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Portable NIR Spectroscopy for Reliable Characterization of High-Intensity Radiating Objects: Statistical vs AI-Based Modelling

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Abstract

Portable near-infrared (NIR) spectroscopy offers a powerful non-contact approach for characterizing high-temperature radiating surfaces, enabling in-situ temperature diagnostics without intrusive sensors. However, achieving measurement reliability under intense thermal emission is challenged by detector nonlinearity, emissivity variation, and calibration instability. This study introduces a portable NIR framework integrating a blackbody calibration device (BBCD) with advanced data-driven modelling to improve accuracy and reproducibility across the 600–1200℃ range. We systematically compare statistical regression methods with AI-based architectures-including fully connected, convolutional, residual, and transformer networks for temperature prediction from spectral data. Results show that AI models, particularly transformer and ResNet architectures, outperform statistical baselines in both accuracy and generalization, especially under irregular sampling and noisy conditions. The findings highlight the importance of BBCD assisted calibration and robust preprocessing in achieving traceable, field-ready temperature measurements, advancing the application of portable NIR spectroscopy in industrial and scientific diagnostics.

1 Introduction

Portable near-infrared (NIR) spectroscopy is an increasingly vital technology for the non-destructive, in-situ characterization of materials. Its adoption is rapidly growing across diverse fields, from agriculture and pharmaceuticals to industrial process control, driven by the development of robust, cost-effective handheld instruments. In industrial settings, this technology is particularly valuable for characterizing high-temperature, incandescent ("blackbody-like") objects, offering a safe and immediate method for monitoring processes reaching up to 1200°C. By analysing the thermal radiation emitted directly from a surface, portable NIR pyrometry eliminates the need for sample extraction and reduces operator exposure to hazardous environments, aligning with the principles of green analytical chemistry [1].

Despite its potential, achieving accurate and repeatable temperature measurements of incandescent emitters with portable NIR spectroscopy presents significant challengees. The measurement integrity is often compromised by factors such as instrumental drift, spectral noise, and fluctuating ambient conditions. More critically, the high-intensity radiation can lead to detector saturation, while the target's surface emissivity, its efficiency in emitting thermal energy can vary significantly with temperature and oxidation state, introducing a primary source of error [2].

To address these challenges in thermal analysis, black-body calibration devices (BBCDs) serve as an essential reference standard. A BBCD provides a highly stable and uniform radiation source that approximates an ideal emitter (emissivity ≈ 1.0), allowing for the precise characterization and correction of the spectrometer's response. By calibrating the instrument against a traceable black-body source, it becomes possible to account for instrumental distortions and create a valid basis for converting spectral radiance measurements into accurate temperature predictions. This calibration step is critical for ensuring that the data collected in harsh field or factory environments is both reliable and comparable. By interleaving measurements of the unknown hot surface with calibration against BBCD spectra, one can better understand and constrain spectral system deviations and thus im-prove the robustness of downstream modelling.

Against this backdrop, the aim of the present study is to systematically compare two modelling paradigms—classical statistical calibration methods versus modern AI-based (machine learning or neural network) approaches—for the prediction of surface temperature from NIR spectral data of high-temperature radiating objects. We use a portable NIR spectrometer in conjunction with a calibrated BBCD reference to collect training and test spectra, then evaluate and benchmark the accuracy, repeatability, and robustness of both modelling approaches. Our goal is to assess which of these two approaches offers superior performance (or under what conditions each excels) in the context of high-intensity thermal emission, thereby guiding future design of portable NIR systems for high-temperature applications.

2 State of The Art

Portable NIR spectroscopy has rapidly evolved from compositional analysis to applications in thermal emission and temperature diagnostics. Advances in sensor miniaturization and calibration stability now enable reliable operation in high-temperature environments, supporting integration into industrial monitoring and quality control systems [3]. The fusion of NIR sensing with pyrometric modelling allows non-contact surface temperature estimation, providing a viable alternative to contact thermometry. Yet, most studies remain limited to laboratory-scale blackbody or bench-top systems, with few addressing the challenges of true portability [4]. Transitioning to field-deployable instruments introduces new uncertainties that demand enhanced hardware precision and data-driven analytical approaches.

Despite recent advances, measurement accuracy and reproducibility in portable NIR pyrometry remain challenging. Variations in detector sensitivity, optical alignment, and temperature-dependent emissivity continue to limit precision [5]. Issues such as data scattering, non-linearity, and low signal-to-noise ratios further complicate regression-based temperature estimation. Moreover, calibration transfer between instruments is often unreliable, as environmental effects - vibration, ambient light, and thermal drift - distort spectral responses. Studies by Pohl et al. [5] and Yang et al. [6] show that even with well-characterized blackbody references, maintaining accuracy in field conditions demands dynamic calibration and uncertainty modelling. Hence, standardized calibration frameworks and adaptive, transfer-learning–based models are increasingly required to ensure robustness.

To overcome these limitations, recent research trends are converging toward the integration of blackbody calibration devices (BBCDs) with machine learning and deep learning models to enhance the reliability of thermal spectral analysis [7]. Blackbody-based calibration offers a traceable physical standard that constrains emissivity-related errors, while data-driven models can learn complex, nonlinear mappings between spectra and temperature more effectively than traditional regression [8]. Hybrid approaches that combine physical calibration and AI modelling—such as convolutional neural networks (CNNs) or hybrid chemometric–ML models—have demonstrated improved accuracy in infrared thermography and spectral pyrometry [9]. For instance, Wang et al. [7] used deep convolutional architectures to predict emissivity-corrected temperature fields from NIR spectra, outperforming polynomial regression and PLSR in both accuracy and generalization. Similarly, Zhang et al. [10] reported that transformer-based regression networks achieved higher robustness under varying optical noise conditions compared to statistical baselines. However, systematic benchmarking between purely statistical and AI-based modelling approaches under calibrated, portable measurement conditions remains limited—representing the critical research gap addressed in this study.

3 Materials and Methods

This study explores the integration of portable near-infrared (NIR) spectroscopy with advanced data-driven modelling to achieve reliable temperature estimation of high-temperature radiating (blackbody-like) objects. The work investigates how calibration accuracy, ensured through a Blackbody Calibration Device (BBCD), and model architecture selection influence prediction robustness. We compare the performance of statistical regression and AI-based neural models—including Fully Connected Networks (FCN), Convolutional Neural Networks (CNN1D), Residual Networks (ResNet1D), and Transformer-based architectures—across irregularly sampled temperature datasets (600–1200 °c).

3.1 Black Body Calibration Device and Measurement Reliability

The Blackbody Calibration Device (BBCD) serves as the primary radiometric reference for ensuring the accuracy and reliability of spectral temperature measurements. It provides a uniform and traceable radiation source approximating an ideal blackbody (emissivity 0.99 ± 0.01). The emitted spectral radiance is described by Planck's law:

$$L_\lambda(T) = \frac{2hc^2}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right)-1} \quad (1)$$

Where h is Planck's constant, c the speed of light, k_B the Boltzmann constant, λ the wavelength, and T the temperature.

Under high-radiance conditions (600-1200°C), portable NIR spectrometers can suffer from detector nonlinearity, optical scattering, and spectral drift. By calibrating each measurement against the BBCD spectrum, the system response function $H(\lambda)$ can be characterized:

$$H(\lambda) = \frac{I_{measurement}(\lambda)}{L_\lambda(T_{BBCD})} \quad (2)$$

Where $I_{measurement}(\lambda)$ is the raw detector signal. The corrected spectral intensity of an unknown emitter is then:

$$I_{corrected}(\lambda) = \frac{I_{sample}(\lambda)}{H(\lambda)} \quad (3)$$

This calibration minimizes systematic errors due to grating efficiency and detector sensitivity variations, ensuring that subsequent temperature predictions reflect physical surface emission rather than instrumental artifacts. The BBCD and setup it shown in Figure 1. For data acquisition, an SR-200N-33 black-body radiator was utilized, providing a temperature range of 50 to 1200 °C, with a thermal accuracy of ±2 °C and a thermal stability of ±0.50 °C. The aperture of the black-body radiator was equipped with a protective quartz glass window, a collimator (ThorLabs F260SMA-1550), and an optical fiber (ThorLabs M44L02), which was connected to the NIRQUEST NQ5200147 NIR spectrometer.

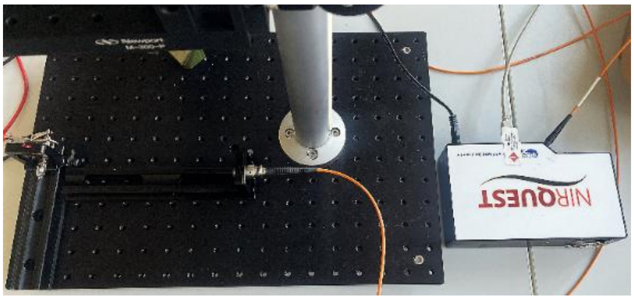

Figure 1 The view on the laboratory set-up used for experimentation.

3.2 Statistical Approach

Using the system response function *H(λ),* the characteristic shape of any measured spectrum can be reconstructed as follows:

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$$I_{reconstructed}(T,\lambda) = L_\lambda(T_{BBCD}) \cdot H(\lambda) \quad (4)$$

The temperature corresponding to the best-fitting reconstructed spectrum is determined by minimizing the quadratic error between the difference of $I_{reconstructed}(T,\lambda)$and $I_{measured}(\lambda)$. For the purposes of calibration and temperature estimation, two separate datasets are utilized. The system response function is determined using the calibration dataset, while temperature estimation is performed on the test dataset. The results are improved by estimating the temperatures of the calibration dataset and subtracting the resulting MAE from each temperature estimation.

3.3 AI-Based Temperature Prediction Models

To complement the calibration-based measurements, this part of the study focuses on data-driven temperature prediction using artificial-intelligence (AI) models [11-13]. The spectral-to-temperature relationship in high-temperature radiating systems is inherently non-linear and multivariate, making conventional regression models less effective when data are noisy, irregularly sampled, or influenced by complex emissions.

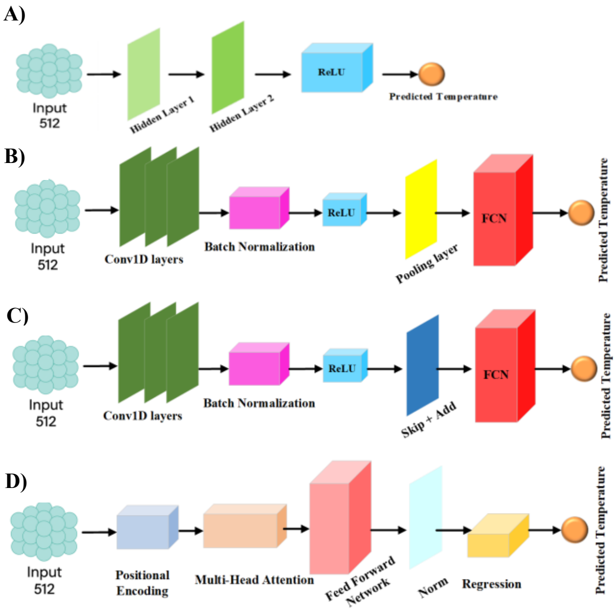

Figure 2 A) FCN architecture diagram. B) 1D-CNN block diagram with convolution and pooling layers. C) Residual block diagram showing skip connection. D) Transformer encoding architecture diagram.

Therefore, we implement and compare four representative deep-learning architectures [14]—Fully Connected Network (FCN), 1D Convolutional Neural Network (CNN1D), Residual Network (ResNet1D), and Transformer Encoder - each designed to capture distinct feature hierarchies within the NIR spectra. Model architectures designed for the study are presented in Figure 2 A-D. These models are trained on both semi-regular and highly irregular datasets (600–1200 °C) to evaluate their ability to generalize under varying sampling conditions. The results provide insight into how architectural choices and learning mechanisms affect robustness, interpretability, and predictive accuracy in portable NIR thermometry.

4 Results

The developed diagnostic pipeline was evaluated on the measured spectral dataset spanning 600–1200°C, where intensity–wavelength curves were collected from irregular temperature intervals. Therefore 80 % of the data were used for training and 20 % for testing to ensure unbiased generalization. The performance of four deep learning models—Fully Connected Network (FCN), 1D Convolutional Neural Network (CNN1D), Residual Network (ResNet1D), and Transformer Encoder—was compared against conventional statistical regression baselines, which yielded notably higher prediction errors. While traditional statistical models struggled to represent the complex, nonlinear relationships between radiative spectral features and temperature, the proposed deep architectures effectively captured spectral dependencies and local emission patterns, resulting in lower Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) – Table 1. This demonstrates the advantage of data-driven learning combined with physics-informed preprocessing, such as baseline correction, smoothing, and normalization.

The dataset comprises NIR emission spectra between 1000 nm and 2200 nm, measured at discrete temperature points from 600-1200°C. The produced irregular and sparsely distributed samples, reflecting realistic industrial monitoring conditions where stable temperature increments cannot always be maintained. To enhance data quality: Asymmetric Least Squares (ALS) baseline correction removed broad background trends. Savitzky–Golay smoothing reduced high-frequency noise. Z-score or percentile normalization ensured intensity comparability across runs.

Among the AI models, the Transformer Encoder achieved the best overall accuracy, followed by FCN, while CNN1D and ResNet1D performed moderately. The FCN showed consistent performance (MAE ≈ 2.4 K), demonstrating its strength in learning global relationships between full-spectrum inputs and temperature. However, its dense architecture lacks spatial awareness of spectral neighbourhoods. The CNN1D and ResNet1D networks leverage convolutional kernels to extract local spectral features, but their performance degraded slightly due to irregular sampling and non-uniform temperature spacing, which weaken the locality assumption of convolutional filters. The Transformer Encoder exhibited the highest robustness to data irregularities. Its self-attention mechanism captures global dependencies between wavelengths, allowing it to dynamically focus on temperature-sensitive spectral regions even when sampling density varies. This explains its superior accuracy and stability across normalization methods.

Two normalization strategies were evaluated: standard-score (z-score) normalization and percentile scaling. As summarized in Table 1, both normalization methods produced comparable overall accuracy trends. However, standard-score normalization yielded slightly better performance for most models, especially for the Transformer Encoder, achieving the lowest MAE (1.97 K) and RMSE

(2.53 K). This suggests that z-score scaling preserved relative spectral dynamics critical for temperature inference, whereas percentile scaling, while more robust to outliers, may have slightly compressed informative radiative contrasts.

The Transformer Encoder, with its attention-based mechanism and positional encoding, remained robust to these irregular patterns, maintaining accuracy even in sparse temperature ranges. Measurement reliability was further influenced by spectral noise, detector saturation, and scattering from oxidation or misalignment. These effects caused baseline drift and distorted emission intensity. To counteract them, an Asymmetric Least Squares (ALS) baseline correction was applied, followed by Savitzky–Golay smoothing, effectively suppressing low-frequency background variations and high-frequency noise while preserving relevant emissivity-driven features.

The results reveal that while statistical models fail to handle complex emission behaviours, deep learning models, particularly the Transformer Encoder, successfully generalize across heterogeneous datasets. The improvement can be attributed to its ability to model non-linear, non-local, and context-dependent spectral interactions that govern thermal emission. The findings emphasize that appropriate normalization, feature-aware model architectures, and physics-informed preprocessing (e.g., BBCD correction) are all critical for reliable temperature prediction under real measurement conditions—especially in portable NIR devices operating under high-radiance and device-dependent transfer functions.

	Normalization method			
	Standard Score		**Percentile**	
Results(K) / **Method**	**MAE**	**RMSE**	**MAE**	**RMSE**
Statistic	-3.15	5.68	-2.83	4.26
FCN	2.43	3.24	2.50	3.24
CNN1D	4.74	6.16	4.28	5.71
ResNet1D	5.09	6.42	4.43	5.53
Transformer Encoder	**1.97**	**2.53**	**2.01**	**2.54**

Table 1 Accuracy comparison of designed models.

5 Conclusions

This study demonstrated the potential of portable NIR spectroscopy for accurate temperature characterization of high-temperature radiating objects in the 600–1200 K range. Through systematic comparison, AI-based models particularly the Transformer and ResNet architectures outperformed classical statistical approaches in accuracy, robustness, and generalization, especially under irregular sampling and noisy measurement conditions. Incorporating blackbody calibration devices (BBCDs) proved essential for maintaining measurement traceability and reducing bias in spectral–temperature mapping. The results highlight that reliable preprocessing, coupled with advanced learning architectures, enables portable NIR systems to achieve laboratory-grade performance in challenging industrial environments.

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