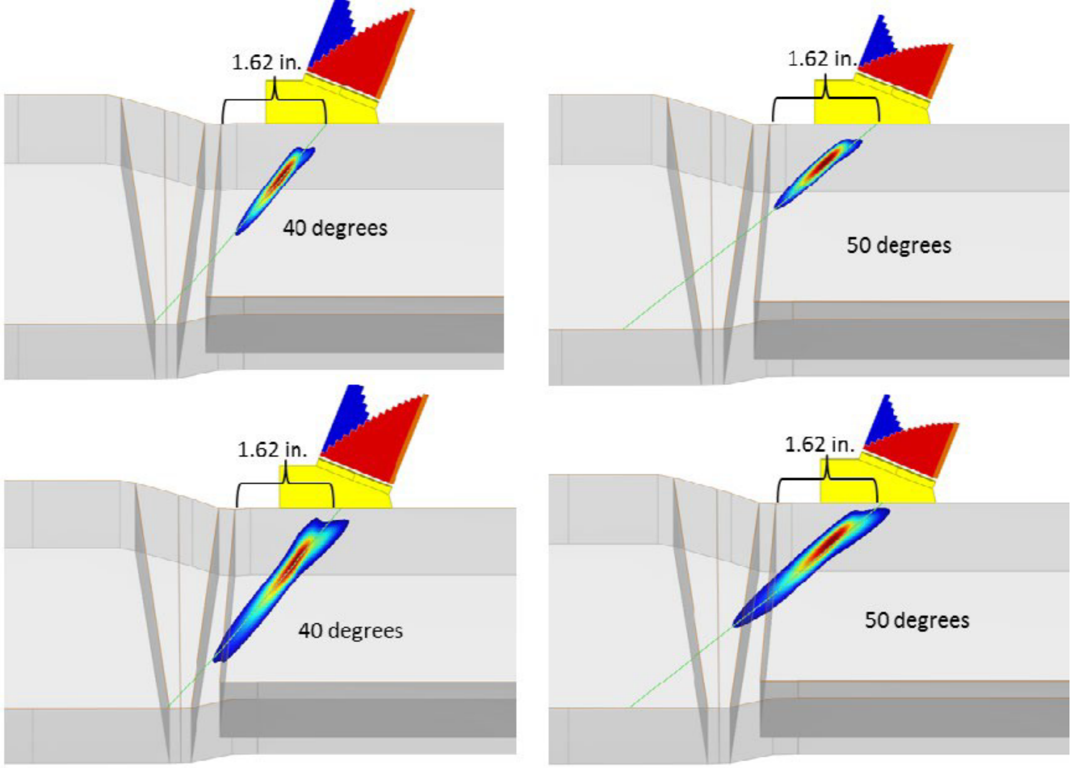

Figure 4.14 Beam Simulations Predicting Coverage at the −6 dB (Top Row) and −12 dB (Bottom Row) Levels at 40° and 50°

Similar to the Calvert Cliffs example in section 4.3, the licensee postulated a 40% through-wall, or 32.5 mm (1.2 in.) deep ID-connected flaw in the susceptible weld material would be the deepest flaw that would go undetected. PNNL modeled the flaw as a planar, semi-elliptical reflector and performed flaw-response simulations similar to those shown in figure 4.11. Note that a semi-elliptical flaw with no surface topology represents a best-case scenario in terms of expected corner and tip echoes. PNNL performed a parametric study using different flaw depths. Results confirmed that the starting position of the probe should be as far back from the weld as possible for the most reliable detection. Results also showed that only modest improvements in flaw detection were realized when flaws were as deep as 50% and 60% through-wall. Based on the simulations, PNNL concluded that a semi-elliptical circumferential planar flaw must be at least 40.6 mm (1.6 in.) deep, or approximately 50% through-wall, before it was reasonable to expect a tip signal response using the PA technique. Overall, the beam coverage plots and defect response simulations indicated that lower inspection angles may increase the overall coverage and likelihood of ID-connected flaw detection.

In this example, the simulations suggested that the licensee's predictions were not conservative enough when considering the size of a flaw that might be missed. The simulations also suggested that using additional inspection angles below 40° may have improved coverage and detectability of ID-connected flaws. As with the examples in sections 4.2 and 4.3, additional simulations may provide insight into whether alternative techniques, such as true-depth focusing or electronic scanning, may be able to improve examination coverage.

4.5 PNNL Test Mockup Design

Harrison et al. evaluated the impacts of limited examination coverage in ultrasonic inspections (Harrison et al. 2020). Incomplete examination coverage is a common issue experienced in every nuclear power plant, so it is important to understand how limited coverage scenarios can affect flaw detectability. The examples shown in subsections 4.2, 4.3, and 4.4 were motivated by limited coverage scenarios, such as OD surface geometry, CASS materials, or physical obstructions. The example in this subsection shows how modeling and simulation can be applied to an experiment by informing mockup design.

PNNL needed to assess coverage limitations in carefully designed mockups under controlled scenarios. One mockup was a stainless-steel plate with an austenitic weld and notches cut at various distances from the weld centerline. Modeling and simulation were used to assure that the flaw locations were appropriate for testing a limited coverage scenario. CIVA was used to generate beam maps and flaw responses when the probe's forward motion was limited by a weld crown.

Probes were modeled based on those used in the study. Models were created using conventional, dual-element, 2 MHz transmit-receive longitudinal probes, one at 45° inspection angle and the other at 60°. The probes were placed with the front edge at the weld toe to imitate the farthest possible forward reach of the probe assuming a weld crown was present. Beam simulation results in figure 4.15 showed that at this position, the leftmost flaw would not be well insonified by the 45° probe, but full coverage should be obtained using the 60° probe. Flaw-response simulations shown in figure 4.16 suggested that the 45° probe may have provided a partial corner signal from the leftmost flaw but no tip response would be visible. The 60° probe gave a full corner signal but a partial tip signal. Results confirmed that the mockup was appropriate for the study.

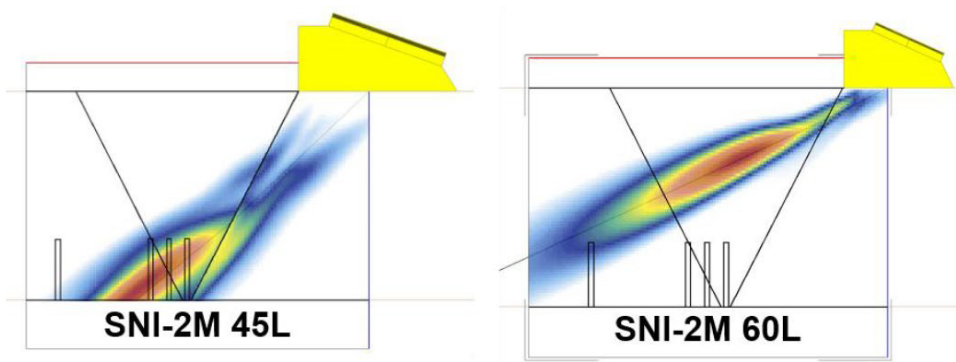

Figure 4.15 CIVA Beam Simulations Showing the Predicted Sound Field through a Homogeneous Weld in a Plate Mockup

The weld and notch positions are outlined. Left: 2 MHz, 45°. Right: 2 MHz 60°. This is Figure 8.6 from PNNL-30238.

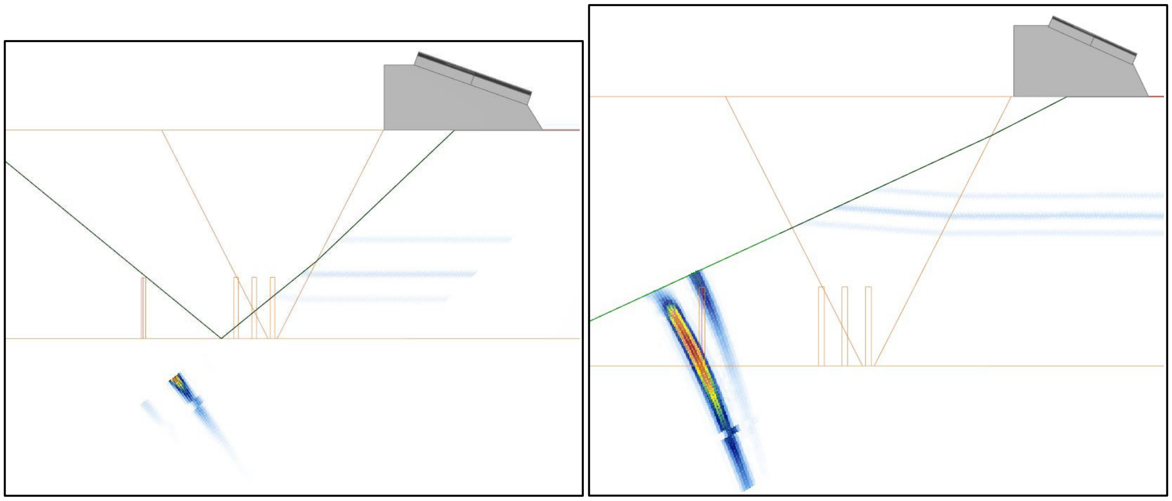

Figure 4.16 CIVA Flaw-Response Simulations Showing the Predicted Flaw Response from the Leftmost Notch

Left: the 45° probe. Right: the 60° probe. This is Figure 8.8 and 8.9 from PNNL-30238.

Note that the simulations were conducted under an ideal scenario where the material properties were treated as isotropic. However, it is well known that the microstructure of austenitic welds has a detrimental effect on the sound beam. Therefore, the simulation results presented a best-case scenario. To illustrate this, beam maps were measured in the laboratory using a laser vibrometer. Figure 4.17 shows the results. The top row illustrates the sound beam transmission through isotropic material and the bottom row, through the weld. The sound beam was distorted as it passed through the weld, but the beam simulations did not account for the distortion. This illustrates that, when interpreting the simulation results, it is important to consider that models do not account for all aspects of a given scenario.

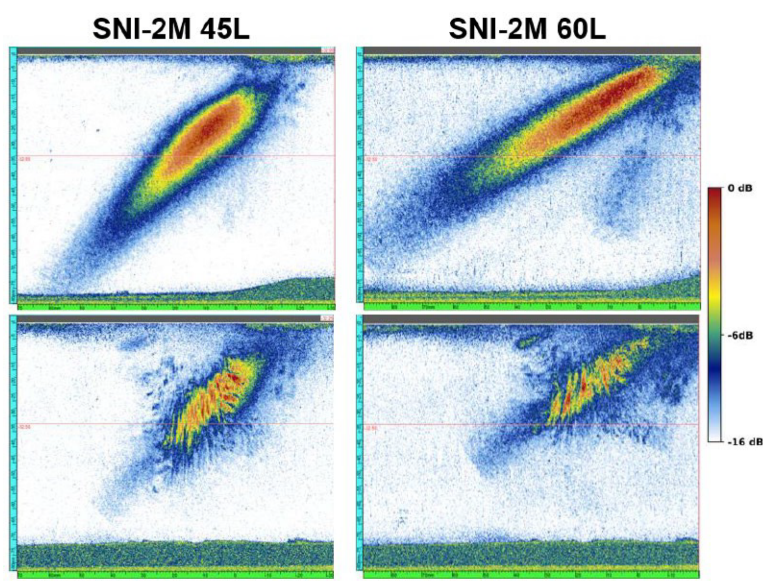

Figure 4.17 Empirical Beam Maps Acquired on the Plate Mockup

Top row: beam maps acquired away from the weld. Bottom row: beam maps acquired through the weld. The red horizontal lines indicate the ID surface of the plate. This is Figure 8.7 from PNNL-30238.

4.6 Riverbend Station Unit 1

This example is described in (Bowerman et al. 1999). In 1989, a crack in an inlet feedwater nozzle to safe-end weld at an operating nuclear power plant was discovered during a routine ultrasonic inspection. The flaw was sized in length and through-wall depth. Over the next three years, the flaw was examined several times to evaluate flaw growth. After three years, the weld was removed and replaced. Destructive analysis was done to establish the root cause of the crack in the safe-end to nozzle weld. Figure 4.18 shows a sketch of the flaw profile.

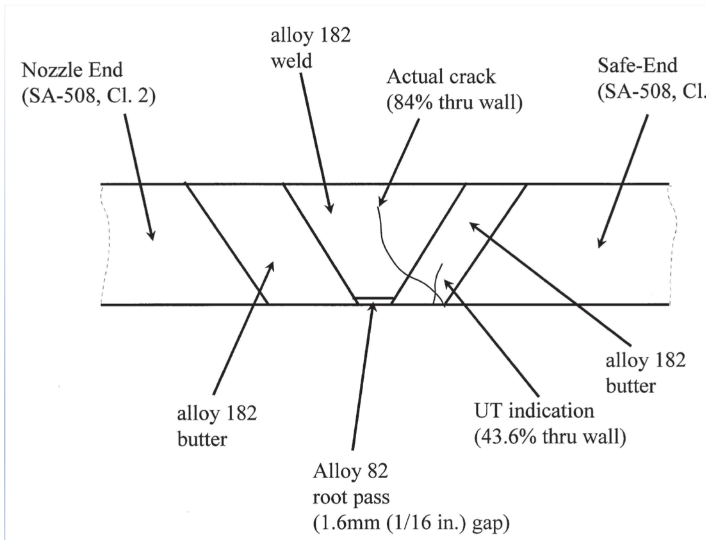

Figure 4.18 Figure from Bowerman et al. (1999) Showing a Schematic of the Specimen and the Flaw Geometry and Location

The flaw's true through-wall depth was found to be 84%, but the UT inspections sized it at 44%. The shape of the flaw was unusual and likely contributed to the difficulty in sizing it properly. Furthermore, the Code-required inspection volume is the inner one-third of the wall thickness, so the probes used were optimized for detection in that region. Confirmatory scans using both non-encoded and encoded approaches validated the inspectors' original results.

In 2020, PNNL implemented modeling and simulation on this flaw to determine if there were any shortcomings in the UT inspection techniques, or if the modeling would confirm the inspection results. Using conventional, dual-element, transmit-receive longitudinal probes at 45° and 60° in the model, results predicted that the flaw tip was not visible and that the flaw through-wall depth was about 40%, similar to the 44% measured by the inspectors (see figure 4.19). It should be noted that the tip of the flaw is well within the near field of the probe, so it is not expected that a good specular echo would come from the tip unless a taller wedge was used.

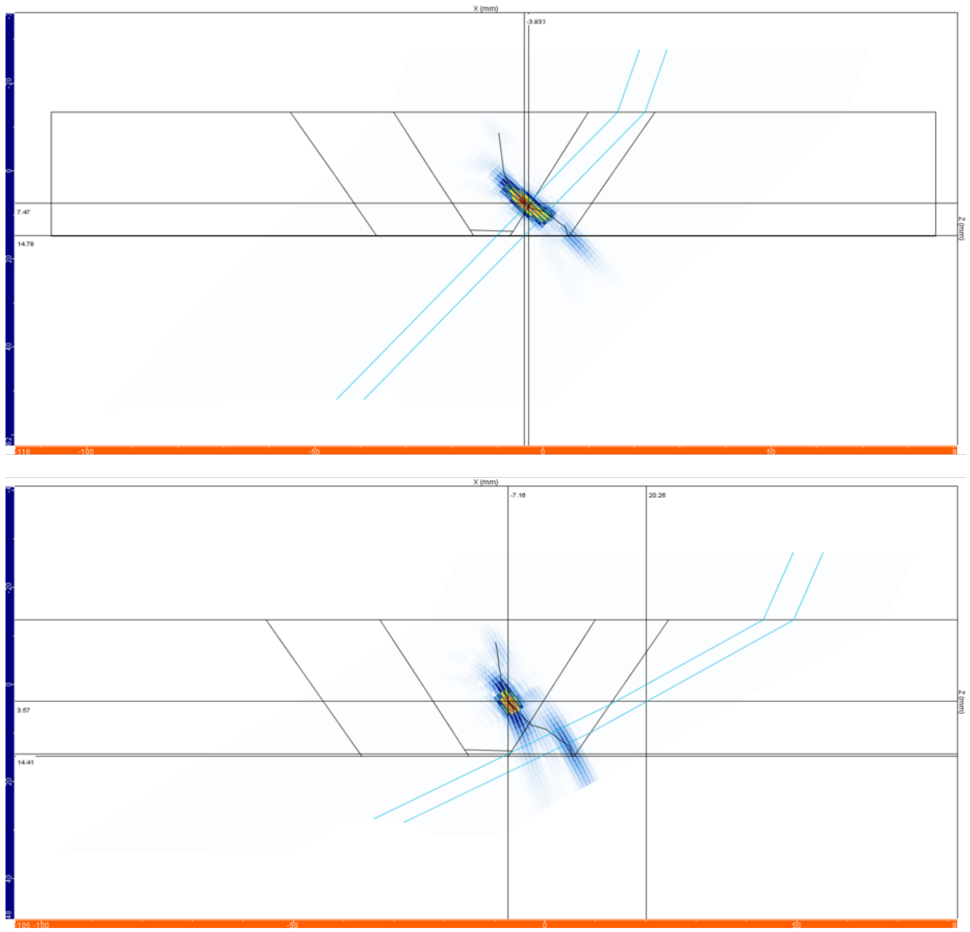

Figure 4.19 Simulation Results at 45° (top) and 60° (Bottom) Confirming the Original Inservice Inspection Findings

Today more advanced UT techniques are available that did not exist when this flaw was originally found, such as phased array, full matrix capture, and plane wave imaging. To investigate the potential advantages of using a PA probe in this situation, another simulation was run with inspection angles ranging from 30°–70° in 8° increments. The simulation results are shown in figure 4.20. The figure shows the combined echoes from all the inspection angles at four different probe positions. Simulations predicted that the deepest part of the flaw (indicated by the arrow) was not detectable, even at 70° or with the probe passing directly over the flaw.

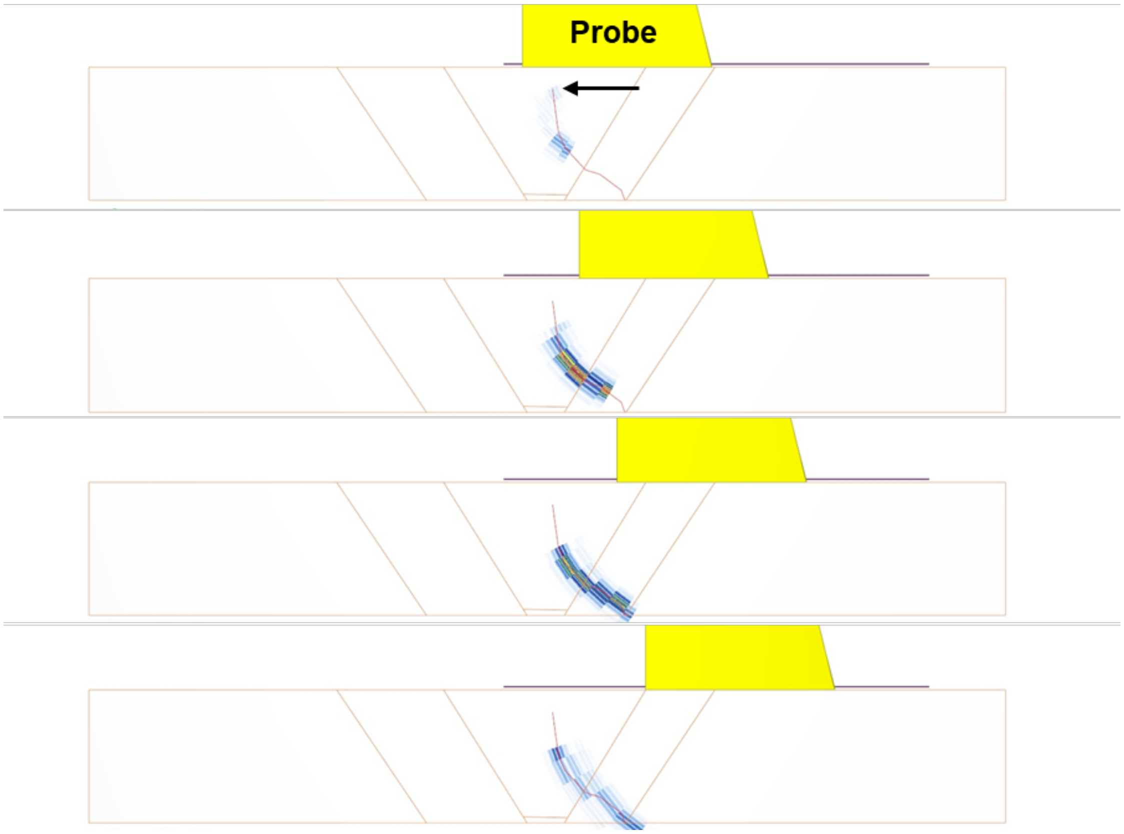

Figure 4.20 Simulation Results Showing the Flaw Response with a Phased-Array Probe

The probe position was incremented from above the flaw (top) to away from the flaw (bottom). The full through-wall depth of the flaw (indicated by the black arrow) was not detected.

Beam simulations can be used to illustrate why the tip of the flaw was not detected. First, simple ray-tracing shows that the highest beam angles are reflected away from the probe, even when the probe is directly over the flaw; see figure 4.21. There are no probe positions which cause direct reflections from the top portion of the flaw. Furthermore, the highest beam angles have relatively low intensities (see figure 4.22), a common issue in phased-array UT, so any direct echoes at high refraction angles would be relatively weak.

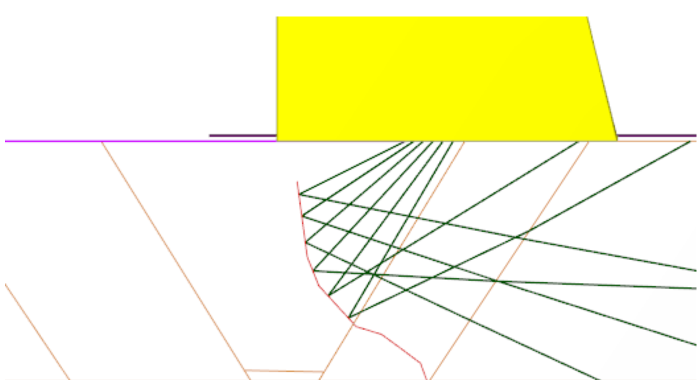

Figure 4.21 Ray-Tracing Diagram of the PA Focal Laws Incident on the Riverbend Flaw

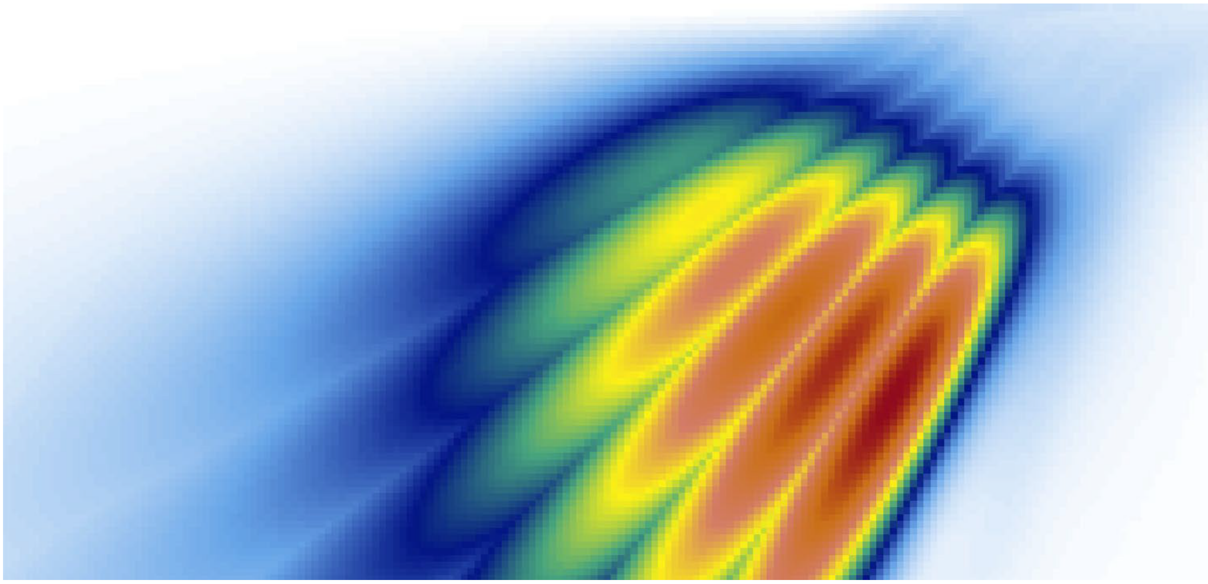

Figure 4.22 Beam Simulations Showing the Relative Intensity of the Different PA Focal Laws from 30° to 70°

This example illustrates how modeling and simulation can be used to predict echo responses from unusual crack geometries. Crack propagation can follow unpredictable paths. Although not every conceivable crack geometry can be modeled, parametric simulations can be used to rapidly explore a large range of scenarios. In this particular example, the simulations vindicated the inspectors' initial findings that the flaw was not as deep as destructive testing found it to be. Simulations also showed that detecting the depth of this flaw would be nearly impossible unless the true depth was known *a priori*.

4.7 Array Probe Design for Steam Generator Tube Inspection

Yoon et al. (2012) described an example of successfully using modeling and simulation to design a custom UT array probe for a specific inspection application. In their study, "experiments were performed by using ultrasonic testing instead of eddy current testing for the inspection of steam generator tubes to detect various kinds of flaws and to see if the detected flaws can be sized accurately." The most common flaws found in Korean nuclear power plant steam generator tubes are primary water stress corrosion cracking. The steam generator tubes are Framatome-type nuclear reactors of the type and geometry found at Uljin Nuclear Power Plant Units 1 and 2. The tubes have an outer diameter of 22.22 mm (0.875 in.) and a wall thickness of 1.27 mm (0.050 in.). Results of their experiments showed that UT was able to accurately size flaws in length and depth using the modeled probe design.

Modeling and simulation in CIVA were used to analyze beam propagation and sound field penetration to account for the tubing curvature while confining the probe to the small tube interior. The overall design comprised a normal-incidence probe to measure wall thickness and four 45° shear wave probes, two to inspect for axial flaws and two for circumferential flaws. Other design requirements included: a focal point at half of the through-wall depth to optimize flaw detection at both the inner and outer surfaces, high frequencies (15 MHz) to enhance detection of small cracks, and beam propagation characteristics optimized for the tubing curvature.

The modeling and simulation work allowed Yoon et al. to assure that the probe design met the inspection specifications. The simulation results allowed the researchers to visualize the sound field and predict the focal depth in the material. The results were then used to inform the probe design and construction. To test the probe, a steam generator tube mockup was designed with 15 flaws from 20% through-wall to 100% through-wall depth on the inner and outer surfaces oriented both axially and circumferentially. All of the flaws were detected.

This example illustrates that modeling and simulation can be successfully applied to the design phase of probe construction. By testing and iterating parameters *in silico*, a significant time and cost savings can be realized over empirical trial-and-error. To enhance the modeling approach, adding flaw-response simulations may have helped determine the minimum flaw length and through-wall depth that the probe would be expected to find. The probe design could then be altered, if necessary, to assure that the flaw detection requirements are met.

5.0 MODEL ASSESSMENT

Verification and validation are critical steps in assessing models and simulation outcomes. Verification is the process of determining that the model's computer code, mathematical approximations, and parameter inputs are correct. Validation is the process of determining the extent to which the simulation outcomes are predictive. In other words, verification asks if the model is correct, while validation asks if the simulation is correct.

There are four possible scenarios with verification and validation, as illustrated in figure 5.10:

- **Verified and valid** – the model is implemented correctly, and the results are predictive. This is the ideal scenario.
- **Verified and invalid** – the model is implemented correctly, but the results are not predictive. In this case, it is possible that the model is not complete. It may also be possible that the empirical results or other validation methods are wrong.
- **Unverified and Invalid** – the model is not implemented correctly, and the results are not predictive. In this case, the computer code, mathematical assumptions, and/or model inputs need to be revisited and carefully checked.
- **Unverified and valid** – the model is not implemented correctly, but the results are predictive. This is the same as getting the right answer for the wrong reasons. **This is the most dangerous scenario**, because the user can be fooled into believing that the model implementation is correct even though it is not and might proceed to draw erroneous conclusions from subsequent simulations.

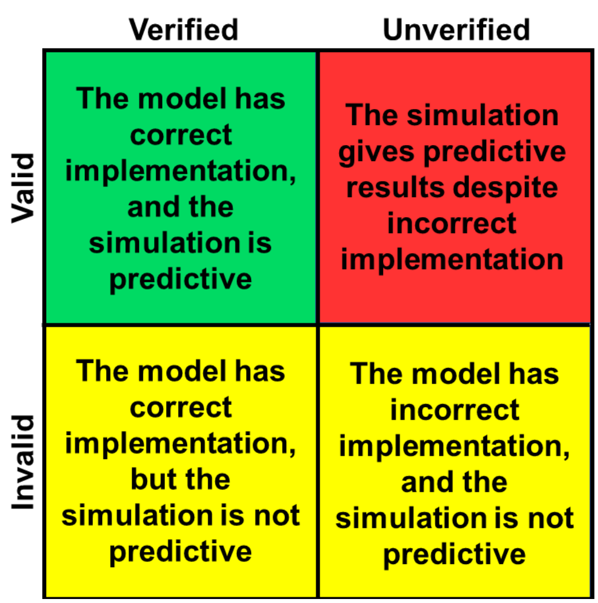

Figure 5.1 Verification and Validation Matrix

The green scenario indicates that it is okay to proceed with the modeling and simulation activities. The yellow scenarios indicate that pause is needed while more model validation and/or verification activities are done. The red scenario indicates danger, as an erroneous model is giving results that appear correct.

Verification requires carefully debugging code and iteratively determining the correctness of mathematical implementations. These steps are typically not possible for end users of commercial software, but problems with code can often be detected through simulation validation steps. If a software bug or problem is suspected, it is important for users to alert the vendor. Verification also requires rigorous measuring and vetting of input parameters. Therefore, both the software creators and the end users have verification responsibilities.

Validation is entirely the responsibility of the end user, who must determine if the model has produced simulated results that are predictive of the modeled scenario. There are many methods of validating simulations, as outlined in Metzger et al. (2014) and Sargent (2010). It is recommended to implement more than one validation method.

Table 5.2 Methods of Model Validation

Validation Method	Description
Compare the results of identical (or nearly identical) simulations performed using different modeling platforms.	Comparing results can be especially useful if 1) the models are fundamentally different, such as FEM versus ray-tracing, and 2) the results are compared to a simulation that has already been verified. For example, CIVA and OnScale use different mathematical approaches to modeling ultrasonic testing. If models are set up in each using identical input parameters, then the results can be compared to one another to determine which model is more predictive. If results are significantly different, then one (or both) of the models will require independent verification. Note that just because one model is more predictive in one scenario does not mean it will be more predictive in all scenarios. Each scenario is unique with respect to model inputs, and each scenario may require different algorithms or code within the model that may affect how predictive a simulation is. Thus, assumptions about model performance cannot be generalized.
Compare the results to empirical data or observations.	This is a critical step in determining if simulation results are predictive. If the simulation results agree with or predict observed data, then this is evidence of validation. As many comparisons as possible or feasible should be made to strengthen the validation. In addition, it is convenient to run simulations of scenarios that are easy to duplicate in the lab. For example, using mockups with side-drilled holes or other machined reflectors that can be well characterized and measured will make it easier to duplicate precise parameters in the model. In more complicated situations, such as with mockups where in situ grown cracks are used, destructive testing will be required to determine the true-state flaw parameters, such as through-wall depth and tilt.
Test the simulation under extreme conditions by using unlikely, but still possible, inputs.	Does pushing the limits of the model yield results that still make physical sense? At what point does the model "break" and no longer give realistic results? It is important to stay within the operational limits of the model.
Ask subject matter experts (SMEs) to gauge whether or not the simulation has	SMEs, such as a UT Level III, have developed experience and intuition about what to expect with ultrasonic testing, such as what realistic flaw responses, scattering, and attenuation look

Validation Method	Description
produced reasonable, logical, and realistic results.	like. They can also determine if scan parameters are realistic or reasonable. One test is to ask if the SME is able to tell the difference between simulation and reality.
Use parametric studies and sensitivity analyses to determine how the simulation outputs are affected by realistic variations in input parameters.	The simulation results should reflect how a real system would behave if the same parameter was varied. Sensitive parameters—those that have stronger effects on the simulation outcomes—should be as accurate as possible in the model. Multiple parameters should be varied at the same time because they often interact with each other in unpredictable ways. The Metamodel function in CIVA was designed for such tests and streamlines the setup and analysis.

In some cases, it is impossible to directly validate a simulation due to lack of data or experience. In such situations, the following three conditions should be met:

1. The model has been verified (a user of commercial software may only be able to verify the model inputs).
2. An array of similar simulations have been validated.
3. The unvalidated simulation is within the envelope of the validated simulations.

For example, consider the following hypothetical scenario. A flaw-response simulation is run to test detectability of a 15 mm deep flaw in carbon steel with a coverage limitation such that only part of the flaw is insonified. There are no empirical data that can be used to validate results on a flaw of this depth. Condition 1 can be met by using a commercial software package that has been well verified for these types of simulations, such as CIVA, and by carefully measuring all of the model inputs, such as the material sound speed, the wedge dimensions, the probe center frequency, etc. Condition 2 can be met by simulating flaw responses using a range of flaw sizes and orientations that can be directly validated with empirical data, for example, by using a mockup that contains machined reflectors of 5 mm, 10 mm, and 20 mm through-wall depths. Finally, condition 3 can be met because the 15 mm flaw in the test situation is within the envelope (size range) of the flaws that have been validated. Although the test simulation was not directly validated, confidence in results can be gained from knowing that the model is verified and that comparable simulations have been validated. Then simple iterations on the model can be run, such as changing the probe range of motion to simulate the limited coverage condition.

5.1 User Considerations

Table 3 lists several questions that the user should be able to answer during the validation process:

Table 5.3 User Considerations

User's Question	Description
Do the results make sense?	If something seems "off," it probably is. All aspects of the model setup should be reconfirmed. If results still do not seem correct, engage with the software technical support for confirmation.
Were the selected options correct? Can the selections be justified?	Software such as CIVA has many user-selectable options that can have strong effects on results. Selected options should be justifiable using experience, expertise, published literature, technical support, or the software user's manual.
Were the model's limitations or assumptions respected?	The software platform is not likely valid for all possible scenarios that the user can execute. The software will probably not give a warning when the model assumptions are violated, so user vigilance is required. For example, it can be easy to violate the high-frequency approximation[5] in CIVA by including structures or flaws that are too small with respect to the probe frequency.
Are the results in line with expectations?	Just because results are unexpected does not mean that they are wrong. However, unexpected results do deserve additional scrutiny. Refer to previous results, SMEs, published literature, and/or theoretical calculations.
Do the results converge? Or do similar simulations produce varying results?	Multiple simulations should be run, and appropriate statistical tests should be used to determine if results are converging on an answer or if they are random.
What are potential sources of uncertainty or error? Can they be better understood with a parametric study?	Try to determine what parameters are introducing the most uncertainty in the results. In presenting results, it is important to explain the sources of uncertainty and what actions were taken to mitigate the uncertainty. It is also important to understand how the uncertainty affects interpretation of the results.
With parametric studies, are there any outliers or results that differ significantly from the others?	Appropriate statistical tests should be used to determine what results are outliers. It must be determined whether outlying results can be trusted or if there is a sound scientific reason for discarding them. Outliers due to errors in the model can be ignored (such as if a parameter was entered incorrectly), but all other outliers should be reported along with any justification for discarding them from the analysis.
Is the variability observed in parametric studies consistent with variability observed empirically?	If empirical data are available, compare the variability in measured results to the variability in simulated results. Ideally, predictive simulations should have about the same variability as empirical data.

5.2 Reviewer Considerations

Simulation results are often used as a basis or justification for decision making. But how does the person reviewing the results, such as a regulator reviewing a relief request, know whether or not to trust the simulation results? It is critical for the basis or justification to include details about

[5] CIVA uses a high-frequency approximation that essentially requires specimen features, such as flaws or surface geometries, be larger than the simulated wavelength.

the model implementation and the validation procedure. The information provided in Table 4 should allow the reviewer to answer important questions.

Table 5.4 Reviewer Considerations

Reviewer's Question	Description
Was the model implemented correctly?	This is an overarching question that will require the reviewer to have knowledge of the software tool used. The reviewer should consider all of the information provided to determine if there were any errors in using the model. The help of an SME may be needed, particularly one with expertise in the software.
What model options were selected and why?	Modeling software may include several user-selectable options, and the reviewer should consider the reasons why the options were selected. With some options there are no right or wrong choices, but it is helpful to know why the choices were made. For example, in CIVA, users have the option of selecting 2D or 3D simulations, of using a plane wave approximation versus a full incident beam, or of including attenuation.
What model parameters were used and why?	Knowing the parameters used is an important step in validating a model and assessing whether the simulation results are reasonable. Model parameters are composed of the user inputs, such as the probe and wedge information, the specimen material properties, and the flaw parameters. Justifications should be provided with any inputs that were approximated or guessed.
How many simulations were run? Was it enough to provide significant results?	The reviewer should gauge if enough simulations were run using a sufficient range of input parameters to fully explore the scope of possible outcomes. A justification (preferably based on a statistical design of experiments or power analysis) should be given to support the number of simulations.
What statistical or mathematical methods were used to analyze the results?	A description of the analysis techniques used should be provided. The reviewer should determine if the appropriate techniques were used. The reviewer should also consider if alternative techniques could be used on the same data to draw different conclusions. In other words, were the analysis methods cherry-picked to support the goals of the work?
Do the results make sense?	This requires some experience on the part of the reviewer. The reviewer should engage with SMEs as necessary to gauge whether the model and parameters used should logically lead to the results shown.
Do the results support the conclusions?	The simulations were run in order to provide evidence or a technical justification for a position or conclusion. It is therefore important to make sure that the correct conclusions were drawn from the results based on the evidence shown. If results are open to multiple interpretations, then additional simulations or analysis may be needed. SMEs may be needed to help answer this question.

6.0 KEY TAKEAWAYS AND GUIDANCE

This section includes key takeaways, specific guidance, and outstanding questions for several of the figure 1.1 roadmap steps. Most of the information in this section was developed using CIVA, but generalizations can be made for other modeling platforms. The lists are not comprehensive but include information and scenarios that were explored in the previous PNNL modeling and simulation reports.

6.1 CASS

6.1.1 Key Takeaways

- Simulations using realistic coarse-grained equiaxed and columnar CASS models based on laboratory specimens are feasible with currently available software tools (Jacob et al. 2022a; Jacob et al. 2022b; Jacob et al. 2020).
- CASS microstructure is random with respect to grain orientation, grain shape, and grain size. The randomness cannot be fully captured by a single model. In other words, no single CASS model will faithfully represent an actual CASS specimen (Jacob et al. 2022a).
- Beam simulations in CIVA using 3D Voronoi regions as surrogates for 2D equiaxed or columnar CASS grains result in more realistic beam maps, as measured by the crossing ratio (Jacob et al. 2022b).
- CASS models using Voronoi regions are much easier to produce than realistic specimen-based models. Voronoi regions produced in CIVA are inherently 3D, load rapidly, and give realistic results (Jacob et al. 2022b; Jacob et al. 2020).
- Models of mixed-grain structures or of a wide variety of grain sizes can be created outside CIVA and imported, but many advantages of using the built-in Voronoi function are lost with this approach (Jacob et al. 2022b; Jacob et al. 2020).
- Flaw-response simulations demonstrate variability in flaw echo amplitudes with different flaw positions in a CASS specimen model (Jacob et al. 2022b).
- DMW specimen models can be created by combining a weld region, a CASS region, and a buttering region. For example, for optimal flexibility and time savings, the user can maintain a library of different regions and combine them as needed in a mix-and-match fashion (Jacob et al. 2022a; Jacob et al. 2022b).

6.1.2 Guidance

- If using CIVA, take advantage of the built-in Voronoi feature when possible as a 3D model of CASS. Note that the current version of CIVA (CIVA 2021) only allows using Voronoi regions in planar or cylindrical specimen geometries. This excludes any weld geometries or custom geometries.
- The number of grains or regions, whether Voronoi or otherwise, will have a significant impact on CIVA's computation time. For a given grain size, minimize the number of grains by minimizing the specimen volume.
- Microstructural randomness will require multiple models and simulations in order to capture an envelope of simulated responses. For example, simply resetting the Voronoi regions in CIVA can change the echo response of a flaw by over 15 Db (Jacob et al. 2022a). It is

important to establish an envelope of simulated and empirical signal responses. Multiple empirical echo responses can be obtained by scanning the corner of a specimen and observing how the signal intensity varies with position, as demonstrated in section 8 of Jacob et al. (2019).

- The optimal value of grain-to-grain velocity variation ΔV in CIVA Voronoi models should be based on available empirical data and trial-and-error in simulations (i.e., parametric studies). A method of determining ΔV is shown in section 7.2.5 of Jacob et al. (2020). For example, PNNL determined in one scenario that ΔV of 6–8% in coarse-grained simulated beam maps provided results comparable to empirical sound field maps, but in other scenarios the value was lower.
- If using CIVA, the accuracy factor should be set appropriately. A parametric study should be used to determine when results converge to an asymptotic value; this can be done by using simplified simulation scenarios, when possible, to reduce simulation time. The lowest accuracy factor that produces convergent results should be used in order to minimize computation time. Section 7.2.4 of Jacob et al. (2020) shows a method of determining the accuracy factor for two CASS scenarios. For FEM-based platforms such as OnScale, the mesh or grid size should be at least 1/15 of a wavelength and small enough to define any grain boundaries to the desired resolution.
- If the type of grain structure to be modeled is unknown (e.g., coarse-grained equiaxed, columnar, banded, etc.), then determine if the granular structure will have a significant impact on simulation results. This can be done by running test simulations with different granular structures and comparing results to available empirical findings, such as the sound field maps shown in Crawford et al. (2014). If empirical data are not available, then completing multiple simulations from a variety of grain models to establish best-case, worst-case, and nominal scenarios will provide a suitable range of results.
- To minimize the time required to complete coarse-grained simulations, start with the lowest level of complexity that the scenario can tolerate and gradually add complexity depending on what the situation warrants until desired results are achieved. Among important items to consider are:
  - beam simulation versus flaw-response simulations,
  - the strength and type of attenuation,
  - the type of material symmetry and the stiffness matrix elements,
  - the number of specimen bounces, whether to include interface interactions,
  - whether to include (and the number of) mode conversions,
  - the size of the computation zone, the number of dimensions to scan (i.e., a 1D A-scan, a 2D B-scan, or a 3D C-scan),
  - and whether to include noise.
- It is critical to compare simulation results to empirical measurements whenever possible. Empirical measurements should be used to adjust model parameters in a careful and informed manner and to assess simulation accuracy. Ideally, these measurements are made in-house, but data found in available reports or papers may also prove useful. Without “ground truth” data, there is no way of evaluating the realism or accuracy of the simulations.

6.1.3 Outstanding Questions

- Multiple simulations should be performed with a range of models in order to determine the bounds of results. How many different CASS or DMW models should be included in a given set of simulations to assure accurate results?
  – Without knowledge of the grain structure of the target specimen, multiple models incorporating a range of microstructure types and sizes should be used. There are five primary types of CASS grain structures: fine-grained equiaxed, coarse-grained equiaxed, fine-grained columnar, coarse-grained columnar, and mixed/banded. Within each of these categories is a continuum of granular geometries, orientations, and sizes. PNNL has only tested coarse-grained equiaxed and fine-grained columnar "realistic" models with a limited set of Euler angles. PNNL also tested fine-grained equiaxed and coarse-grained columnar with CIVA Voronoi regions. The number of necessary models will depend on how well the results converge and the quality of the empirical data used for verification.
- How realistic do the CASS grain structures need to be?
  – Randomness in actual CASS microstructures throughout a given specimen limits the usefulness of very realistic models. The model will only be representative of the specific CASS grains that were modeled and therefore the specific location in the specimen on which the model was based. For simulations in CIVA, 3D Voronoi regions have been shown to be adequate surrogates for realistic CASS grains. The number of scattering interfaces, the sizes of the grains, and the basic grain geometry (i.e., columnar versus equiaxed) are all more important than the specific grain orientations, especially when the number of scattering interfaces is large.

6.2 Weld Models

6.2.1 Key Takeaways

- Beam simulations were performed in OnScale and CIVA using the same austenitic weld model based on electron backscatter diffraction (EBSD) data. The scatter observed in the empirical sound field maps was more similar to the OnScale results than to the CIVA results (Jacob et al. 2022a).
- The weld model used in CIVA predicts the empirically-observed funnel effect, in which there is a stronger sound field, and therefore stronger echo response, at the near-side base of the weld (Jacob et al. 2022b). Simulated results tend to overemphasize the effect, more so at 60° refraction angle than at 45°. Consequently, near-side flaws may be more difficult to detect than simulations predict.
- The weld model used in CIVA predicts the observed shadow effect, where beam scatter from the weld results in a weaker sound field on the far side of the weld (Jacob et al. 2022b). Simulated results tend to overemphasize the effect, meaning that far-side flaws may be easier to detect than simulations predict.
- The specific Euler angles of the weld models affect flaw detectability, although not dramatically in most cases tested. Results of simulations using models of materials with complex microstructure (Jacob et al. 2022b; Jacob et al. 2020), suggest that the number of interfaces and grain sizes have more impact than the specific Euler angle assignments. The ideal grain size is probably on the order of half a wavelength in CIVA. Grains that are too large will not give realistic scatter, while grains that are too small will violate the CIVA high-frequency model assumptions. FEM modeling in OnScale can be used with arbitrarily small

grains, but small grains (especially oddly shaped grains) will require a finer mesh and longer simulation times.

- Accuracy of flaw-response simulations using realistic flaw geometries obtained through destructive testing did not benefit from using a complex austenitic weld model as compared to using an isotropic specimen model or a planar flaw (Jacob et al. 2022a). As with CASS, randomness in weld microstructure cannot be adequately captured, so weld models will always be approximate at best.

6.2.2 Guidance

- It is not critical to exactly model the weld grain microstructure and Euler angles, as long as enough grains and interfaces are used to provide an appropriate degree of scatter. Empirical data should be used to guide what is deemed "appropriate" in the context of a given weld model.
- The grain microstructure of the weld to be inspected is unknown, so multiple weld models should be used to cover a range of scenarios. No single simulation result should be considered representative.
- The funnel effect and shadow effect have been observed empirically and confirmed with simulations. Such confirmation supports the usefulness of simulations in predicting coverage and flaw responses in austenitic weld scenarios.
- Different probes and refraction angles should be simulated separately. Do not assume that one set of simulation results will be representative of all probes or angles.
- A variety of austenitic weld models can be created by starting with a basic weld model microstructure, duplicating it for the number of desired weld models, then populating each model with random Euler angle assignments. This could be a rapid and efficient method of developing a weld model library. If desired, individual models could be tested against empirical results to characterize them and allow models that cause outlier results to be discarded.

6.2.3 Outstanding Questions

- Multiple simulations should be performed with a range of model inputs in order to determine the bounds of results. How many different weld models should be included in a given set of simulations to assure accurate results?
  - The answer hinges on more statistical strength than the four weld models and one empirical dataset used in Jacob et al. (2022b) allow. However, based on the data available, three or four weld models appear to provide a good prediction of empirical results. More would probably be better.
- How realistic do the weld models need to be? Should the different weld models be based on actual EBSD data, or can they have arbitrary grain geometries and random Euler angle assignments?
  - PNNL's work showed no compelling benefit to using an EBSD-based model over a random weld model. In some cases, one or more of the random models gave results that agreed better with experiment, and in other cases the EBSD model did. Due to inherent randomness in any specimen's weld microstructure, the number of grain boundaries and the grain sizes is likely more important than the specific grain shapes and property definitions. (This also appears to hold true for CASS simulations.)

- Sets of simulations on complex weld geometries can take a long time. Should a different set of simulations be performed for each probe?
  - Each probe should be simulated separately, preferably starting with a beam simulation through isotropic material to characterize probe performance. However, similar probes (similar aperture, frequency, and inspection angle) were shown to produce similar results in Jacob et al. (2020). If time is limited, then it may be possible to extrapolate simulation results across probes. This is not recommended and should only be done with strong justification.

6.3 Noise

6.3.1 Key Takeaways

- Simulating noise in CIVA is straightforward, but it can require considerable trial-and-error to achieve a noise field that matches empirical results (Jacob et al. 2022b).
- When compared to empirical scans of coarse-grained materials, structural noise simulated in OnScale appeared to be more realistic than the noise simulated in CIVA (Jacob et al. 2022a).
- Noise can be simulated in CIVA flaw-response simulations but is not an option in beam simulations (Jacob et al. 2022b).
- Adding noise to a CIVA model can increase computation times dramatically (Jacob et al. 2022b).
- Adding noise to an OnScale or a finite element model requires embedding noise reflectors within the specimen model (Jacob et al. 2022a). Computation times are not increased substantially just by adding noise reflectors, but the mesh density should be adjusted so that each noise reflector is adequately resolved. Increasing the mesh density to resolve small reflectors will increase computation time.
- In CIVA, structural noise reflectors are always the same size and shape. In OnScale, the properties of the noise reflectors, including the size, spatial density, spatial distribution, and composition, are individually tailored by the user (Jacob et al. 2022a).
- Adding noise to a CIVA model does not diminish the flaw-response amplitude since the noise and signal are computed independently (Jacob et al. 2022b). Thus, when simulating noise in CIVA, the signal-to-noise ratio is affected only by a change in noise and not by a change of signal.
- Adding noise to an OnScale model affects the flaw-response amplitude, because less sound energy is able to reach the flaw (Jacob et al. 2022a). This is consistent with what is expected empirically.
- CIVA noise reflectors are randomly redistributed for each simulation. Rerunning a simulation with identical parameters gives a different noise pattern (Jacob et al. 2022b). A controlled test of flaw response with variable flaw parameters but a constant noise distribution is not possible in CIVA. This can be a problem if, for example, a noise reflector happens to lie on the flaw in some simulations but not in others because the noise added to the flaw response makes the flaw response appear stronger. Noise reflectors in OnScale can be distributed however the user chooses since they are not automatically generated by the software (Jacob et al. 2022a).

6.3.2 Guidance

- CIVA has two noise parameters, ρ (reflector density) and A (reflector strength). The noise amplitude decreases when ρ decreases, since fewer reflectors are available. This can be compensated for by increasing A, although the amplitude increase is not proportional to the reflector density decrease. In other words, decreasing ρ by a factor of 10 does not result in a tenfold noise amplitude decrease. For intermediate values of ρ, a tenfold decrease in ρ can be compensated for by about a threefold increase in A (Jacob et al. 2022b). This relationship breaks down for low values of ρ and may vary for different simulation scenarios, so it should only be taken as a rule of thumb.
- Simulating noise in OnScale requires changing the specimen model by adding noise reflectors. This can be done by adding a random distribution of pores. The pore reflectivity can be adjusted by changing the pore size, spatial density, and composition (Jacob et al. 2022a). The MATLAB toolbox can be used to generate the noise reflectors. It is important to remember to adjust the mesh density so that the pores are adequately defined.
- When using CIVA's structural noise option, the noise pattern appears to remain essentially constant beyond a certain ρ threshold. Increasing ρ beyond this threshold appears to have no practical advantage but dramatically increases the simulation time. Based on the preliminary studies, the threshold is in the range of ρ ≈ 1 to 10 reflectors/mm^3 and is frequency dependent (Jacob et al. 2022b). Higher frequencies result in smaller noise echoes, so a higher density of noise reflectors may be needed.
- The CIVA parameter ρ need not be restricted to integers or to numbers greater than 1. The default value is ρ = 1 reflectors/mm^3, but lower values can be used. The smallest ρ tested was 0.001 reflectors/mm^3 (Jacob et al. 2022b).
- CIVA computation time is a very strong function of ρ, so minimizing ρ is advantageous. In PNNL's tests, simulation times were increased by well over a factor of 10,000 from a simulation with no noise to one with ρ = 100 reflector/mm^3 (Jacob et al. 2022b). Low reflector densities, such as ρ ≈ 0.001 to 0.01 reflector/mm^3, have little impact on simulation time in the scenarios that PNNL tested. Again, the appropriate value of ρ should be determined iteratively.
- A multifaceted flaw placed along the surface of the specimen can effectively simulate surface noise by providing echo responses that are similar in appearance to empirical surface noise (Jacob et al. 2022b). The geometry and shape of the surface flaw should be iterated until the desired noise signature is achieved.
- CIVA noise reflectors are randomly placed throughout the specimen. Occasionally, a reflector will be positioned such that it will generate a very strong and anomalous-looking response. It may be best to rerun such instances. Also, if a noise reflector is coincident with a flaw, then the flaw signal will appear to increase. The user should be careful not to misinterpret results with regard to flaw detectability.
- Flaw-response simulations in CASS materials can be simulated using CIVA Voronoi regions as models for grains, but structural noise cannot be added to simulations with Voronoi regions. Combining noise simulations with flaw-response simulations through simple image addition appears to result in a good representation of a noisy simulation (Jacob et al. 2022b). Such addition can be done in software platforms such as Python and MATLAB. More sophisticated methods of combining images may be useful, for example, in generating virtual flaws for data analysis training, but that is beyond the scope of this work.

6.3.3 Outstanding Questions

- There are multiple options for adding noise in CIVA. Should structural, polycrystalline, or surface noise be used in a CIVA simulation?
  - In general, granular noise or noise from inclusions should be simulated using the structural noise option. Polycrystalline noise may be appropriate for certain applications that have not been investigated by PNNL. The surface noise approach can be used in special cases where surface clutter dominates.
- What method should be used to simulate surface echoes caused by geometric features, such as weld root and counterbore?
  - The noise approaches discussed here should not be used to simulate echoes from ID surface geometry. The best approach is to include all geometrical features directly into the specimen model.
- This discussion focuses primarily on structural noise. What method should be used to simulate electronics noise?
  - Noise from the electronics cannot be avoided empirically. Well-calibrated commercial systems typically have very low noise backgrounds that have a smooth appearance, in dramatic contrast to CASS structural noise, so simulating that background noise is probably not necessary. If simulating electronics noise is needed, then using a high spatial density of noise reflectors and a low reflectivity may provide the best results, but this was not tested by PNNL. Note, however, that high reflector densities in CIVA will increase simulation times dramatically, with completion times estimated to be as high as months or years. Other sources of spurious noise should be handled on a case-by-case basis.

6.4 Attenuation

6.4.1 Key Takeaways

- Attenuation is straightforward to simulate and adds little to computation time while potentially adding realism to models with high frequencies or long sound paths (Jacob et al. 2022a; Jacob et al. 2022b).
- For CIVA Voronoi models of coarse-grained specimens, material attenuation is not an available parameter. However, the grain size and sound field scattering parameters can be adjusted to simulate attenuation (Jacob et al. 2022b).

6.4.2 Guidance

- Attenuation is a strong function of frequency. The correct attenuation function and parameter values should be measured or obtained from the literature.
- Simulating attenuation is probably not necessary for most isotropic steel piping models at frequencies $\lesssim$5 MHz, but this should be evaluated on a case-by-case basis.
- Calibration signals should always be used when comparing simulated attenuation so that a baseline signal can be established.
- Attenuation parameters must be added separately to each region of a multi-region specimen model.

- For CIVA Voronoi models, attenuation can be adjusted by iterating the grain size and ΔV parameters. It will take some trial-and-error to match attenuation observed empirically.

6.4.3 Outstanding Questions

- When should attenuation be added to a model?
  - Simulating attenuation may be valuable when the accuracy of a flaw-response amplitude is expected to be affected by beam attenuation. This may be especially useful in granular materials like CASS, in highly-attenuative materials like many plastics or rubber, or when the beam path is long, as with multiple surface reflections. Accurately simulating attenuation requires well-characterized material attenuation properties and a well-calibrated flaw response, such as from a side-drilled hole. Material properties may be found in the literature or can be measured directly. Adding attenuation is not computationally expensive, but simulating attenuation incorrectly can give misleading results.
- Should attenuation in the wedge or water path be simulated?
  - Again, this depends on parameters such as the probe frequency, wedge material, water path length, etc. Empirical data should be used to guide whether attenuation is needed in a simulation.
- How is the frequency response affected by attenuation?
  - As with empirical scans, attenuation is a function of frequency. Probes with large bandwidths will experience more attenuation at the upper frequencies of the bandwidth. It is important to consider the bandwidth of the probe, the frequency dependence of the attenuation, and the observed effects in empirical scans.

6.5 Quantitative Metrics

6.5.1 Key Takeaways

- Quantitative metrics are useful for making direct comparisons between different simulation results or between simulated and empirical results (Dib et al. 2017; Dib et al. 2018; Jacob et al. 2020).
- Ideally, comparisons should be made by using a consistent calibration signal, such as the echo response from a side-drilled hole (Dib et al. 2018). However, such calibration signals are not always available, especially in empirical scans. Also, calibration signals cannot be used to compare sound beam scatter patterns.
- Different metrics can be developed for different purposes. There is no single “correct” or standard metric, and some situations may require multiple metrics (Dib et al. 2017; Dib et al. 2018; Jacob et al. 2022a; Jacob et al. 2020).

6.5.2 Guidance

- Before trying to develop or implement a metric, it is important to determine the quantity or aspect that is being measured. For example, if comparing signal responses with different simulation settings, the responses can be measured by the height of a peak or by integrating the peak. It may be unclear which measurement makes most sense until after the data are collected and different metrics are tested. As another example, similarity between images can be measured by using a correlation coefficient, mean square error, ora structural similarity index. It may be that measuring multiple metrics will give the most insight.

- It is important to avoid bias in analyses and ensure that the metrics can be applied objectively.
- It is important to understand when similarities or differences in measured quantities are statistically significant. Acquiring multiple measurement is critical for calculating comparative parameters such as correlation coefficients and p-values[6].

6.5.3 Outstanding Questions

- When do quantitative metrics need to be used?
  - Metrics should be used when a verifiable and objective claim is being made about an observation or result. Judgment or opinion should not be relied on except in the most obvious of cases.
- What metrics should be used?
  - Choosing the appropriate metrics is often a function of judgment, experience, and trial-and-error. Most of the time, well-established metrics can be used, such as echodynamics, signal-to-noise ratios, means, medians, and standard deviations. In more complicated circumstances, metrics may need to be developed or borrowed from other disciplines. Sometimes, multiple metrics are needed because a single metric cannot capture the complexity of a situation.
- How many measurements are needed for metrics to be meaningful?
  - It is useful to engage a statistician in the early stages of experimental planning to determine what metrics will be useful and how many measurements will be needed for the metrics to be meaningful. With enough information, a statistician can run a statistical power analysis to guide the number and type of data needed.

6.6 Probe/Wedge Properties

6.6.1 Key Takeaways

- Probe and wedge properties can have a significant impact on simulation outcomes (Dib et al. 2017).
- Probes that are nominally identical may have different performance characteristics (Dib et al. 2018). For example, two probes that are the same model number may have different near-field/far-field dimensions, effective apertures, beam spread/divergence angle, bandwidths, or peak and nominal center frequencies. The differences are typically small but can have a significant impact on simulation outcomes.
- Simulating phased-array probes is straightforward in UV and CIVA. After defining the probe characteristics, the user can define a focal depth, or range of focal depths, and UV or CIVA will calculate the delay laws (Dib et al. 2018). In OnScale, a 3D, multi-element probe model must be created, and the phased-array laws must be calculated externally and imported into OnScale along with the probe model.

[6] The p-value is a statistical measure of significance used to determine the probability that one set of data differs from another set of data.

6.6.2 Guidance

- When modeling a specific probe, it is important to measure all the relevant parameters, including the wedge dimensions and angle, the speed of sound in the wedge material, the probe aperture, the bandwidth, the center frequency, and the shape of the excitation impulse. Other parameters may be needed depending on the requirements of the modeling software.
- PA delay laws in CIVA should be calculated with the probe on an isotropic material model, otherwise a set of adapted delay laws[7] will be calculated that may be valid for only a specific location on the specimen. Once the delay laws are calculated, they can be saved and reloaded as needed. When loading delay laws from a file, do not recalculate the delay laws even if CIVA gives a warning that they need to be calculated—CIVA will use the delay laws as loaded from the file.
- OnScale requires careful and detailed definitions of probe properties, including the piezoelectric crystal type. The user must develop the probe and wedge independently, and an appropriate mesh density should be used to avoid stair-step patterns in the angled wedge surface (Jacob et al. 2022a). The boundary conditions applied to the internal surfaces of the wedge should be set to *absorbing* to avoid having spurious sound reflect within the wedge before entering the simulation volume.

6.6.3 Outstanding Questions

- What can be done if only the *nominal* probe or wedge parameters are known?
  - The impact of using nominal values can be tested by using metamodels in CIVA or by conducting a parametric study. Once the expected variability caused by a given parameter is understood, efforts can be made to measure it or account for it in the simulations. For example, consider a hypothetical scenario where a user found that there is some uncertainty of the precise wedge angle, wedge height, and wedge curvature due to wear. Using a metamodel, the user determined that small variations in the wedge angle have a large impact on the echo response, but the other two parameters have minimal impact. Based on these results, action can be taken to measure the actual wedge angle more frequently and more precisely to assure that it remains within tolerance.

6.7 <u>Beam Simulations</u>

6.7.1 Key Takeaways

- Beam simulations are useful for visualizing how the predicted sound field propagates through a material. The sound path, beam spread, sound intensity, and volumetric coverage can be assessed (Dib et al. 2018; Jacob et al. 2022a; Jacob et al. 2022b; Jacob et al. 2020).
- Beam simulations can be used to help design probes that meet certain requirements (Dib et al. 2018).

[7] Adapted delay laws are calculated to provide the desired refraction angle in the presence of material anisotropy. For example, if the model material deflects the sound beam at an internal interface, adapted delay laws will account for the deflection. However, in real world scenarios, the material properties are unknown to the delay law calculator and adapted delay laws are not used. The delay law calculator assumes that the material is isotropic.

- It is not recommended to use beam simulations to predict flaw-response amplitudes or the ability to detect flaws. While beam simulations can predict how well a region is insonified, they are not a surrogate for flaw-response simulations (Dib et al. 2018; Jacob et al. 2020).
- Beam models through non-isotropic materials, such as austenitic weld models or CASS models, can be illustrative of scattering effects and attenuation (Jacob et al. 2022a; Jacob et al. 2022b; Jacob et al. 2020).

6.7.2 Guidance

- When setting up a flaw-response simulation, it is useful to first simulate the beam to assure that the expected sound field is produced. This is particularly important when modeling a new probe or specimen.
- After performing a beam simulation in CIVA, a flaw-response simulation can easily be set up using identical probe and material parameters. With the beam model open, navigate to the dashboard and select "Inspection Simulation." A dialog box will ask for confirmation to use the current settings.
- Beam simulations cannot be run with flaws in CIVA. If it is desired to visualize the sound field incident on a flaw, the flaw must be drawn as part of the specimen. The 2D or 3D CAD editor in CIVA can be used to create custom specimens.
- It is necessary to pay careful attention to boundary conditions when simulating sound fields in OnScale. Oblique reflections and absorbing boundary conditions can have unanticipated effects on the simulation results. When simulating the beam at a specific location such as a specimen surface, it is useful to expand the size of the specimen by at least a wavelength to eliminate boundary effects (Jacob et al. 2022a). Expanding the specimen size prevents boundary artifacts by effectively giving the sound energy room to propagate out of the region of interest.

6.7.3 Outstanding Questions

- What do the beam simulations actually show? For example, do they show acoustic pressure, particle velocity, particle displacement?
  - Beam simulations can show a variety of calculated results, depending on the options chosen. For example, the CIVA default is to display the displacement magnitude, but components of the displacement or velocity, in addition to other options, are available. It is important to keep this in mind when looking at results across platforms so that an apples-to-apples comparison can be made.
- Can beam simulations be used to predict whether full coverage is obtained in a Section XI inspection?
  - Beam simulations are expected to be a useful tool in predicting beam coverage in an examination volume; however, this has not yet been validated. Like any other modeling scenario, multiple simulations that cover the range of input parameter variability, including material microstructure, should be explored. Section 3.0 of this report gives a hypothetical example of using beam simulations to predict coverage.

6.8 Flaw-Response Simulations

6.8.1 Key Takeaways

- Flaw-response simulations are useful for predicting flaw signals. They may be especially useful in complicated or unusual geometries, when testing probe parameters, or when determining scan parameters (Dib et al. 2018; Jacob et al. 2022a; Jacob et al. 2022b).
- Flaw-response simulations in materials with random grain sizes or distributions, such as coarse-grained CASS, may not accurately reflect empirical results in comparable materials. The random effects of the material microstructure on the sound field will often give results that vary from empirical data (Jacob et al. 2022a).

6.8.2 Guidance

- In CIVA, flaw-response simulations with complex grain structures, such as CASS or austenitic welds, may need to be analyzed outside of CIVA so that straight-line beam paths are used.
- To avoid violating the high-frequency approximation used in CIVA, flaw dimensions should be approximately one wavelength or greater. A parametric study should be performed with flaw size or probe frequency as a parameter to see where simulation accuracy begins to diminish.
- In order to assure proper sound field properties and coverage, a beam simulation should be performed prior to flaw-response simulations, particularly when modeling a new specimen or probe.

6.8.3 Outstanding Questions

- Many mockups do not have reflectors that are appropriate for calibration signals, such as a side-drilled hole. How can the results of a flaw-response simulation be quantitatively analyzed in the absence of a calibration signal?
  - In the absence of a well-characterized reflector or end-of-block corner response, other parameters may be used to quantify flaw-response results. One option is to measure the ratio of the corner echo amplitude to the tip echo amplitude in the empirical data and the simulated data. This will provide a relative echo strength of a tip signal. Another option is to compare multiple flaw responses to look for consistency between empirical and simulated results.
- How are simulated flaw responses affected by the specimen geometry and microstructure?
  - The modeled microstructure can have a large impact on the simulated flaw response, so it is important to perform enough simulations with different microstructures to cover a range of responses and define an appropriate response envelope. Changes to a CASS microstructure or the position of a flaw with respect to the weld centerline can have significant effects. Simulated noise can also impact the flaw response. Specimen geometry should be included in the model when possible to account for additional echoes or reflections. The only way to answer this question for certain is to perform testing with different model scenarios.

7.0 SUMMARY

Over the past several years, PNNL has researched the effectiveness and limitations of modeling and simulation of ultrasonic inspections. PNNL evaluated three different modeling and simulation software platforms. The roadmap discussed in section 1.2 summarizes all the topics that were covered, including:

- Developing quantitative metrics to compare simulated and empirical data,
- Understanding the sources and propagation of simulation uncertainties,
- Understanding the effects of model parameter variability on simulation outcomes,
- Determining the relationship between beam simulations and flaw-response simulations,
- Exploring the effects of different weld models on simulated flaw detectability,
- Exploring the ability to accurately simulate beams and flaw responses in coarse-grain microstructure and in dissimilar metal welds,
- Demonstrating the modeling software's capability to simulate noise and attenuation in different scenarios,
- Establishing the accuracy and predictiveness of flaw-response simulations through laboratory scan results and destructive testing.

The culmination of the modeling and simulation effort is this NUREG/CR report that summarizes the challenges faced by ultrasonic modeling (section 3.0) and gives several real-world examples of simulations used in the nuclear industry (section 4.0). Key challenges include:

- Knowing the input parameters and understanding how to deal with uncertainty of parameters that cannot be measured (such as microstructure) or accounted for in the model (such as human factors),
- Understanding sources of uncertainty, whether from approximations made in the mathematical models or from measurements of input parameters,
- Accurately assessing the simulation results and using empirical data for validation,
- Determining the predictability of the results so that correct conclusions can be drawn.

Section 5.0 of this NUREG/CR provides guidance of verification and validation of models. This information is intended to be useful to the users, or individuals who are setting up and executing the models, as well as those who are assessing the outcomes, or the reviewers. Delving a bit deeper, section 5.1 provides guidance specifically to the user while section 5.2 is geared toward the reviewer. The sections provide key questions for the user and reviewer to consider for assurance that the conclusions drawn from the simulations are as sound as possible.

Finally, section 6.0 has practical key takeaways and guidance from several of the roadmap topic areas. The information in this section is intended to familiarize users with common issues and provide guidance. Gaps in the form of outstanding questions are also addressed.

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10. SUPPLEMENTARY NOTES

11. ABSTRACT (200 words or less)

The guidance and conclusions provided in this report are the result of a multi-year effort to understand the potential role of modeling and simulation in improving the efficiency and efficacy of ultrasonic inspections of nuclear power plant components. Conclusions are coalesced from previous work, and strategies and best practices are suggested for successful implementation of modeling and assessment of simulation outcomes. An overview of challenges in modeling and simulation is given, along with strategies for overcoming these challenges. Methods of validation and verification are outlined to help assure that models and simulation outcomes are reliable. Specific direction for implementing the models is provided as well as guidance for assessing the outcomes. In addition, key takeaways and lessons learned for different modeling scenarios are listed. The guidance and conclusions summarized in this report are intended to form the technical framework for development of a nondestructive evaluation modeling and simulation best practices document that will support standardization of modeling practices across the commercial nuclear power industry.

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