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A case study in engineering model validation using new wavelet-based methods

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Abstract
Simulation model validation is an important part of simulation development and use. An emerging challenge is the examination of functional data systems and the validation of the simulations built to represent them. While validation methods do exist, there is a gap in the engineering and statistical approaches used for functional model validation. This case study demonstrates the use of recently developed methods based on the use of wavelets to bridge the engineering-statistical gap in functional simulation model validation. Two methods are used to provide insight regarding model validity, and a third method is used to identify areas of system-simulation disagreement when model validity fails to hold.

KEYWORDS
engineering, functional data, validation, WANOVA, wavelets

1 | INTRODUCTION

It is an exciting time to be involved in quantitative analytics. Statistical analyses have seen a tremendous growth in appreciation under newer labels such as "machine learning" or "statistical learning." Increasingly complex optimization problems are being tackled through the use of heuristics and large-scale or super computing. Bayesian methods are increasingly in use and are transforming how test and analysis results obtained throughout the product life cycle can be brought into use for decision making later in that product life cycle. A final example, and our particular focus, is the use of rigorous and sometimes detailed simulations, or models, currently used in a wide variety of domains and envisioned to eventually help design new systems in silico, thereby avoiding costly physical prototype and test cycles. For such virtual design to occur, however, there is a crucial characteristic these simulations or models must have. These models must be deemed valid for their intended purpose before they can be used with any reasonable confidence. The focus of this case study is the validation of these types of important engineering models and simulations.

Simulation and model validation is a fairly new technology because computer simulations are really not that old either. However, the simulation validation literature is quite well developed but does appear to fall into two nondistinct ways of thinking about the topic. One way of thinking is the engineering perspective whereby the methods are sometimes quite subjective, based on graphical outputs or on numerical measures of agreement between a model and a system output. Another way, which we label here as the operations research perspective, casts the validation problem into a statistical framework within which one can construct and test statistical hypotheses of model to system agreement. Our methods, demonstrated in this case study, bridges these perspectives, providing an engineering look using statistical principles. Simulation and model validation is a fairly new process because computer simulations are a relatively new development. Despite being fairly new, the simulation validation literature is quite well developed and comprises two nondistinct ways of considering the topic. One viewpoint is the engineering perspective whereby the methods are sometimes quite subjective, based on graphical outputs or on numerical measures of agreement between a model and a system output. Another approach, which we label here as the operations research perspective, casts the validation problem into a statistical framework within which one can construct and test statistical hypotheses of simulation-to-system agreement. Our methods, demonstrated in this case study, bridge these perspectives by synthesizing the engineering perspective with statistical principles.

This paper is organized as follows. In the next section, we provide a brief review of the model validation field particularly emphasizing the two perspectives of validation. We then set the context for the validation case study scenario in Section 3 and describe the new wavelet-based validation approach in Section 4. The case study results are provided in Section 5, and we close with a summary and concluding remarks in Section 6.

2 | LITERATURE REVIEW

Computer simulations are powerful tools for system design. Simulations are used in all aspects of system design. Simulations also hold promise for eventually developing and testing new systems in a fully virtual environment. However, the use of simulations for this design task, actually for any specific task, comes with an important condition; simulation verification and validation (V&V).

Validation is arguably the more difficult (and more crucial) aspect of V&V and is our focus. Validation ensures the simulation suitably represents the system it is meant to represent. Verification ensures the simulation is built as designed. In validation, the focus is whether or not the simulation output suitably represents (or matches) the corresponding system output. Simulation output comes in either discrete or functional (continuous) form, and validation methods vary according to the output form.

Validation methodologies are a relatively new field, with computer simulation emerging in the late 1960s.[1] However, the use of computer simulation has exploded, a growth that correlates quite well with the exponential growth in computing power. Simulation validation methodology is fairly well established although there are some critical gaps. A gap of particular interest involves the use of statistical methods for functional output validation. Further, simulation validation methods fall into what we see as two nondistinct schools of thought, the operations research approach and the engineering approach, but by recognizing these approaches, one can devise new methods to fill the methodological gaps and bridge the validation approaches.

The operations research approaches are best represented by the work of Balci,[2] Sargent,[3] and Kleijnen.[4] A comprehensive historical account is given in Sargent.[5] These approaches combine the use of informal methods, such as graphical comparisons and expert opinion, with more formal, statistically-based methods. These methods are generally applied to discrete output simulations. These simulations tend to focus on processes; process improvement; and large scale, system-of-systems models. Applicable examples include manufacturing plant design, distribution planning, or aircraft repair processes.[6] The formal methods used to compare the simulation output to the corresponding system output include hypothesis testing, confidence interval comparisons, and various multivariate tests. Atkinson[7] provides a comprehensive summary of these approaches.

The engineering approaches are generally more focused on system, and subsystem, modeling and design, and thus, the engineering simulations tend to produce continuous output. Such systems are also called dynamical or functional systems. Thus, the engineering approach is more focused on the physical systems functioning within the higher level process or system of systems examined than found in the operations research simulations. Leading work in this area is found in Oberkampf and Barone[8] as well as in Oberkampf and Trucano.[9] The methods in the engineering approach focus on the use of informal methods of comparing simulation and system output and the use of metrics of agreement between the simulation and system output streams. Again, Atkinson[7] provides a thorough summary of the various metrics proposed and in use.

What is needed for engineering validation are methods that combine useful aspects of each of the operations research and engineering approaches. To characterize, the operations research approaches provide the statistical framework but do not adequately address functional output, while the engineering approaches accommodate the functional output but do not provide the full statistical basis of comparison. The approach we have developed in other works and demonstrate in this case study accommodates the functional output, yields metrics of agreement between the simulation and system output, and provides a statistical basis for the validation decision. Specifically, wavelet decomposition of both the simulation and the system signals, and subsequent comparisons of those decompositions, serves as a recently developed means to meet this simulation validation need (Atkinson et al[10-12]).

3 | WAVELET ANALYSIS

Wavelets are a relatively recent development in the field of mathematics but have had a significant impact thus far.[13,14] Wavelets apply in a variety of situations, and there is potential for the use of wavelets as a method for simulation model validation. Wavelet analysis is a powerful tool for evaluating data signals by transforming them from the time domain to the time-frequency or wavelet domain. This enables the denoising of a signal via a process called wavelet thresholding. It is also possible to perform statistical inference on high-dimensional data by implementing wavelet analysis of variance (WANOVA).[15] These capabilities allow the analyst to more accurately compare functional system and simulation data to perform a validity assessment.

This validation capability comes with certain assumptions: The system and simulation output are generated under comparable conditions; the signals being compared occur over similar time ranges; and the collection times in each signal align. These assumptions are quite reasonable in practice.

Wavelets transform signals or functions using a mother wavelet (ψ) and father wavelet (ϕ). These are used to generate a family of wavelets through dilations (j) and translations (k), so that a function may be expressed as

$$f(t) = \sum_k c_{j_0,k}\phi_{j_0,k} + \sum_{j \geq j_0} \sum_k d_{j,k}\psi_{j,k}\,, \tag{1}$$

where $c_{j,k}$ and $d_{j,k}$ are wavelet coefficients. The discrete wavelet transform (DWT) calculates the inner products of the signal and wavelet functions and is used to estimate the wavelet coefficients. Wavelets are able to transform nonstationary data and offer increased computational efficiency. For additional information regarding wavelets, see Burrus et al,[13] Ogden,[14] and Girimurugan et al.[16]

As alluded to previously, wavelet thresholding is the process for denoising a signal. This was first explored by Donoho and Johnstone[17] who define a universal threshold,

$$\lambda = \hat{\sigma}\sqrt{2log(n)}, \tag{2}$$

where $\hat{\sigma}$ is an estimate of the standard deviation of the noise and n is the sample size. Wavelet coefficients are modified according to the threshold, and the resulting signal represents the denoised signal.

The use of wavelets led to two new validation approaches, a metric approach[11] and a WANOVA approach,[12] each of which are described next and demonstrated in our subsequent case study. Additionally, if either approach indicates a failure to declare the simulation valid, a search method called the wavelet bisection method should be employed. This method is also described below and demonstrated in the case study.

3.1 | Validation metric of thresholded signals

Validation metrics[18,19] are a common and effective method for assessing functional model data, such as time-series data. However, when analyzing extremely noisy data, the results from using a model validation metric may be skewed and inaccurate. This is because the signal noise may increase the estimated discrepancy between the system and model data, incorrectly resulting in an invalid model assessment. The signal noise may be due to pure error encountered during system observations and therefore does not represent true model bias. Accordingly, Atkinson et al[11] propose a dynamic model validation metric based on wavelet thresholded signals. In this approach, the system and model data signals are denoised using wavelet thresholding and then compared using a model validation metric. The model validation metric assesses the shape, phase, and magnitude errors to produce a comprehensive validation metric, R^*. This metric is calculated as

$$R^* = \alpha_1\left(\frac{1-\rho_{xy}}{2}\right) + \alpha_2\left|\frac{\tau}{T}\right| + \alpha_3(m)\,, \tag{3}$$

where ρ_{xy} is the correlation coefficient, τ is the lag, T is the signal length, m is the magnitude error component, and α_i represents weighting coefficients. This method is very effective at removing the signal noise prior to calculating a validation metric value. However, this technique does require that the analyst specify an "acceptable validation metric value" to judge whether the model is valid or invalid. As with other validation metrics, there is no specific value, or range of values, for the cutoff. Values used are based on best practice or expert opinion. We have future work planned to focus on more rigorous definition of these cutoff values. This designation currently requires subjective input and is therefore a limitation of the current method.

3.2 | Wavelet analysis of variance

WANOVA performs statistical inference in the wavelet domain. Girimurugan et al[15] present a WANOVA methodology that tests for statistical differences among functional data. They adapt a functional analysis of variance (FANOVA) model with response Y_{ijk}, for case, $i = 1, 2,...,t$; replicate, $j = 1, 2,...,r_i$; and response, $k = 1, 2,...,n$, while assuming multivariate normal noise. The wavelet representation yields a test statistic,

$$\kappa_\eta = \sum_{i=1}^{t}\sum_{k=1}^{n}\tilde{\theta}_{ik}^2. \quad (4)$$

In Equation 4, $\tilde{\theta}_{ik}$ represents the thresholded wavelet coefficients associated with case i. The κ_η test statistic is compared with a critical value to test the null hypothesis that the t sets of functional data are statistically equivalent.

Atkinson et al[12] extend WANOVA for use in model validation assessments. The WANOVA method compares the system data signal, s, to the simulation data signal, m, and tests the hypotheses that

$$H_0\!:\mathbf{s} = \mathbf{m},$$
$$H_1\!:\mathbf{s} \neq \mathbf{m}.$$

This hypothesis assumes a valid model data signal should be statistically equivalent to the system data. If the test statistic exceeds a critical value, the null hypothesis is rejected, and the model is deemed invalid.

3.3 | WANOVA bisection method

Most model validation methods conclude upon assessing whether a model is valid or invalid. However, for the engineer or simulation model developer seeking to build and improve the simulation model, this approach is incomplete. If the model is deemed invalid, the developer has no further information on the nature of the discrepancy. It would be valuable to know if the discrepancy is located over a particular range in the functional data. Similarly, it would be worthwhile to know if some intervals of the model data show strong agreement with the system data. Atkinson et al[10] present a WANOVA Bisection method that identifies a range in the functional data over which the model is most biased in relation to the system. The approach employed in this paper uses WANOVA and the bisection method to demonstrate how such an approach aids developers in correcting the necessary elements of the simulation.

Thus, given an invalid model, the WANOVA bisection method bisects the system and model data signals and performs WANOVA on each half of the signal. The two test statistics are compared, and the half with the larger statistic value is the half containing the greater model bias. These steps are repeated until the desired interval length is reached. The resulting interval represents the region over which the the model data differ most from the system data.This technique may also be used to determine over what region the model data are least biased and more elaborate search processes could find multiple regions of model disagreement. This is discussed further in Atkinson et al.[10]

4 | MODEL VALIDATION SCENARIO CONSIDERED

Modern military aircrafts are extremely capable in terms of their military power and, as a result, are very complex systems. Next generation aircraft will be even more capable and even more complex. One cost for this increase in system capability is an increased reliance on electronic systems. This increases not only the power demands of the system but also the heat generated by the system and the heat used within the system. Consequently, there will be tremendous demands on thermal management systems (TMS) within these future aircraft weapon systems.

Thermal efficiency is maintained by an aircraft TMS since thermal loads through the aircraft affect all aspects of aircraft performance. The next generation military aircraft requires an accurate design of not only the TMS but also all those systems that use the thermal energy in the aircraft. Advanced modeling and simulation tools can provide the capability required to investigate and assess the thermal loads expected. Specifically, these models will comprise a suite of models examining subsystems through system performance. Not only is building the models a challenge but validating these models for specific use presents a challenge as well.

One component of the TMS is an air cycle machine (ACM). The ACM handles air flowing through an aircraft system, such as avionics components or turbines. In the ACM, "air is compressed and then routed through a heat exchanger or series ofheat exchangers before being expanded again by a turbine, which provides the mechanical work for the compressor."[20]

The ACM in the current setting mimics a reverse Brayton cycle where air is cooled using turbomachinery. For an ACM, the main stream air is taken in and heated. The heated air is pressure controlled using a regulating valve. The air is compressed and then cooled using a heat exchanger. This heat exchanger has ambient air blown over it. The cooled air is expanded again in the turbine after which the air exits the system through an expanding duct. Figure 1 is an abstracted version of the ACM built and modeled in Bracey's research.[20]

Bracey[20] developed a bench-top experimental version of an ACM along with a simulation model of that ACM unit in a MATLAB-Simulink code. Specific details on the experimental unit and the model are found in Bracey's thesis.[20] Our focus is on the validation of the

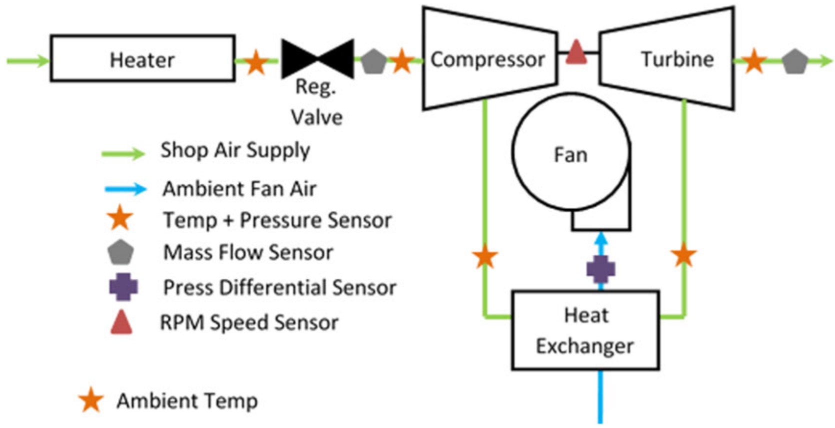


FIGURE 1 Diagram of abstracted air cycle machine modeled and tested[20] [Colour figure can be viewed at wileyonlinelibrary.com]

model against the bench-top experimental unit. Data samples from the bench-top unit were available. The specific data examined are the temperature and pressure readings just after the compressor but before the turbine (see red triangle in Figure 1).

5 | VALIDATION CASE STUDY RESULTS

The new validation methods described in section 3.1 are applied to the functional data generated during system and simulation model testing of the ACM component of the TMS. For this analysis, there are 44 samples each for the system at a common configuration, with measures on both temperature (T) and pressure (P). Simulations are run to collect temperature and pressure data to compare with the system data. Therefore, we conduct a total of 88 validity assessments to evaluate the ACM model. We compare a system data signal and a simulation data signal each for a single variable, temperature, and pressure, over all 44 cases. These system data signals have a length of 3751 data points with a simulation model sampling rate of 25 samples per second for the time required to obtain a sufficient sample to compare with the system sample.

These data signals lend themselves perfectly to analysis via our new model validation methods. The noise in the functional data is well evaluated and accounted for by the process of wavelet thresholding. Then, the model data are evaluated using the model validation metric to assess the sources of error between the system and model data. Additionally, WANOVA provides an objective and statistically based evaluation of the model data. Finally, in cases where the methods deem the model invalid, the WANOVA bisection method is used to locate the interval(s) of model discrepancy so that developers can make the necessary corrections and improvements. Thus, this application serves as an effective case study through which to employ and evaluate the efficacy of wavelet-based validation techniques in modeling and simulation validation.

The wavelet threshold method requires a critical value choice for the metric. This choice is based on domain knowledge. For this case, a value of 0.001 was selected. Although all cases were examined, only two cases are presented in detail here. The two discussed, case 19 for temperature and pressure, were selected to demonstrate the use of our wavelet analysis methodology for functional system validation. The narrative provided on the two selected cases applies equally as well to the other 44. The appendix contains the WANOVA validation results for all the cases considered.

Figure 2 presents the plots associated with sample 19 and the temperature reading associated with that sample. Sample 19 was selected for discussion, as it is a comprehensive representation of the results across all the samples, and it provides applicable visualization results to

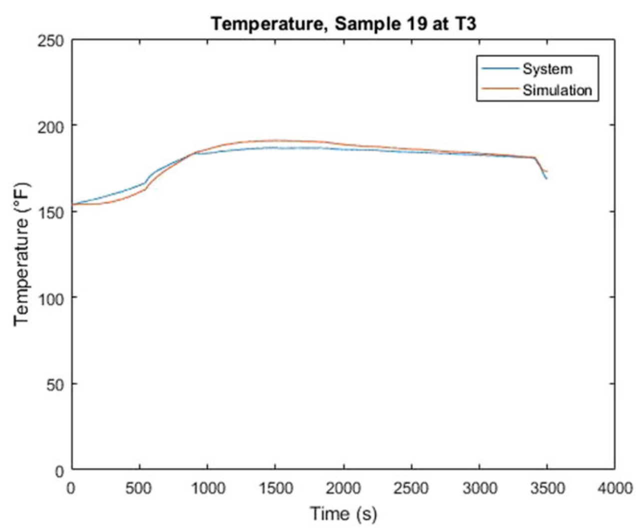


FIGURE 2 Sample 19, temperature measurement results, system versus simulation output [Colour figure can be viewed at wileyonlinelibrary.com]

support the method components we highlight. The validation metric value was calculated as 0.0021, which leads to rejection of the model as valid. The WANOVA method was then applied yielding a measure of 16 154, which is far greater than the critical value of 1870. The critical value used in this WANOVA hypothesis test is based on the denoised WANOVA statistic. Specifically, the theoretical distribution of this statistic along with the defined level of significance is used to calculate the critical value. Details are in Atkinson et al.[10] This result also provides agreement with an invalid model conclusion.

Figure 3 presents WANOVA bisection results. Note how the method focused directly on that portion of the model signal with the larger difference from the system signal. The takeaway is that the use of an objective, quantitative approach to locating areas of system-model output disagreement provides a viable mechanism to help engineers and modelers isolate the issues arising in model validation efforts.

The second example demonstrates using the method not only to isolate a problem but also to confirm the positive results of the corrective action taken with the model. Figure 4 shows the results again from sample 19 but with specific focus on the pressure reading. The validation metric of 0.0016 and WANOVA value of 2889.7 both support an invalid model assessment.

In some instances, engineers report the need to adjust the model pressure by a constant, such as in this case by 1.5035. Figure 5 adds the new functional line onto Figure 4. Metrics for this new model are 0.0007 for the validation metric and 165.5 for the WANOVA. Both measures now indicate that the model is valid, supporting the positive results of the model changes.

Table A1 provides the results for all cases considered. Note the multisample results help provide statistically significant evidence of the validity of the simulation with

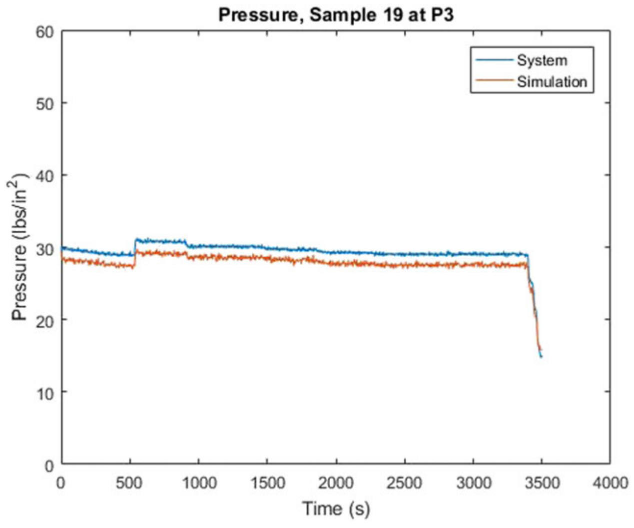
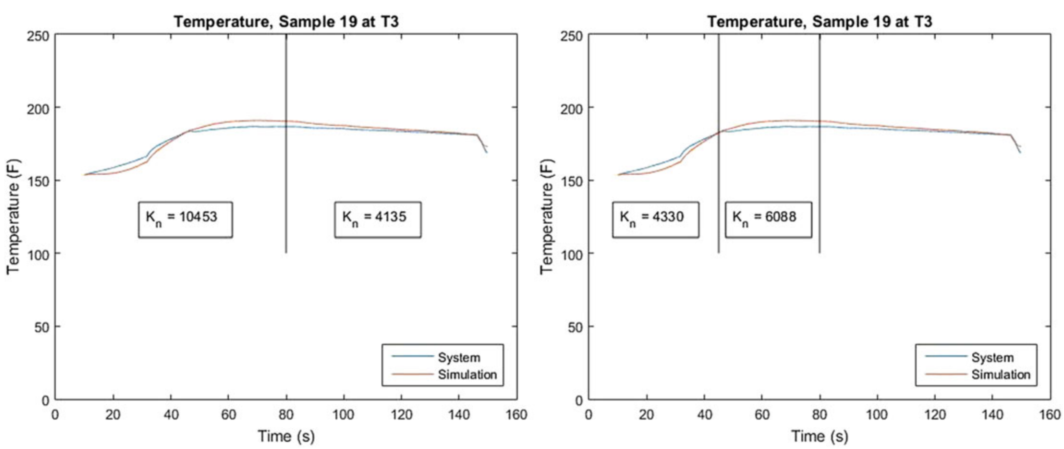


FIGURE 4 Sample 19, pressure measurement results, system versus simulation output [Colour figure can be viewed at wileyonlinelibrary.com]

respect to the system. Across all 44 cases, 21 were deemed not valid at temperature. This supports a multisample conclusion that the simulation is not valid with respect to its temperature results. Five of the pressure samples were invalid, but none were invalid when the correction was implemented. This suggest a multisample conclusion that the simulation is valid with respect to pressure results, especially when a small bias is present.

The two cases represent the use of a quantitative validation method that bridges the operations research and engineering approaches to model validation. The method employs an engineering metric, a statistical hypothesis test approach, and a search method to identify regions of model disagreement. In the end, our results indicate model validity for the temperature and pressure variables considered individually, which presumably would also



(A) First iteration (B) Second iteration

FIGURE 3 Sample 19, temperature wavelet analysis-of-variance bisection method results. The left side depicts the first iteration, and the right side the second iteration that hones in on where the problem exists [Colour figure can be viewed at wileyonlinelibrary.com]

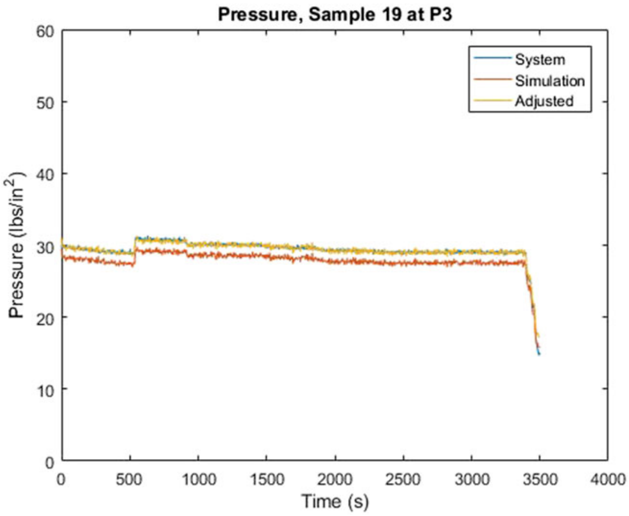


FIGURE 5 Sample 19, pressure measurement results, system versus original and modified simulation results [Colour figure can be viewed at wileyonlinelibrary.com]

hold when considered simultaneously. Such multivariate approaches to model validation are areas of future research.

6 | SUMMARY AND CONCLUSION

This work demonstrates how newly developed methods for functional data simulation validation can be applied not only to assess simulation model validity but also to pinpoint where the system and simulation disagree in the time-series, functional data output. The case study used represents a single case that compares an engineering bench-level model against a simulation of that system, but provides a starting point for future extensions of the methodology.

Future work on these validation methods involves extending the family of wavelet functions considered, possibly extending the work to multidimensional surfaces, developing an improved statistical basis for the validation metric employed, and building computational packages for implementing the validation methods employed. These improvements will coincide with additional applications of the methods to actual system-simulation validation efforts.

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DISCLAIMER

The views expressed in this article are those of the authors and do not reflect the official policy or position of the United States Air Force, Department of Defense, or the US Government.

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APPENDIX

TABLE A1 Results of WANOVA testing over all cases

Trial	Pressure, Original	Pressure, Corrected	Temperature
1	832.8	46.5	1357.7
2	1704.8	94.5	3138.7
3	797.5	38.9	3072.9
4	7321.9	139.2	3135.5
5	188.5	23.4	714.2
6	521.5	39.2	782.3
7	721.3	61.5	7453.6
8	1355.0	210.8	9255.6
9	200.4	22.3	1016.0
10	422.9	60.3	211.8
11	7895.1	519.2	35 799.0
12	806.6	50.9	6818.1
13	1264.8	74.9	7054.9
14	1307.9	58.5	1355.4
15	586.3	45.8	2924.9
16	537.5	38.0	6012.2
17	517.5	26.5	1639.9
18	2254.9	211.2	17 253.0
19	2889.7	165.5	16 154.0
20	177.1	7.7	2640.8
21	893.4	95.0	8832.0
22	1059.3	41.4	4819.9
23	758.0	35.1	1020.0
24	170.1	18.9	842.4
25	104.3	14.5	438.8
26	1194.4	51.2	1413.6
27	207.3	20.2	26.1
28	181.8	14.3	144.3
29	420.5	24.9	2401.6
30	164.3	15.7	558.0
31	265.8	21.0	1097.1
32	144.2	15.7	988.8
33	344.4	20.3	2116.4
34	167.7	14.8	733.2
35	556.7	38.8	1303.8
36	1363.3	155.8	4116.9
37	566.2	61.0	5938.0
38	2979.9	153.3	4890.7
39	418.9	55.9	3287.5
40	313.2	16.8	1590.2
41	238.2	15.5	78.9
42	65.2	8.0	241.5
43	647.3	38.4	2103.8
44	1440.7	62.0	1607.6

Abbreviation: WANOVA, wavelet analysis of variance.