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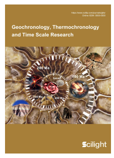

Article

Sensitivity Analysis in Thermal Structure and Thermochronology Calculations

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Abstract: Sensitivity analysis should be an essential part of quantitative studies in the geosciences. It serves as an important first step in evaluating our confidence in the results of a numerical calculation, and it helps us identify what input parameters should be high-priority targets for further research to improve confidence in our modeling results. Here, we explore the fundamentals of sensitivity analysis as it applies to calculations related to the thermal structure of the lithosphere and thermochronologic calculations. After presenting simple examples using well-known approaches, we compare the results obtained using a less familiar approach: the Taguchi Method. Although the Taguchi Method is underutilized in the geosciences, it is often used in process engineering to reduce the number of experiments necessary to determine the sensitivity of systems to large numbers of interdependent variables. We demonstrate that the Taguchi Method yields sensitivity rankings comparable to those produced by more conventional approaches, while requiring substantially fewer model runs. This efficiency makes it particularly well-suited to the analysis of complex thermal-kinematic models, where high dimensionality and long compute times often limit systematic uncertainty evaluation. The method's ability to identify dominant sources of uncertainty across parameter types provides a practical framework for guiding future data collection efforts.

Keywords: thermal-kinematic modeling; exhumation rates; sensitivity analysis; Taguchi Method; orthogonal array design

1. Introduction

Thermochronology enables the reconstruction of rock cooling histories through time by modeling the temperature-sensitive behavior of radiogenic systems, which are influenced by the crustal thermal structure. As a result, thermochronologic interpretations inherently depend on assumptions about the thermal field through time and space. Uncertainties in primary assumptions and constraints that are used as inputs to thermal-kinetic and thermal-kinematic models directly impact the reliability of results and, ultimately, the robustness of geological interpretations. While such modeling is gaining popularity in the thermochronometry community (e.g., [1–5]), attempts to express uncertainty in modeling results are usually focused on the range of acceptable model fits that are, themselves, largely a function of thermochronometer uncertainties. However, modeling exercises also incorporate a large number of parameters for which no uncertainties are explicitly incorporated. Here, we emphasize an essential first step toward rectifying this omission: a comprehensive sensitivity analysis. In addition to reviewing well-known, traditional approaches to sensitivity analysis, we present and advocate a less-well-known approach—the Taguchi Method [6]—which is particularly well-suited to sensitivity analyses for calculations based on complex systems of equations such as those encountered frequently in modeling thermochronologic datasets.

2. Sensitivity Analysis

The sensitivity analysis of an equation asks how much each parameter influences the solution of the equation. While general awareness of uncertainty informs our understanding of confidence in model results, sensitivity analysis clarifies which parameter uncertainties most significantly constrain that confidence. This is extremely important. For example, suppose we know our estimate for a high-leverage parameter is very uncertain. In that case, we should place less confidence in the result of a calculation or model and exercise caution in our geologic interpretation of the result. More broadly, sensitivity analysis can identify new, high-priority research directions for improving confidence in key parameter estimates that, in turn, improve the quality of our geologic modeling.

The most straightforward approach to sensitivity analysis is sometimes referred to as a "one-at-a-time" (*OAAT*) analysis [7]. The procedure involves changing one estimated parameter in a calculation while not changing all other parameters and then repeating this experiment for all other parameters, one by one. By comparing the experimental results with the results of the original calculation made using the assumed parameter values, we can establish the rank order of sensitivity on specific parameters. While this approach is straightforward, it does not account for possible interactions among parameters that might affect the rank order. A more sophisticated and statistically robust approach when the variables may be interdependent involves a full permutation of all parameter combinations within uncertainty limits, known as full factorial "design of experiments" or *FF-DOE* (e.g., [8,9]).

2.1. Examples of OAAT and FF-DOE Sensitivity Analysis

We illustrate both approaches using two simple physical models pertinent to thermochronology and thermal history modeling. First, we consider one standard formulation of a steady-state geothermal gradient for the crust, which considers both conduction and an exponentially decreasing heat production contribution with depth after [10]:

$$T = T_s + \frac{zq_m}{k} + \left(1 - exp\left(-\frac{z}{z_\tau}\right)\right)\frac{H_{ne}{z_r}^2}{k} \tag{1}$$

Equation (1) solves for temperature (*T*) at a specified depth (*z*) as a function of five independent variables: T_s, surface temperature; q_m, mantle heat flux; k, thermal conductivity; z_r, an e-folding depth for a distribution of heat production that decreases exponentially with depth; and H_{ns}, volumetric heat production. Nominal estimates for the five independent variables are shown in Table 1, and the calculated geotherm based on these reference values is shown as the thicker solid black curve in Figure 1. All simulations and plotting of the results were performed in MATLAB.

A simple *OAAT* analysis might involve evaluating *T* at a single depth (15 km) by perturbing each of five independent variables from its reference value by +10% of its nominal value, one at a time, and solving for temperature. These temperatures are then compared with the calculated temperature at a depth of 15 km based on the nominal values for all parameters. We find that the least percentage change in calculated temperature is obtained for a +10% change in surface temperature, T_s. That change in calculated temperature serves as a baseline for the *OAAT* analysis. We define an influence factor (*IF*), which has its minimum value of 1.0 for the percent change associated with the +10% perturbation in T_s, and then divide the calculated differences for all other independent variables after perturbation by the perturbed *Ts* difference to define an *IF* for each parameter. These values for the *OAAT* analysis are listed to two significant digits in the second column of Table 2. Higher IF values correlate with increasing importance of uncertainty in the temperature calculation. This exercise shows that the most influential parameter is thermal conductivity, which is roughly 11 times more influential than surface temperature. In fact, Column 2 of the table shows that all other parameters are much more influential than T_s. Based on this list, we can also assign a ranking of the influences for each parameter in Column 3—with a ranking of 1 being the most influential—to each parameter. (Note that lower ranks correlate with higher IF).

Table 1. Reference values for geothermal gradient sensitivity analysis.

Parameter	Value	Unit
T_s	288.15	K
q_m	0.028	W/m^2
k	2.5	W/m·K
z_r	1.0×10^4	m
H_{ns}	2.04×10^{-6}	W/m^3

Sources: [10,11].

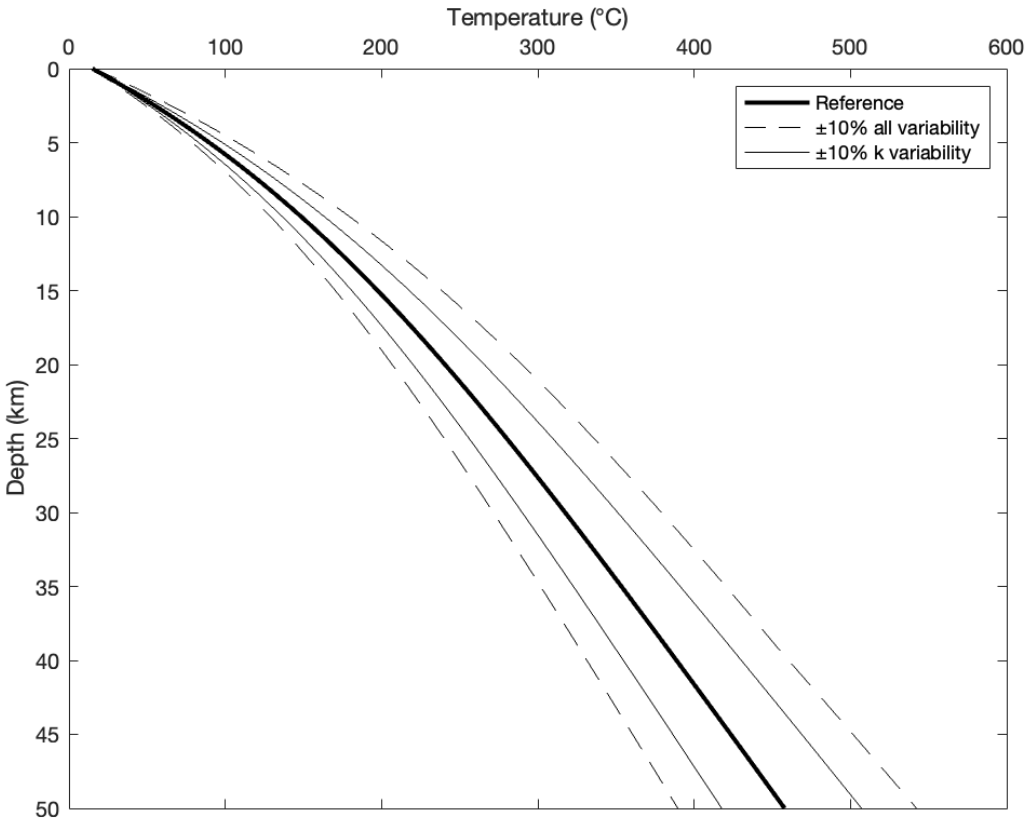

Figure 1. Geothermal gradient using parameter reference values of [12] (thick solid black line). The dashed black lines represent uncertainty in predicted exhumation rates from a Monte Carlo simulation using 10,000 realizations and varying all model parameters simultaneously by ±10%. The thin solid black line shows the result when only the top-ranked parameter (as identified by the Taguchi Method) is varied by ±10%. The comparison illustrates that this parameter alone accounts for a substantial portion of total uncertainty, supporting its identified significance.

Table 2. Comparison of rankings of significance (1 being most significant) for input parameters to geothermal gradient equation using the (a) "one-at-a-time" sensitivity analysis, (b) full factorial analysis, and (c) Taguchi analysis.

	One-at-a-Time		Full Factorial		Taguchi	
Parameter	**IF**	**Rank**	**IF**	**Rank**	**IF**	**Rank**
T_s	1.0	5	1.0	5	1.0	5
q_m	6.8	3	6.8	3	2.4	2
k	11	1	11	1	2.7	1
z_r	8.5	2	8.5	2	2.1	3
H_{ns}	5.4	4	5.4	4	2.1	4

An *FF-DOE* sensitivity analysis of Equation (1) requires evaluating how its solution changes from that yielded by reference values when we explore all possible variable combinations, assuming that each variable value can be at the reference value or a specified perturbation from that value, in this example +10%. These model solutions are typically called "experiments" in the design of experiments statistical literature. Each variable can be at one of two "levels" during this exercise: the reference level (Table 1) or at a level that is +10% of that value. The number of experiments that must be conducted (N_e) is 32, based on the equation

$$N_{ex} = L^{v} \tag{2}$$

where L is the number of levels and v is the number of variables. For Equation (1), *FF-DOE* analysis yields identical rankings of the influences of variables and influence factors from those obtained using the *OAAT* (Table 2).

In addition to accounting for possible influences among variables, the *FF-DOE* approach is also more easily adapted to sensitivity analysis when we wish to test the effects of multiple levels of perturbations. For example, Equation (2) tells us that, with 243 experiments, we could test the sensitivity of the Equation (1) solution at three levels: one using reference values, one using values +10%, and one using values −10%. Unfortunately, Equation (2) also hints that *FF-DOE* sensitivity analysis becomes cumbersome for systems of equations with large numbers of independent variables, a problem for which we offer a solution in the next section.

In order to evaluate the efficacy of the *OOAT* and *FF-DOE* approaches for more complicated equations with few variables, we also applied them to the classical "Dodson's equation" [13], which is often used to estimate the bulk closure temperature (T_{cb}) for a mineral-isotopic system from experimental diffusion data assuming a cooling rate (dT/dt):

$$T_{cb} = \frac{E}{Rln\left(\left(AD_oRT_{cb}{}^2\right)/\left(a^2E\left(\frac{dT}{dt}\right)\right)\right)} \tag{3}$$

Equation (3) includes parameters related to the intrinsic diffusivity of the daughter product of a radioactive decay scheme: the activation energy (E), the diffusivity at infinite temperature (D_o), and the effective diffusion dimension (a) for a dated mineral. It also includes the gas constant *R* and a constant (*A*) which reflects the presumed diffusion geometry. Typical values for some of these parameters are compiled by [14] and are also used in this study. While Equation (3) contains fewer independent variables than Equation (1), it is more complex because it cannot be rewritten to solve directly for T_{cb} and must be solved iteratively.

For a sensitivity analysis of Equation (3), we explored the relative effects of +10% variations in *a*, D_o, and *E* on calculations of the closure temperature of the apatite (U-Th)/He thermochronometer assuming a cooling rate of 10 °C/Ma, a geometry factor of 27 (cylindrical), and using reference values from [15] (Table 3). The results (Table 4) show that the *OAAT* and *FF-DOE approaches* yield the same result: comparing + 10% perturbations in independent variables, a calculated T_{cb} is least influenced by D_o and, by far, most influenced by the activation energy, *E*.

Table 3. Reference values for bulk closure temperature sensitivity analysis and Taguchi Method experiments for the apatite (U-Th)/He thermochronometric system.

Parameter	Value	Unit
E	142	kJ/mol
A	27	-
D_o	0.009	m^2/s
a	50	µm
dT/*dt*	10	K/s

Sources: Diffusion parameters for He in apatite from [15], other parameters from [14].

Table 4. Comparison of rankings of significance (1 being most significant) for input parameters to Dodson equation using the (a) "one-at-a-time" sensitivity analysis, (b) full factorial analysis, and (c) Taguchi analysis.

	One-at-a-Time		**Full Factorial**		**Taguchi**	
Parameter	**IF**	**Rank**	**IF**	**Rank**	**IF**	**Rank**
E	53	1	53	1	46	1
D_o	1.0	3	1.0	3	1.0	3
a	2.0	2	2.0	2	1.9	2

2.2. The Taguchi Method—A Fractional Factorial Approach

When the number of variables is large in design of experiment applications, statisticians often turn to fractional-factorial approaches, which efficiently evaluate only a subset of all possible parameter combinations to identify dominant effects [9]. One of these—the Taguchi Method [6]—uses orthogonal arrays to reduce the number of experiments necessary to determine likely cause-and-effect relationships. Applications of the Taguchi Method (*TM-DOE*) begin with a recasting of Equation (2) as follows:

$$N_{ex} = L^j \tag{4}$$

The new parameter *j* is the smallest integer that will satisfy the relationship:

$$P = \frac{L^{j-1}}{L-1} \tag{5}$$

where P is the number of parameters (also known as factors). For our geothermal gradient analysis, with five independent variables tested at two levels (the reference level and the reference level plus 10%), Equation (5) requires $j = 3$, and Equation (4) suggests that only 8 experiments are required to establish the relative sensitivity of calculations made using Equation (1) to +10% perturbations in variable values. This represents a substantial reduction in the computational overhead of the *FF-DOE* approach ($N_{ex} = 8$ vs. $N_{ex} = 32$), and such reductions are much more valuable for equations or systems of equations with many more variables. Once N_{ex} is established, the specific experiments necessary are established using orthogonal arrays [16]. Additional information regarding the Taguchi Method and its application to sensitivity analysis may be found in the supplement as well as in [17–19]. Orthogonal array construction is explained further in [20].

All calculations using the Taguchi Method were implemented in MATLAB R2024a using custom scripts. In [21], we provide a standalone MATLAB program that demonstrates the application of the *TM-DOE* to evaluate the relative influence of model input parameters on solutions to Equation (1). The results (Table 2) show that, for most variables, *TM-DOE* yields the same relative rankings as the *OAAT* and *FF-DOE*, emphasizing that thermal conductivity is the most influential variable, while surface temperature and volumetric heat production are the least influential. However, the relative rank of the second and third most influential variables is reversed from the *OAAT* and *FF-DOE* results. Inasmuch as *FF-DOE* is a more comprehensive technique, the observed difference suggests that the reduced set of equations used for the *TM-DOE* analysis does not fully capture the full range of variable interactions. In contrast, *the TM-DOE* analysis of Equation (3) (Table 4) produces the same relative rankings as the other two methods. A comparison of influence factors among the three methods illustrates that IF calculations, while generally useful as guidelines, are not exact and depend on how the sensitivity analysis is performed.

3. Discussion

In this contribution, we have reviewed three ways to analyze the sensitivity of solutions to basic calculations pertinent to understanding the thermal structure of the lithosphere and modeling thermochronological data. The results imply that all three provide similar—and, for many input parameters, identical—results. The *OAAT* approach is straightforward and easily understood. However, it does not perform reliably when there are influences among variables, and it requires many independent experiments when an equation or a system of equations contains many variables. The *FF-DOE* approach is reliable, thorough, and effectively accounts for influences among variables, but it can still become cumbersome with many variables. The *TM-DOE* approach retains the effective management of influences and is much more computationally efficient. However, our experience is that it is most reliable for identifying the most and least impactful variables and less reliable for nuanced evaluation of the relative significance of variables between extremes. If the difference between two variables determined to be of intermediate significance is important for a particular study, we suggest relying instead on the *FF-DOE* approach.

3.1. Visualization of the Control of High-Influence Variables on Calculation Uncertainties

Armed with the knowledge of which variables are most influential in the result of a calculation, it is possible to explore how much fully propagated uncertainties for calculations depend on highly influential variables. For example, Figure 1 illustrates such an analysis of the geotherm equation over depths ranging from 0 to 50 km. The reference values in Table 1 yield a modeled geotherm shown as a thick line in the figure. We then used a Monte Carlo approach [22,23] to explore how ±10% perturbations in all independent variables would permit variations in the modeled geotherm over the entire 50 km depth interval. The bounding curves for these models are shown in Figure 1 as dashed lines. Remembering that thermal conductivity (k) was ranked first in our sensitivity exercise, we next repeated the Monte Carlo exercise, holding all variable values at the reference values except the thermal conductivity, which we allowed to vary randomly between ±10% of the reference value. Thin solid lines in the figure represent the bounding curves for these models. Figure 1 reinforces our initial conclusion that thermal conductivity is a highly influential variable in Equation (1); at great depths, k variation accounts for over 50% of the total variations in temperature permitted by a full ±10% perturbation in all variables. Figure 2 shows the results of a similar exercise for Equation (3), reinforcing the extremely strong influence of E on calculations of closure temperature as a function of cooling rate.

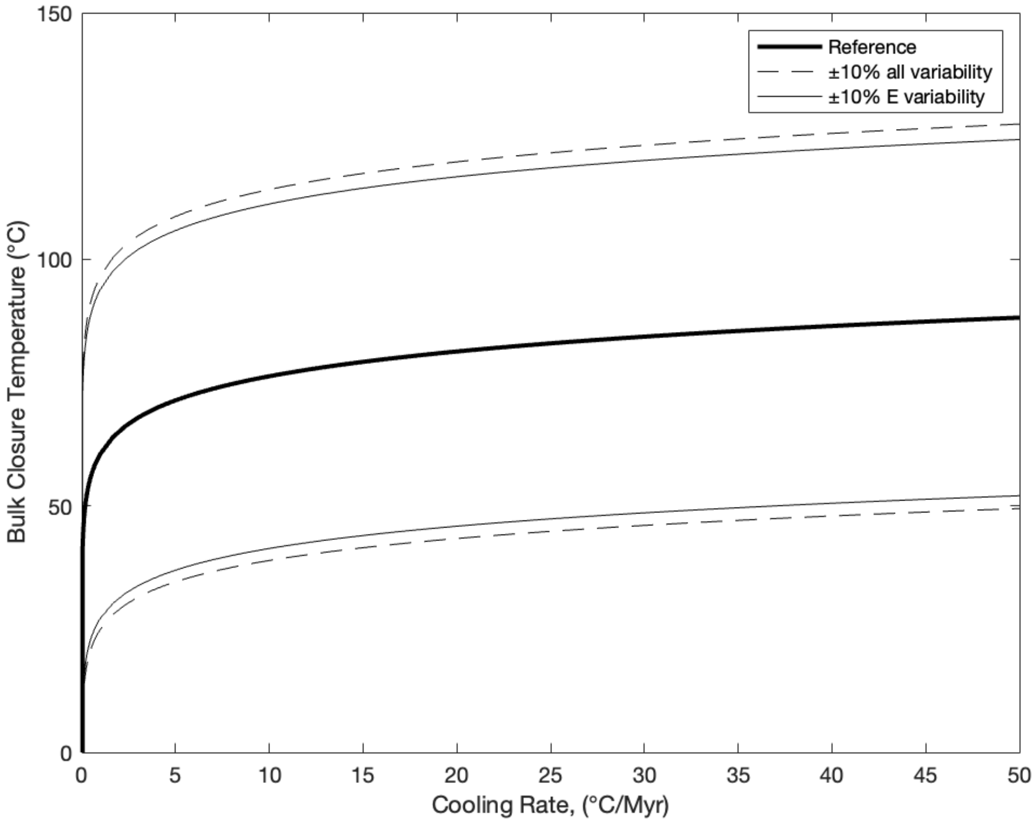

Figure 2. Bulk closure temperature change with cooling rate using parameter reference values of [15] (thick solid black line). The dashed black lines represent uncertainty in predicted exhumation rates from a Monte Carlo simulation using 10,000 realizations and varying all model parameters simultaneously by ±10%. The thin solid black line shows the result when only the top-ranked parameter (as identified by the Taguchi Method) is varied by ±10%. The comparison illustrates that this parameter alone accounts for a substantial portion of total uncertainty, supporting its identified significance.

3.2. Avoiding Misinterpretations of Sensitivity Analysis Results

Our study focused on the relative influences of parameters, each perturbed by a notional +10%. The same methods can be extended easily to test the impact of ± 10% perturbations by increasing the number of levels and, consequently, the number of experiments. In addition, the perturbations need not be a uniform percentage of the reference values. This is important because some reference variables are known better than others, and thus, a sensitivity analysis using a fixed percentage perturbation, as was the case for our study, could lead to misleading results if conducted uncritically.

One important caveat is that real-world applications of sensitivity analysis should use variations based on our understanding of reasonable uncertainty, whether that uncertainty is unquantifiable or quantifiable through experimentation. For example, thermal conductivity in the crust varies significantly by mineralogy and rock type and is inherently a function of both depth and temperature [11,24], such that our assumption of a ± 10% variability in k in this contribution is likely somewhat too low for practical applications. More significantly, volumetric heat production—H_{ns}—varies widely and three-dimensionally in the crust in ways not captured by a simple, one-dimensional model like that described by Equation (1) [11]. For this variable, realistic variations of up to 200% are plausible. Such differences among independent parameters could result in practical differences in the rank ordering of variables in Table 1.

3.3. Implications for Uncertainty Estimation in Thermochroology

It is not difficult to modify the sensitivity analyses described above to gain insights regarding how uncertainties in input parameters propagate into uncertainties in the results of calculations. However, for a more detailed assessment of how uncertainties propagate into modeling results, we favor using Monte Carlo methods because they are simple to implement and perform well (e.g., [25]). In some cases, however, the systems of equations necessary for such calculations are computationally cumbersome; for example, thermal-kinematic models require solving a transient heat equation in multiple dimensions. When paired with inverse approaches like Monte Carlo sampling, the computational cost of repeated forward model evaluations becomes a limiting factor. Those cases benefit from sensitivity analysis prior to complete uncertainty propagation to identify the most influential parameters and focus on their effects on modeling outcomes. In a companion paper, we will explore such exercises in detail.

For the presentation of thermochronologic data and either thermal-kinetic or thermal-kinematic modeling of those data, there is a widespread tendency for researchers to focus on the propagation of analytical and measurement uncertainties into model uncertainties (e.g., [25–29]). While this is understandable, the sensitivity analyses presented here suggest we ignore other sources of uncertainty at our peril. For example, all thermal history or thermal-kinematic modeling exercises rely either on (1) assumed closure temperatures for thermochronometers or (2) the diffusion or annealing parameters used to calculate closure temperatures. Our analysis of Equation (3) underscores the strong dependence of calculated closure temperature on activation energy. From the experimental study upon which Table 3 is based [15], the value for E derived from the experimental data carries a 3.5% 2σ uncertainty. Propagating just that uncertainty into Equation (3) results in a 16% uncertainty in closure temperature, assuming a 10 °C/Ma cooling rate. It is good practice to propagate all uncertainties—or at least all of the most impactful uncertainties—in thermal-kinetic or thermal-kinematic modeling studies.

4. Conclusions

We have reviewed two familiar approaches to sensitivity analysis, applying them to simple equations pertinent to thermal structure and closure temperature calculations. The results compared favorably with those obtained with the less familiar Taguchi Method, a widely used approach to sensitivity analysis in process engineering. The Taguchi Method is significantly more computationally efficient than fully exhaustive methods using full factorial or one-at-a-time designs and permits focused study of the most significant parameters in complex modeling exercises in thermal history and exhumation history research. Subsequent studies emphasizing improving input parameter definitions and minimizing uncertainties should improve overall modeling quality for more complex scenarios.

Author Contributions

S.S.: conceptualization; methodology; software; writing—original draft preparation; visualization K.H.: conceptualization; supervision; writing—reviewing and editing. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement

Not applicable.

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Conflicts of Interest

The authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

AI tools were utilized to improve the clarity and efficiency of author-generated MATLAB scripts used in this paper.

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