

Article

Experimental and Statistical Analysis of Iron Powder for Green Heat Production

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Abstract: In the current investigation, a novel methodology was employed to assess iron powder as a recyclable and sustainable energy carrier. Concurrently, an examination of the modeling of iron powder ignition and the ensuing heat output from the burner was undertaken. The flame temperature was determined by examining the light intensity emitted by the particles as they melted, which is directly related to the particle's cross-sectional area. An account of the characterization of the experimental procedure, validation, and calibration is presented. Through measurements, distinct one-to-one correlations have been established between the scales of flame combustion and the temperatures of particles of varying sizes of iron. Additionally, a theoretical model for the combustion of expanding particles, particularly iron, within the diffusion-limited regime has been rigorously developed. This model delves into the spectra acquired from particle flames within the burner, utilizing Partial Least Squares Regression (PLSR) and Principal Component Analysis (PCA). This study investigates the use of optical fiber spectroscopy to predict flame temperature and assess iron powder size. The aim was to investigate how different sizes of iron powder affect flame temperature and to create calibration models for non-destructive prediction. The study shows that smaller particles had an average temperature of 1381 °C while larger particles reach up to 1842 °C, demonstrating the significant impact of particle size on combustion efficiency. The results were confirmed using advanced statistical methods, including PLSR and PCA, with PCA effectively differentiating between particle sizes and PLSR achieving an R^2 value of 0.90 for the 30 μm particles.

Keywords: iron powder; sustainable energy; flame combustion; PCA; PLSR



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1. Introduction

In order to address the pressing issue of greenhouse gas emissions, the exploration of novel combustion technologies and alternative fuels has become imperative. Among these innovations, metal fuel cycles have emerged as promising avenues for clean power generation, as delineated in recent literature [1–3]. This approach offers several distinct advantages [4]. First, metal powders offer significantly higher energy density than hydrogen, thereby improving both storage and transportation efficiency. Second, combustion of metals incurs no CO₂ emissions, thereby presenting a viable solution to environmental concerns and mitigating the impacts of global warming. Third, the combustion byproducts, primarily metal oxides, can be captured and regenerated into metal powders through the utilization of renewable energy sources like solar and wind power, rendering metal powders as highly sustainable energy carriers [4,5]. Metals such as magnesium, boron, and aluminum, which are sometimes mentioned as energy carrier or additives due to their highly exothermic reactions have recently attracted great interest as viable candidates for metal fuel cycles. Conversely, despite its comparatively lower energy release, iron holds promise as a viable metal fuel owing to its widespread availability, cost-effectiveness,

moderate flame temperature, and propensity for heterogeneous combustion. However, the understanding of iron combustion remains in its infancy, with scant literature available on both the theoretical and experimental fronts. Comprehensive investigations into the flame temperatures of iron powder and its flame propagation were recently carried out by researchers at McGill University and Eindhoven University of Technology [4–9], building upon pioneering efforts in the field initiated approximately three decades ago by Sun et al. [10–12]. Concurrently, the utilization of iron powders as a sustainable energy carrier has garnered increasing interest among researchers [13–15]. Iron powder, known for its high energy density, has the potential to generate high-temperature flames. Reducing emissions from high energy-density carriers is crucial for advancing our understanding of the dynamic optimization of combustion processes and enhancing the application of these fuels in combustion chambers [16]. However, experimental investigations into iron particle combustion remain limited. Recent studies have increasingly focused on the ignition of iron powder in air as a means to generate clean and renewable heat. These efforts have also led to the development of systems capable of utilizing iron powder as a renewable energy source [7]. Despite these efforts, research on the spectral analysis of iron powder flames remains limited, and statistical analyses of these spectra have not yet been conducted. Preprocessing is a critical step in most spectrometric analyses, with the choice of method dependent on the specific data and requiring either domain expertise or a trial-and-error approach to achieve optimal results [17]. Recent work by Yao et al. explored the impact of accounting for the spectral characteristics of ignited iron powder flame, specifically focusing on the spectral range between 600 and 1000 nm [18]. Additionally, their study examined the relationship between spectral emission and particle temperature as a function of wavelength. Additionally, Ning et al. estimated the temperature of ignited particles using spectrometry and spectral fitting techniques [19]. Tang et al. examined the flame spread of iron dust suspensions (3–27 μm) in vertical tubes, where gravity served as a force multiplier. They determined the temperature of the burning particles by applying Planck's equation to linearly fit the spectral intensity, following the spectroscopic recording of typical iron flame spectra. Their findings revealed that the emitted particles had wavelengths ranging between 500 and 850 nm [20]. The current research aims to introduce a novel concept: the iron powder flame, characterized by its distinct stabilization within a radiant burner employing a vortex configuration. The creation of a bespoke apparatus tailored to stabilize vortex-based, counterflow iron flames marks a significant advancement in facilitating the thorough investigation of fundamental flame characteristics. This undertaking integrates state-of-the-art optical diagnostics, including absorption and emission spectroscopy techniques [21–23]. Essentially, comprehending the fundamental properties of iron flames is paramount in the design of metal fuel combustors and engines. These advancements play a pivotal role in advancing the realization of a sustainable, low-carbon economy rooted in the utilization of metal-based fuels [24–26]. This research focused on the investigation of light reflection, emission, and absorption across different energy levels in various materials, providing valuable insights into the samples. However, due to the high-dimensional and potentially highly correlated nature of the data, analysis and interpretation can be challenging. Preprocessing is often required to remove extraneous variance, such as effects caused by fluctuations in temperature, or light scattering. Analytical techniques like partial least squares regression (PLSR) and principal component analysis (PCA) are commonly employed to address these challenges [17,27]. This research introduces a novel approach for assessing iron powder combustion as a sustainable energy carrier. By using optical fiber spectroscopy and statistical methods (PLSR and PCA), it investigates the impact of iron powder size on flame temperature and combustion efficiency. Unlike previous studies, this work provides comprehensive spectral analysis and predictive modeling, offering insights for optimizing iron-based combustion systems and enhancing burner designs for cleaner energy production. This study aims to investigate the effectiveness of optical fiber spectroscopy in predicting flame temperature and assessing iron powder size at four different levels. The research will analyze the influence of iron powder size and develop calibration

models for non-destructive prediction of flame temperature. It will also determine the ability to discriminate flames based on particle size using Principal Component Analysis (PCA) on the PC plot for each specific iron powder composition. The research will utilize spectral processing techniques and contrast these methods with empirical data obtained from flame temperature measurements using data acquisition sensors. This comparative study will provide a comprehensive insight into the effects of iron particle size on exhaust gas temperature, which is crucial for the development of an efficient iron burner design. In the study, the ignition mechanism of the iron particles is investigated using a fiber optic spectrometer that measures the temperature of the iron powder particles and simultaneously records their movement with a camera. The temperature of the burner exhaust gas is analyzed in relation to the fluctuations of the iron powder particle size at the burner outlet.

2. Materials and Methods

In this study, the TU/e's (Eindhoven University of Technology) MC² burner is applied [7,26] for the experiments conducted, while micron-sized iron particles were employed, obtained from TLS Technik GmbH & Co., Niedernberg, Germany. These particles have a nominal diameter ranging from 20 to 50 μm and exhibit a purity of 99.8%.

The initial particle ensemble was fractionated using a vibratory sieve shaker (RETSCH AS 200, Haan, Germany, vibratory sieve shaker equipped with RETSCH woven wire mesh sieves). Following this, the particle size distributions, represented as projected area diameters for each fraction, were assessed with a calibrated optical microscope, coupled with the standard particle analysis functions of ImageJ software version 1.52; the particle size distribution of sieved fractions is shown in Figure 1. On the other hand, the image of the unsieved iron powder is shown in Figure 2. Powders closer to the scanning electron microscope camera are brighter here, and those further away are darker.

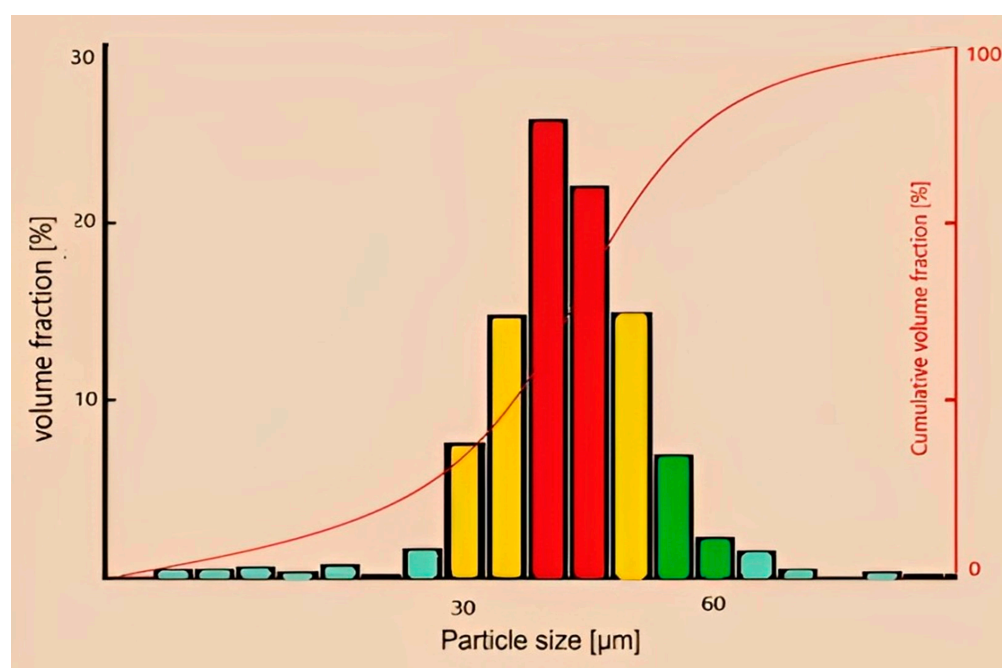


Figure 1. Analysis of the particle size distribution of sieved fractions, including the arithmetic mean and the cumulative distribution curve. Adapted from [25].

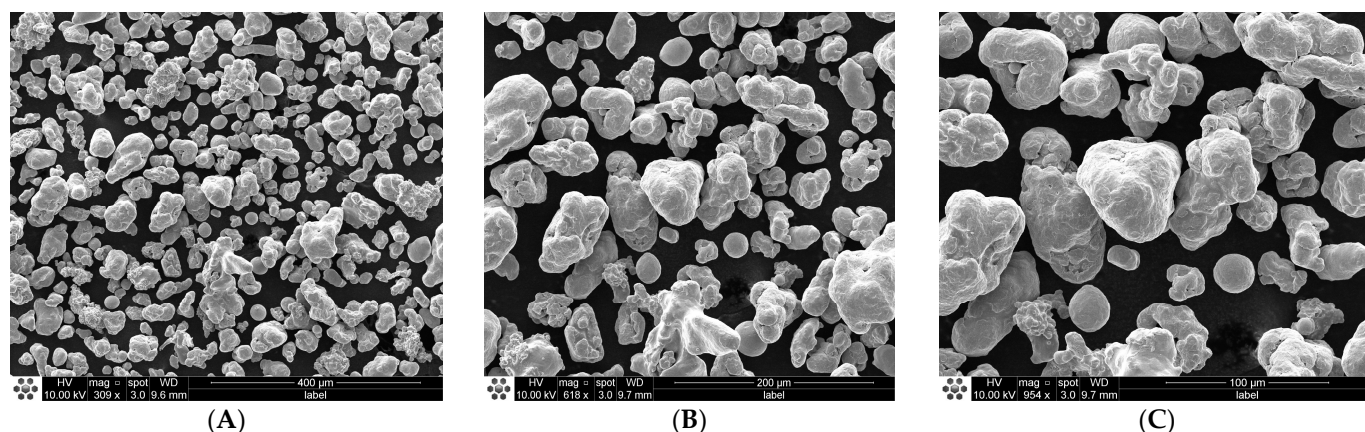


Figure 2. Scanning Electron Microscope (SEM) image of unsieved iron powder (amorphous-shaped iron powder from POMETON Co). Images in order from left to right from large scale to small scale, (A): 400 μm , (B): 200 μm , and (C): 100 μm .

2.1. Estimation of the Flame Spectrum

A StellarNet Inc, Tampa, FL, USA, infrared spectrometer, with a wavelength range extending from 877 to 1755 nm and a resolution of approximately 0.5 nm, was utilized to acquire time-integrated spectra of the combusting particles. To ensure accuracy, the spectrometer was calibrated using a reference lamp source using a tungsten ribbon. The spectrometer was calibrated using a certified tungsten ribbon lamp calibrated by the National Institute of Standards and Technology (NIST) [25]. During the experimental procedure, light emissions from incandescent particles combusting within a 2 s interval were captured using a collimator and transmitted to a spectrometer through a fiber-optic cable. The collimator was positioned 15 cm from the burner tip, consistent with the distance used during the calibration of the tungsten ribbon (see Figure 3 for a typical iron flame in the burner). To process the raw spectral data, background noise was first subtracted, and the resulting signal was then multiplied by calibration coefficients. The spectra were subsequently analyzed within the wavelength range of 1000–1600 nm. This range was selected due to the enhanced sensitivity of the spectrometer in this region, which facilitates accurate determination of the particle temperatures. Assuming that the emissivity of iron is invariant with wavelength in the current wavelength window—thus, treating it as a grey body—temperature determination was conducted by fitting Planck’s law to the recorded spectral data using the least-squares method. This approach is conventionally known as multi-wavelength pyrometry. It is noteworthy that the time-integrated spectrum predominantly reflects radiation from particles at or near their peak temperature. As a result, the temperature recorded by the spectrometer is a close approximation of the peak temperature of these particles, which is chiefly determined by those exhibiting higher thermal energy. The iron particles underwent spectral analysis within the visible/near-infrared spectrum, spanning from 1000 to 1600 nanometers, utilizing a portable analytical system (see Figure 4 for a typical plot of a spectrometer and Figure 5 for a typical iron flame in the burner and the position of the spectrometer). As shown in Figure 4, the initial spectrum is this way so that no preprocessing has been done on it; so, it is the spectrum of the iron powder flame. This primary spectrum is used for fitting in order to obtain the flame temperature. These primary spectra are later pre-processed, and then statistical analysis is performed on them. In Figure 4 the x -axis spans from approximately 800 nm to 1800 nm. This range corresponds to the near-infrared (NIR) part of the electromagnetic spectrum. The y -axis (counts) represents the intensity or the number of photons detected at each wavelength. Higher counts indicate a stronger detected signal at that specific wavelength. The dip observed between 1300 nm and 1400 nm suggests some form of absorption or scattering event occurring at this wavelength. This could indicate the presence

of a material or compound that absorbs light in that specific region, causing a reduction in the detected signal.

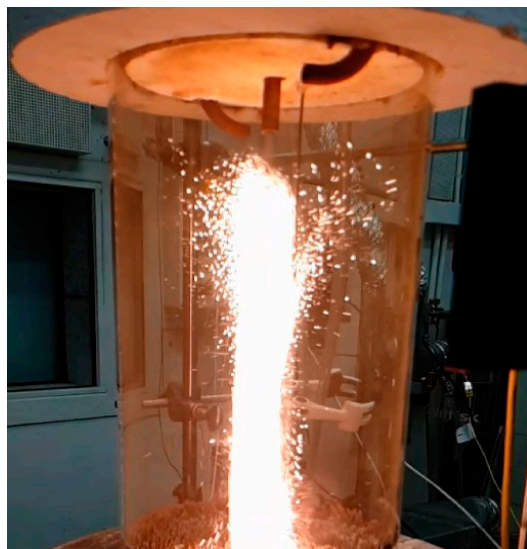


Figure 3. Iron powder flame inside the burner.

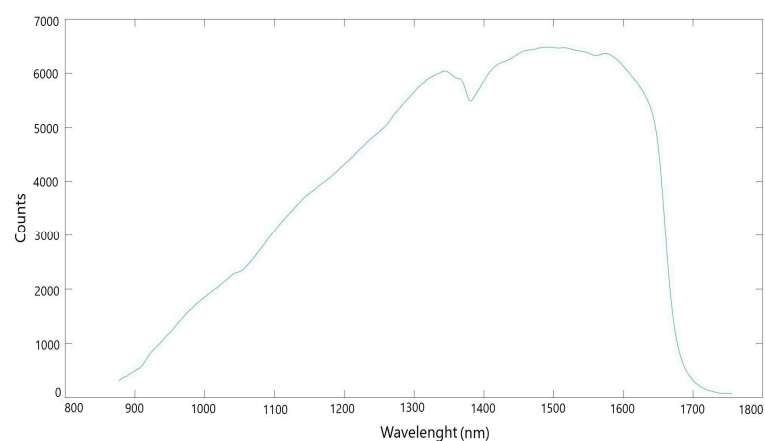


Figure 4. Example of spectrum without preprocessing.

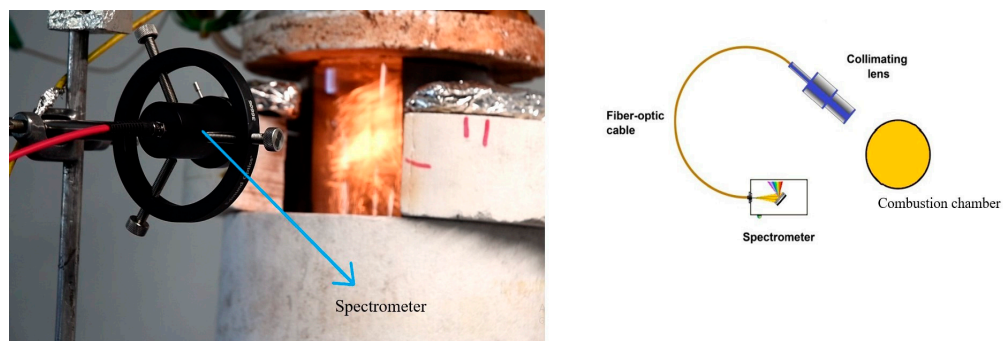


Figure 5. Placing the spectrometer next to the ignition chamber.

In this arrangement, the reflected constituent was quantified through a spectrometer. The data acquisition process was orchestrated seamlessly via the specialized software.

The instrument setup comprised an amalgamation of four components. First, a portable spectrometer was carefully integrated with a fiber optic probe. The investigation

utilized a specialized “step index” fiber optic probe, originating from the StellarNet Inc. infrared spectrometer. Operating in unison, this spectrometer was paired with a CCD sensor, characterized by a high-resolution 2048-pixel matrix. The sensor is able to discern the intensity of each wavelength signal with a wavelength resolution of 0.577 nanometers.

2.2. Iron Powder Mixing and Injection Systems

The experimental apparatus comprises several integral components: the air inlet, which regulates essential airflow; the metal powder dispersion system, ensuring a consistent supply of iron powder for combustion; spectroscopy, capturing and analyzing emitted light to provide insights into the combustion process; and the data collector device, which organizes and records the data from the spectroscopy. This coordinated arrangement is critical for performing experiments and obtaining accurate data on iron powder combustion.

The experimental setup, involves putting iron powders inside a bottle-shaped container, where a controlled airflow carrier gas is introduced at one end. This system ensures precise interaction between the iron powder and the airflow, crucial for achieving the study’s experimental objectives. The energy generation process begins by introducing air through tubes arranged to create a swirling motion, followed by the addition of iron–air dust through a fuel inlet. The burner is preheated with a pair of semi-cylindrical radiant electric heater ignition aids while a cyclone enhances suspension dynamics, promoting effective component separation. Gas temperature monitoring is conducted using thermocouples strategically placed at key points, including beneath the outlet and atop the radiant heater, allowing for detailed thermal behavior analysis. A ceramic fiber insulation plate, 50 mm thick, serves as the lid, maintaining system stability and contributing to efficient energy generation (see Figure 6) [26].

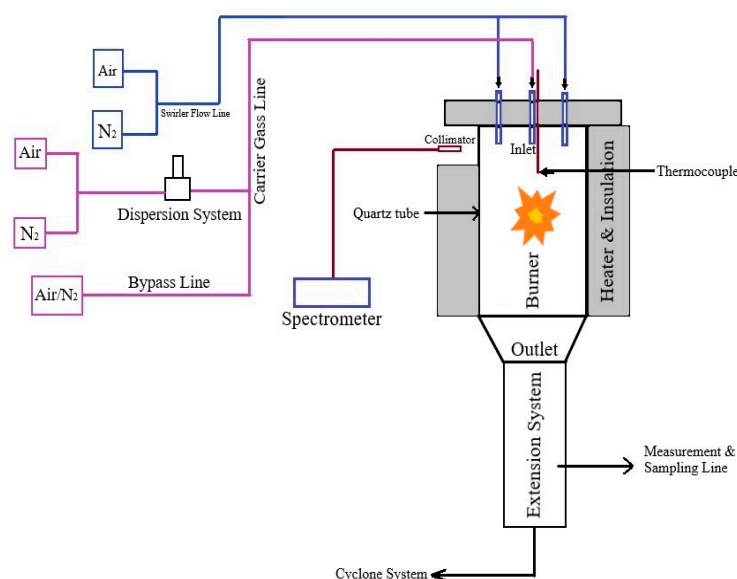


Figure 6. Schematic of cyclonic combustion.

The burner configuration features two Type VF 180 12 heating elements from Fibercraft, each with a power output of 1.7 KW, housed in a quartz tube from Squall Hapert with an inner diameter of 130 mm, a length of 500 mm, and a volume capacity of 0.007 m³. The iron powders, sifted and carefully selected, were used in the MC² burner with a mass flow rate of 0.6 g/s across all experiments. Additionally, the study examined the combustion behavior of iron particles smaller than 20 µm, 30 µm, 40 µm, and 50 µm. A customized MATLAB (version R2021b) algorithm, developed with components from the IDL particle tracking library, was used to analyze captured images. This algorithm accurately determined the centroid coordinates, sizes, and intensities of flames by summing the grayscale values of pixels within each bright region, providing comprehensive insights into the particle

flame behavior [28–30]. Utilizing a scanning electron microscope (SEM), we captured detailed images and analyzed dispersion patterns to determine particle sizes, significantly enhancing our understanding of combustion residue behavior and positively influencing research decision-making.

2.3. Experimental Analysis

At the beginning of the test, the heaters were activated to allow sufficient time to reach a level in which the temperature inside the burner stabilized. Then, the temperature inside the burner was measured and the heating by the electric heater resumed until it reached 800 °C. Then, the test began with the initiation of the air inlet and the combustion of the iron powder. After a stabilized flame was established, the electric heater was turned off. It should be noted that the air flow has no direct influence on the surface temperature, which is why the surface temperature is considered constant throughout the test [31].

The exhaust pathway of the burner, equipped with a temperature sensor, facilitates the release of combustion byproducts and continuously provides real-time temperature data. This data, which is influenced by variables such as iron powder particle size, is crucial for analyzing and optimizing combustion efficiency. Monitoring temperature fluctuations helps researchers understand how these factors impact combustion processes, thereby aiding in the design and operation of such burner systems. The exhaust gas temperature is checked alongside the particle flame temperature to provide a comprehensive understanding of the combustion process. By measuring both temperatures, researchers can better understand heat transfer, identify potential inefficiencies or incomplete combustion, control emissions, and detect any abnormal conditions that could affect the system's operation. Temperature measurements were conducted using thermocouples and a spectrometer, which analyzed the flame spectra between 1000–1600 nm. A fiber-optic probe captured light emissions, and pre-calibrated tools ensured accuracy in temperature determination via fitting of Planck's law.

2.4. Spectral Preprocessing (MSC, SNV, Derivatives, and Smoothing)

For this purpose, the spectra taken from the flame particles of iron powder, which includes data in the nanometer wavelength, were examined (an example of the spectrum is shown in Figure 4). Spectral data obtained from spectroscopy are often high-dimensional and can exhibit strong correlations, making analysis and interpretation challenging. Preprocessing is necessary to remove extraneous variance, such as effects caused by temperature fluctuations or light scattering. In this study, the analysis was conducted using the Unscrambler software (version 10.5, Camo process, Norway), employing Principal Component Analysis (PCA) on Vis/NIR spectral data along the wavelength for each size of iron powder with 20 repetitions for each size to identify sample groupings and outliers. The preprocessing of spectra involved Multiplicative Scatter Correction (MSC) and derivative calculations via the Savitzky–Golay transformation to enhance the quality of the data. These processed spectra were then utilized to develop calibration models correlating with the parameter of interest—the particle flame temperature—using PLSR [32,33]. The study highlights the importance of pretreatment methods such as smoothing and baseline correction to reduce noise and correct baseline variations in experimental data. Savitzky–Golay smoothing was used to address noise in the spectra, while MSC corrected baseline shifts caused by light scattering phenomena in fresh samples. The Standard Normal Variate (SNV) technique was employed to correct slope variations and scatter effects, with derivative methods enhancing spectral differences but potentially increasing noise. To manage this, initial smoothing was applied using the Savitzky–Golay algorithm to ensure accurate data analysis [34].

2.5. Partial Least Squares Regression (PLSR) and Principal Component Analysis (PCA)

In PLSR, latent variables are iteratively constructed to maximize the covariance between the spectral matrix and the response variable of particle flame temperature, with outliers identified as measurement errors being excluded before reconstructing and rede-

veloping the models using the Unscrambler software [35]. Principal Component Analysis (PCA), introduced by Pearson and Hotelling, transforms correlated variables into a set of uncorrelated principal components, with the number of components equal to or fewer than the original variables. PCA optimizes variance capture through orthogonal components, simplifying datasets by reducing the number of variables while retaining the information of the original data [33]. PCA was selected to reduce the dimensionality of high-dimensional spectral data, revealing patterns and groupings in particle sizes. PLSR was employed to create accurate predictive models for flame temperature, maximizing covariance between spectral data and response variables.

3. Results and Discussion

3.1. Experimental Results

The study employed spectrometry to measure the temperatures of burning iron particles of varying sizes, with precise calibration to ensure accuracy. The analysis of particles categorized into four size ranges: under 20 μm , 30 μm , 40 μm , and 50 μm ; revealed a near linear relationship between particle size and temperature. Smaller particles averaged 1381 $^{\circ}\text{C}$, while larger particles reached temperatures up to 1842 $^{\circ}\text{C}$ (as shown in Figure 7). This trend underscores the effect of particle size on particle flame temperature, with larger particles generating higher temperatures. These findings are pivotal for optimizing combustion processes and advancing combustion science, leading to enhanced control and efficiency in energy utilization [31].

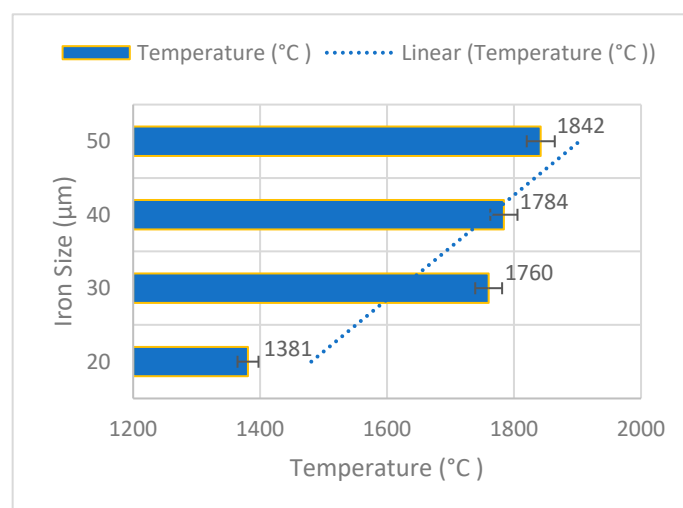


Figure 7. Mean temperature variations of iron particles.

In this investigation, after the start of the test, the gas temperature of the outlet emanating from the burner was recorded as a fraction of time after ignition. Subsequently, the temperature readings were consistently monitored until the conclusion of the test. In total, data points were acquired at distinct junctures throughout the duration of the experiment. The data are shown in Figure 8.

Following the findings depicted in Figure 8, there is a concurrent rise in the gas temperature recorded at the outlet for each iron particle size. Specifically, there is a discernible elevation in the temperature at the outlet of the burner chamber with time. This empirical relationship underscores the direct correlation between these influential parameters and the resultant temperature profile within the chamber. Smaller particles displayed a steeper temperature increase gradient compared to larger particles, influenced by their heating intensity and heat release rate. Specifically, particles smaller than 20 μm increased at 0.357 $^{\circ}\text{C/s}$ (70 $^{\circ}\text{C}$ to 228 $^{\circ}\text{C}$ in 490 s), 30 μm particles at 0.352 $^{\circ}\text{C/s}$ (58 $^{\circ}\text{C}$ to 222 $^{\circ}\text{C}$ in 460 s), 40 μm particles at 0.169 $^{\circ}\text{C/s}$ (26 $^{\circ}\text{C}$ to 118 $^{\circ}\text{C}$ in 550 s), and 50 μm particles at 0.156 $^{\circ}\text{C/s}$ (32 $^{\circ}\text{C}$ to 100 $^{\circ}\text{C}$ in 430 s). These findings highlight the impact of particle size

on combustion dynamics, with smaller particles leading to faster temperature increases, providing critical insights into how different iron powder sizes affect temperature changes during combustion [36,37]. The observed relationship between iron particle size and combustion temperature is critical for enhancing iron powder combustion technology. By optimizing particle sizes, industries can achieve higher combustion efficiency, leading to more sustainable energy generation, particularly in high-temperature industrial processes. To gain a comprehensive understanding of the combustion process, it is essential to measure not only the temperature of the particle flame but also the temperature of the exhaust gas. By assessing both temperatures, researchers can better comprehend heat transfer, identify inefficiencies or incomplete combustion, regulate emissions, and detect any anomalous variables that may affect the system's performance [27]. In this experiment, the study's controlled lab environment might not fully reflect real-world combustion systems, potentially affecting the generalizability of the results.

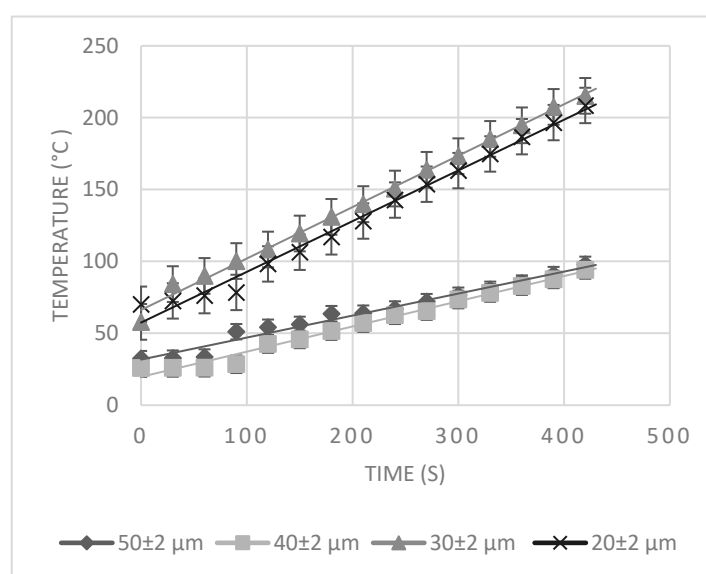


Figure 8. Influence of iron powder size on the exit temperature from the burner.

The results obtained from the Scanning Electron Microscopy (SEM) analysis are depicted in Figure 9, with an emphasis on particles smaller than 20 μm and those around 50 μm in size. Figure 9A is for particles smaller than 20 μm , and Figure 9B,C is shown for particles with a size of 50 μm . As demonstrated in Figure 9, an increase in particle size is associated with a higher frequency of cracks, which is consistent with the research of Ali et al. [38]. Future work could explore a broader range of particle sizes and environmental conditions to better understand their impact on combustion dynamics. Investigating the role of oxygen concentration and other external factors could further optimize combustion processes for various industrial applications.

3.2. Results of PLS Analysis

The outcomes of Partial Least Squares Regression (PLSR) models for iron powder ranging in sizes from below 20 μm to 50 μm , are delineated through calibration models for predicting the outlet temperature. The R-squared of the measured flame temperature and the predicted flame temperature by the input data were calculated by the Unscrambler software. This parameter is a statistical measure used in machine learning to evaluate the quality of a regression model. It measures how well the model fits the data by assessing the proportion of variance in the dependent variable explained by the independent variables. Full cross-validation substantiates the predictive capability of these models. R^2_{CV} proves the predictive ability of these models, and R^2_C also proves the ability to predict the mea-

sured values. Notably, the most noteworthy performance was observed for particles sized at 30 μm , attaining an R^2 value of 0.90, as illustrated in Figure 10.

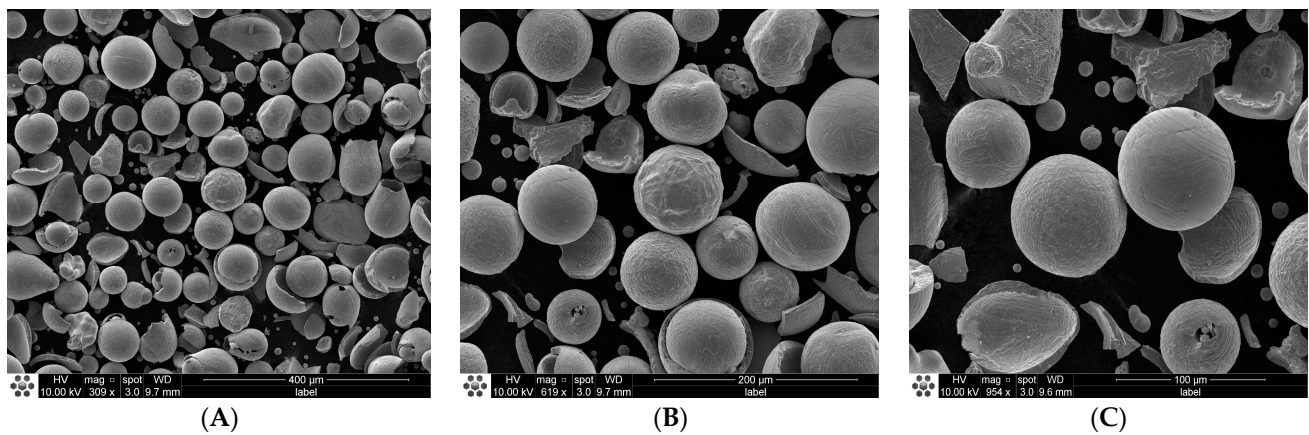


Figure 9. Scanning Electron Microscope (SEM) images of ignited iron powder, images in order from left to right from large scale to small scale, (A): 400 μm (smaller than 20 μm), (B): 200 μm (50 μm), and (C): 100 μm (50 μm).

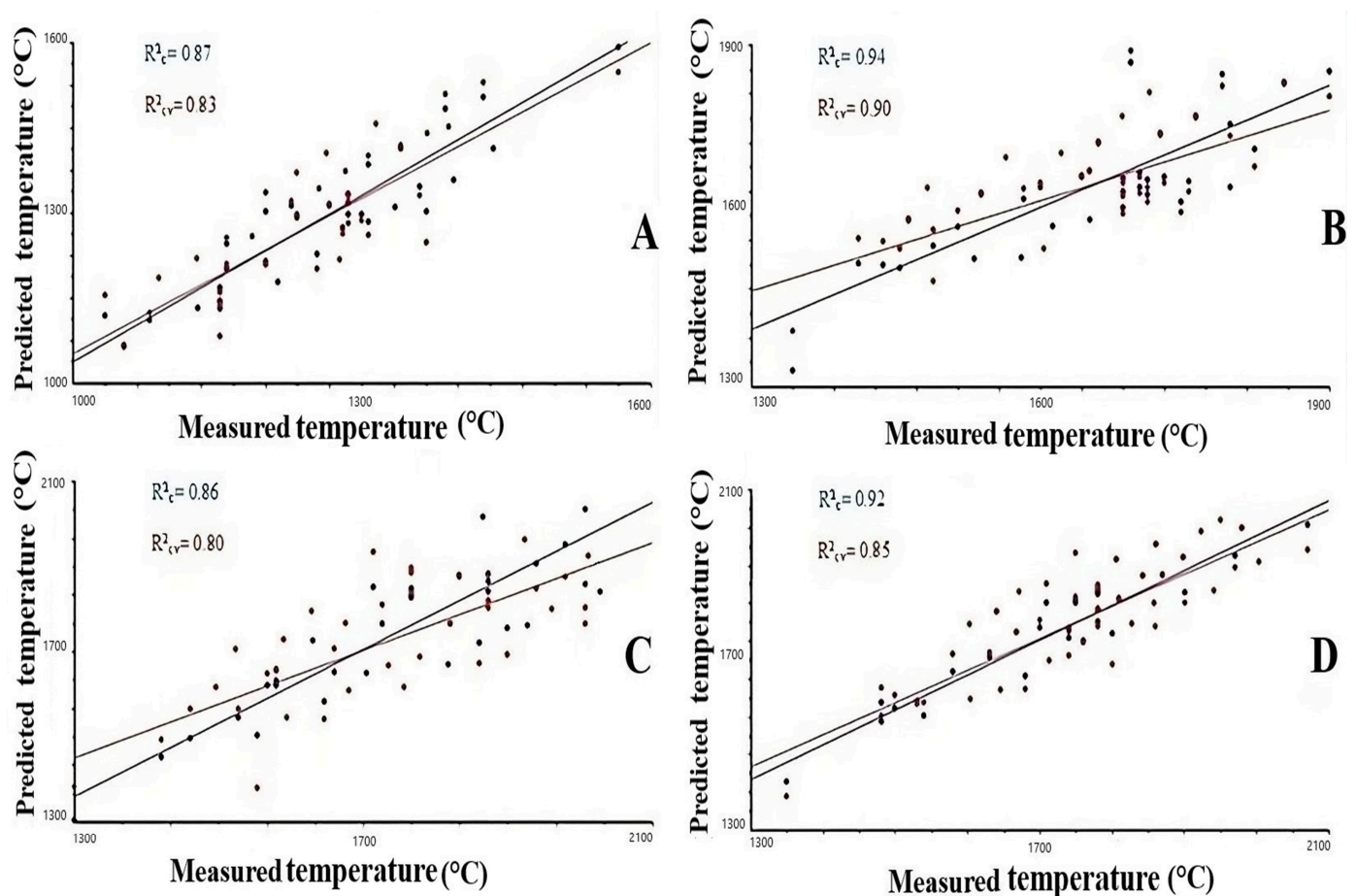


Figure 10. Predicted temperature vs. reference measured temperature of outlet iron powder of the prediction set for the optimal PLS models ((A): 20 μm , (B): 30 μm , (C): 40 μm , and (D): 50 μm).

This finding echoes the study conducted by Buchheiser et al., wherein an R^2 value of 0.90 was achieved for estimating temperature in iron microparticles utilizing Near-Infrared (NIR) spectroscopy [39,40]. Additionally, similar outcomes were reported by [6], utilizing NIR spectroscopy to quantify the outlet temperature of a burner.

3.3. Results of PCA Analysis

Principal Component Analysis (PCA) was utilized to categorize the different sizes of iron powder based on their spectral characteristics in the visible range. A PC chart was generated to visualize the distinctions among the various powder sizes. External factors, particularly those discernible within the visible spectrum, were identified as pivotal discriminants. Notably, the suitability of the visible region for the separation of iron powder was underscored, as fiber optic spectroscopy can effectively leverage this spectral domain [41]. The best results were obtained from the SNV and D2 preprocessing.

First, the flame spectral data of the different sizes of the iron powder were given to the software to perform PCA. PCA is able to separate these data into two principal components due to the high amount of spectral data. Based on the spectral data for 4 types of flames for different sizes of iron powder, the following results were obtained. For flames from powders below 20 μm and 50 μm compared to 30 μm and 40 μm , PCA was able to work with a resolution of 74%, so that 74% of the spectral data of these flames could be separated from each other, which is equivalent to the first principal component PC-1. In contrast, PCA was unable to distinguish between the spectra of flames with sizes of 30 μm and 40 μm , which is of course due to the similar behavior of the spectra of flames of these two sizes. There was a 20% difference between the flame spectra of particles smaller than 20 μm and those of 50 μm along the second principal component PC-2. The optimal resolution for iron powder particles of different sizes was achieved with PC-1, which accounted for 74% of the total variance. As shown in Figure 11, PC-1 discriminates 74% between particles smaller than 20 μm , 30 μm , 40 μm , and 50 μm . In contrast, PC-2 showed a separation rate of only 20%.

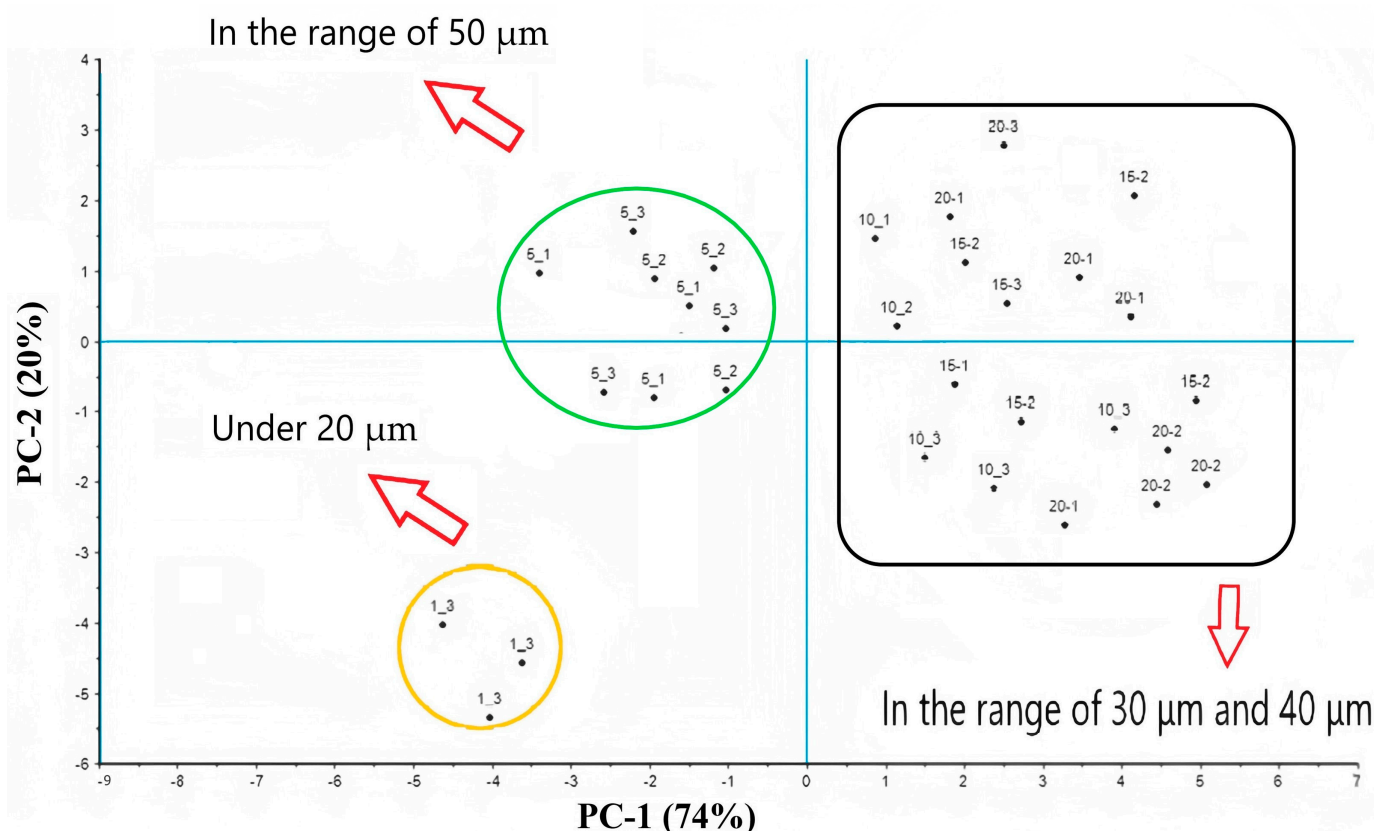


Figure 11. PCA graph for iron powder in four different sizes based on spectrometer graph flame. PC-1 serves as the primary principal component, while PC-2 represents the secondary one.

A comprehensive investigation employing Principal Component Analysis (PCA) was conducted on a dataset comprising 138 samples of spectral varieties of iron powders within

the visible region of the spectrum. The analysis revealed distinct clustering patterns among the four groups categorized by particle size; namely, those under 20 μm , 30 μm , 40 μm , and 50 μm , as depicted in Figures 11 and 12.

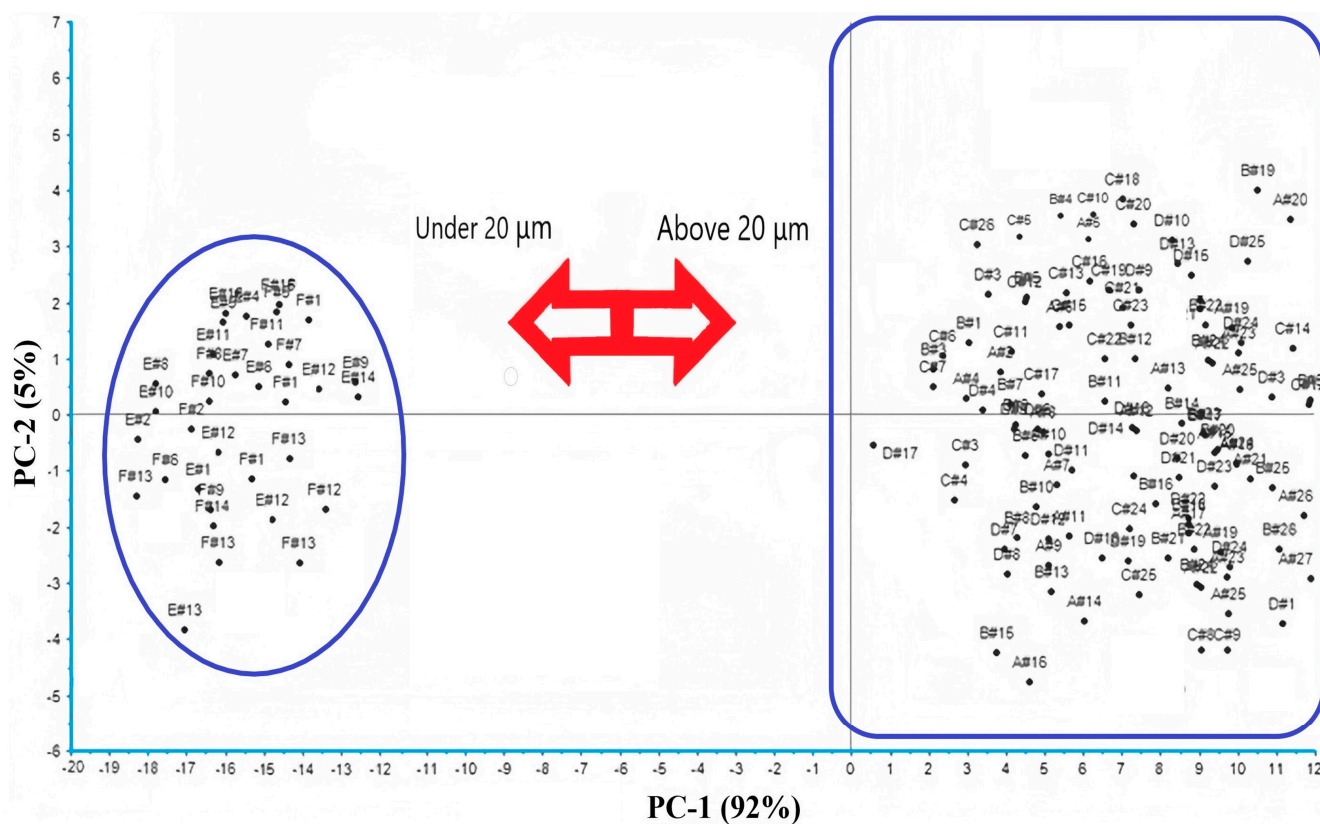


Figure 12. PCA graph for iron powder in two sides, under 20 μm and above 20 μm . PC-1 serves as the primary principal component, while PC-2 represents the secondary one.

Samples larger than 20 μm generally show PC-1 values above zero, while those smaller than 20 μm have PC-1 values below zero. These findings underscore the efficacy of fiber optic spectroscopy in conjunction with PCA for robust categorization of different flame spectra across distinct size categories. This assertion is reinforced by other studies, providing further validation of the methodology's potential for effective statistical separation of particle size from the particle spectra [42,43]. It also shows the spectrometer's ability to separate iron flames based on physical size characteristics using statistical preprocessing.

4. Conclusions

In summary, this study investigates the effectiveness of optical fiber spectroscopy in predicting flame temperature and assessing iron powder size at four different levels. This study aims to analyze the impact of iron powder size on the particle spectra used to measure the flame temperature of particles and subsequently develop calibration models for non-invasive predictions of particle size. Additionally, it seeks to determine the capability of differentiating flames based on particle size using Principal Component Analysis (PCA) on the PC plot for each specific iron powder composition. Particle size and combustion temperature was established, with smaller particles (under 20 μm) averaging 1381 $^{\circ}\text{C}$ and larger particles (up to 50 μm) reaching temperatures of 1842 $^{\circ}\text{C}$. This finding underscores the significant influence of particle size on combustion efficiency, offering valuable insights for optimizing industrial combustion processes. Advanced statistical techniques, including Partial Least Squares Regression (PLSR) and Principal Component Analysis (PCA), were employed to further validate the findings. PLSR models achieved an R^2 value of 0.90 for 30 μm particles, corroborating the predictive power of the model. PCA facilitated the

effective categorization of particle sizes, with PC-1 accounting for 74% of the total variance. These statistical analyses not only reinforce the experimental results but also highlight the utility of spectroscopic methods in characterizing particle combustion properties, paving the way for improved control and optimization in combustion applications. These results demonstrate the potential of using optical fiber spectroscopy and advanced statistical techniques to optimize combustion processes, leading to more efficient energy production and reducing the environmental impact of industrial applications.

Author Contributions: M.S.: conceptualization, formal analysis, investigation, methodology, software, validation, and writing—original draft. B.G.: project administration, resources, and supervision. G.N.: supervision and validation. W.P.: formal analysis, validation, and writing—review. M.B.: formal analysis, validation, and writing—review. P.d.G.: project administration, resources, supervision, and writing—review. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

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