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Intensity-Preserving Robust Fusion for Multi-Frame Spatial Heterodyne Spectral Recovery Toward Atmospheric Remote Sensing

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Abstract

Compact spatial heterodyne spectroscopy (SHS) is useful for atmospheric remote sensing, but repeated interferogram acquisition alone does not guarantee stable recovered spectral intensity. An intensity-preserving framework based on self-calibrated quality-gated robust fusion (SC-QGRF) was evaluated for multi-frame SHS spectral recovery. Frame weights are derived from image and spectral quality descriptors while avoiding framewise spectral normalization. Test spectral measurements were carried out using potassium and xenon lamps, which served as controlled laboratory cases for line spectrum and broadband spectrum recovery, respectively. Random Single, Image Average, Spectrum Mean, Spectrum Median, and the proposed strategy were compared under a common recovery and evaluation setting. Complete frame and exposure response analyses retained the main spectral profiles and showed no evident exposure-dependent intensity bias in this laboratory setting. Repeated subsampling provided the main stability evidence. SC-QGRF achieved the lowest variability in all four core metrics: coefficient of variation (CV) of K-AreaRatio = 0.0445%, CV of the full width at half maximum of the second K peak (K-FWHM2) = 0.0395%, CV of Xe-BandIntegral = 1.1770%, and standard deviation (STD) of Xe-SpectralCentroid = 0.0786 nm. The method can be used as a spectral quality control and fusion step for repeated SHS observations toward atmospheric remote sensing, while gas cell and field measurements remain necessary for retrieval-level validation.

Keywords: spatial heterodyne spectroscopy; atmospheric remote sensing; spectral recovery; intensity preservation; robust fusion; spectral quality control



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1. Introduction

Atmospheric remote sensing relies on recovered spectra with stable intensity, not only on profiles that can be visually recognized. In trace-gas retrieval and broadband radiance analysis, weak absorption features, band-integrated quantities, spectral centroid positions, and exposure-dependent responses may enter calibration checks and retrieval preprocessing. Greenhouse gas retrieval studies have linked uncertainty to instrument

terms, radiometric gain, spectral calibration, surface reflectance, and forward model inputs [1,2]. Work on MethaneAIR, TROPOMI, and broader satellite methane observation products also indicates that stable spectral information and controlled preprocessing are needed before retrieval-level use [3–6].

Repeated acquisition can improve measurement reliability for compact satellite, ground-based, or unmanned platforms. Its value, however, is conditional on the stability of the recovered spectral quantities. Satellite methane emission studies and validation studies support this requirement in both satellite and ground-based observation settings [7–9]. Recent work on plume detection and methane emission monitoring makes the same point: repeated observations remain useful only to the extent that the spectral quantities are traceable [10,11]. Long-term satellite imagery studies of atmospheric cloud properties further show that remote sensing records are useful only when the observation products are consistently processed and interpretable [12].

SHS provides a compact route for atmospheric spectral observation. It encodes wavelength information in the spatial frequency of a stationary two-dimensional interferogram and avoids macroscopic optical path scanning. The Greenhouse Gases Monitoring Instrument on GaoFen 5 satellite II is a recent SHS example for greenhouse gas monitoring, and its on orbit spectral calibration work shows that wavelength offset correction is needed before quantitative use [13,14]. For SHS and related greenhouse gas spectrometers, studies have examined phase distortion, instrumental line-shape characterization, and wavelength calibration error analysis [15–17]. Satellite missions such as GaoFen 5/GaoFen 5B, GOSAT, Copernicus/Sentinel platforms, and Landsat differ in observation objectives, instrument concepts, and data products. The present study is therefore limited to intensity-preserving SHS spectral recovery preprocessing and does not attempt a cross-mission retrieval performance comparison.

SHS has also been used or investigated in atmospheric nitrogen dioxide observation, compact space spectrograph modelling, and visible gas sensing [18–20]. Work on high dynamic range imaging, signal-to-noise ratio, SHS development, and instrumental function characterization suggests that recovered spectral quality is shaped by both optical configuration and post-acquisition processing [21–24]. The original SHS concept remains the interferometric basis of these later implementations [25].

For SHS instruments, the interferogram is an intermediate record. Later analysis uses a one-dimensional recovered spectrum and metrics such as line area, full width at half maximum (FWHM), band-integrated intensity, and spectral centroid. Local dark regions, bright-tail anomalies, weak saturation, detector response variation, frame dimension anomalies, and fringe modulation changes may appear after Fourier domain recovery as spectral intensity fluctuation, line-shape variation, or centroid shift. This issue matters for atmospheric optical instruments, since instrumental line-shape degradation, satellite instrument characteristics, and reference spectrometer stability can affect retrieval-level analysis and validation [26–28].

Intensity preservation is therefore a separate constraint. Framewise min–max scaling, peak normalization, or area normalization may improve visual overlap, but they disturb the physical intensity relationship among repeated spectra. They can also hide real exposure-dependent response differences. An atmospheric SHS processing chain should reduce unreliable frame contributions while leaving the recovered intensity scale unchanged.

Most SHS and greenhouse gas instrument studies have focused on optical design, calibration, phase correction, instrumental line shape, signal-to-noise modelling, dynamic range extension, and spectral reconstruction. Repeated frame fusion has received less attention, particularly when frame quality varies and recovered spectral intensity must be preserved.

To isolate the effect of the fusion rule, four representative baselines were considered under a common recovery operator: selecting a single frame, averaging interferograms before recovery, averaging recovered spectra, and taking the pointwise spectral median. These baselines were not intended to cover all SHS processing methods. Instead, they provide transparent reference strategies for testing how repeated frame processing affects intensity-preserving spectral recovery. Single-frame selection, image averaging, and spectral domain averaging or median fusion each provide a simple reference strategy, but they do not jointly consider image domain defects, spectral consistency, and frame-level contribution traceability. This limitation motivates the use of a quality-guided fusion strategy that reduces unreliable frame contributions while preserving the recovered intensity scale.

Single-frame selection is the most direct strategy because it leaves the detector scale intensity of one interferogram unchanged; however, it makes the recovered spectrum dependent on a single acquisition and does not use the redundancy provided by repeated measurements. Image averaging can reduce uncorrelated image noise before Fourier domain recovery, but it combines fringe records before Fourier centering, sideband selection, and projection. For SHS and related spectral systems, preprocessing operations applied before spectral recovery can affect the information carried by the interferogram or spectrum [19,29]. When frame-to-frame background variation, local defects, fringe contrast changes, or weak phase differences are present, interferogram domain averaging may alter the effective modulation entering spectral recovery.

Spectral-mean fusion avoids interferogram domain averaging because each frame is recovered before fusion, but all recovered spectra are assigned equal confidence. This makes the result sensitive to frames affected by image defects or spectral inconsistency. Pointwise spectral median fusion is more resistant to isolated spectral outliers, but it does not use image domain-quality evidence and does not provide explicit frame-level contribution weights. These limitations are consistent with common issues in spectral and hyperspectral data handling, where preprocessing and outlier treatment can influence quantitative spectral metrics [30].

For this reason, an intensity-preserving evaluation framework was developed using SC-QGRF as the quality-guided fusion strategy for multi-frame SHS spectral recovery toward atmospheric remote sensing. Frame weights are estimated from image defect descriptors and spectral consistency descriptors using within-group robust statistics. Median-based robust deviation measures and Huber-type residual weighting provide the statistical basis for reducing abnormal frame contributions, while an effective frame constraint prevents the weighted fusion from collapsing into an implicit single-frame selection [31,32]. This design does not require an external ground-truth spectrum for every acquisition group and preserves the recovered intensity scale during fusion.

Potassium and xenon lamp measurements are used as laboratory validation data rather than atmospheric constituents. In this laboratory validation setting, they provide controlled line spectrum and broadband spectrum cases for evaluating spectral recovery stability before gas cell or field atmospheric measurements. Five strategies are compared under the same wavelength axis, recovery operator, projection setting, and metric definitions. The evaluation includes complete frame spectral recovery, exposure response, repeated subsampling stability, and frame weight redistribution.

2. Materials and Methods

2.1. Laboratory SHS System and Validation Data

The validation data were acquired using a laboratory spatial heterodyne spectrometer for controlled spectral recovery tests. Figure 1a shows the optical configuration. The incident beam was collimated, split into two interferometric arms, diffracted by two fixed

tilted gratings, recombined, and recorded as a two-dimensional interferogram by a scientific sCMOS detector. Spectral information was therefore encoded in the spatial frequency content of a stationary interferogram, without mechanical optical path scanning. Table 1 lists the main acquisition and recovery parameters.

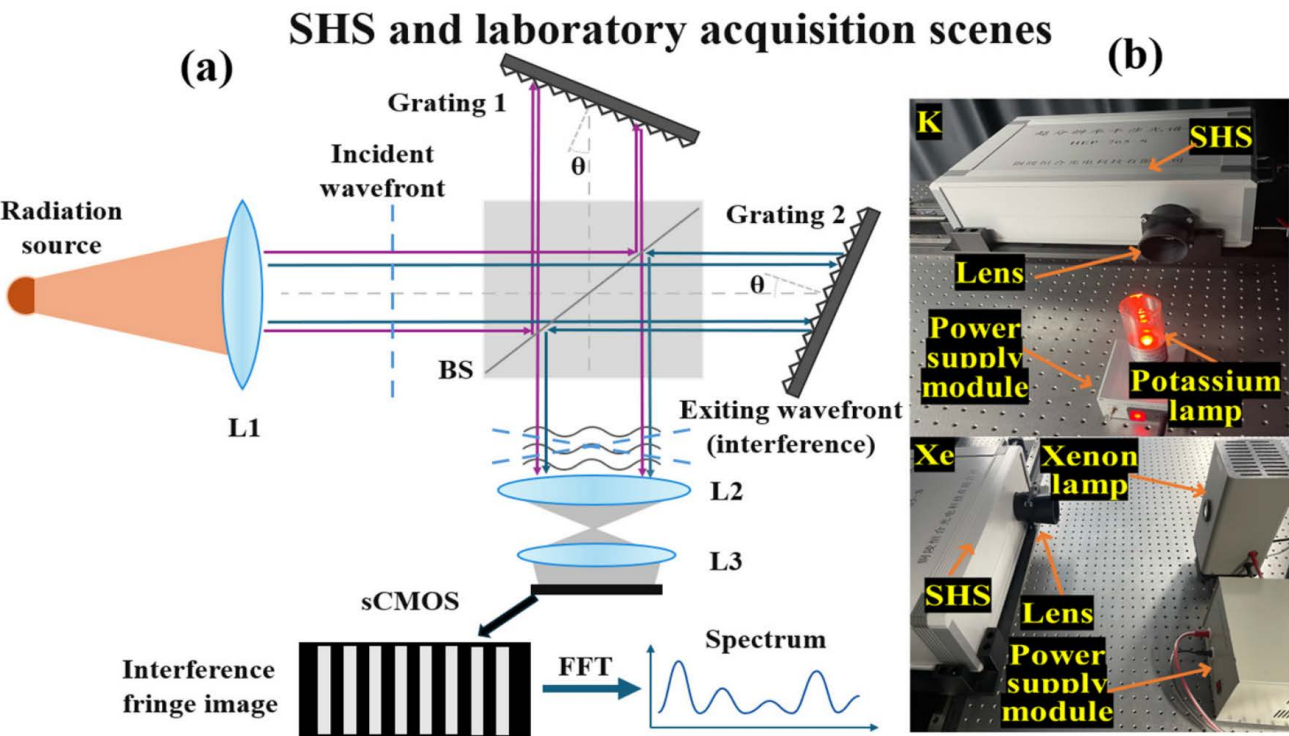


Figure 1. Laboratory SHS system and acquisition scenes. (a) Optical layout of the spatial heterodyne spectrometer. L1–L3 are lenses, BS is the beam splitter, FFT indicates Fourier transform spectral recovery, and the interferogram is recorded by an sCMOS detector. (b) Potassium and xenon lamp measurements used as controlled line spectrum and broadband spectrum validation cases before gas cell or field atmospheric measurements.

Table 1. Main acquisition and spectral recovery parameters.

Parameter	Value
Grating groove density	600 lines/mm
Detector	pco.panda 4.2 sCMOS
Image size	2048 × 2048 pixels
Pixel size	6.5 μm × 6.5 μm
Raw data format	16 bit ASC
Potassium exposure series	20–220 ms, step 20 ms
Xenon exposure series	5–80 ms, step 5 ms
Reference wavelength	$\lambda_0 = 756.65172413 \text{ nm}$
Spectral sampling interval	$\Delta\lambda = 0.029 \text{ nm/channel}$

Two lamp sources were used to provide controlled spectral conditions. The potassium lamp was used as an emission-line source for testing narrow feature recovery, including weak peak stability and line-shape-related metrics. It was not used as a reflective target, and no potassium reflectance was measured or analyzed. The xenon lamp provided a broadband case for evaluating band-integrated intensity and spectral centroid stability. In this setting, the lamp spectra were not treated as atmospheric constituents. They were used to test line and broadband SHS spectral recovery stability before gas cell or field atmospheric measurements.

During each exposure series, the lamp condition, optical alignment, and acquisition geometry were kept unchanged. The potassium exposure time ranged from 20 ms to 220 ms with a step of 20 ms, and the xenon exposure time ranged from 5 ms to 80 ms with a step of 5 ms. For each exposure time, 50 signal interferograms and 50 dark frames were acquired. A pixelwise median dark frame was constructed from the 50 dark frames at the same exposure time, and this exposure-matched median dark frame was subtracted from the corresponding signal interferograms.

Before spectral recovery, all signal frames were checked by a frame size audit. Frames whose dimensions did not match the valid acquisition size were excluded from recovery, fusion, and metric calculation. The analysis used valid interferograms with a size of 2048×2048 pixels, and each exposure group contained 50 valid signal frames after the audit. After dark subtraction, negative pixel values were set to zero before spectral recovery. This operation was applied uniformly to all frames and all processing strategies.

No method-dependent clipping, rescaling, min–max normalization, peak normalization, area normalization, or frame-wise spectral normalization was used for quantitative analysis. The recovered spectra were kept on a common detector intensity scale after dark correction. DC or near DC cropping and display contrast adjustment were used only for visualization; quantitative metrics were calculated from the full recovered spectra. Conditional on this data processing setting, the exposure response discussed below refers to the consistency of recovered spectral metrics across exposure time, not to absolute radiometric calibration.

2.2. Processing Framework

Figure 2 gives the processing framework used throughout the analysis. After frame size audit and exposure-matched dark correction, valid interferograms were grouped by source type and exposure time. In this framework, preprocessing refers to frame size audit, exposure-matched median dark frame subtraction, negative value clipping after dark correction, and source/exposure grouping. These steps were completed before method comparison, and the same preprocessed valid frame pool was supplied to all five strategies. Each exposure group was treated as a common valid frame pool. The same pool was then used for Random Single, Image Average, Spectrum Mean, Spectrum Median, and SC-QGRF, so that all five strategies were compared under the same source and exposure condition.

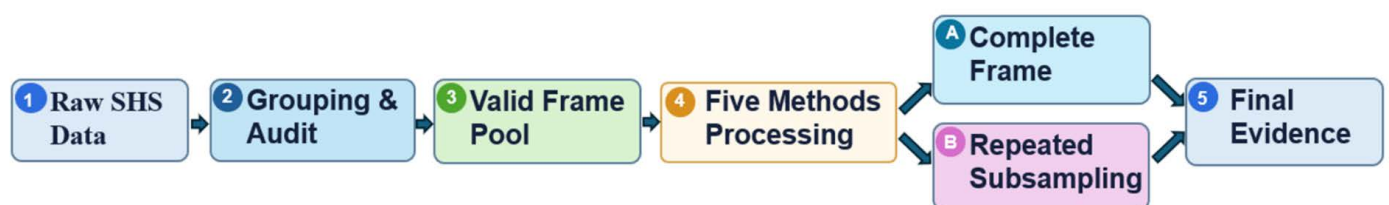


Figure 2. Processing framework for complete frame and repeated subsampling analyses.

Two analysis paths were built from this pool. Complete frame analysis used all valid frames in an exposure group to obtain full group spectra and exposure response results. For SC-QGRF, this path also provided frame weight diagnostics. Repeated subsampling analysis used selected frame subsets from the same pool to test sensitivity to frame subset perturbation. Within a given subsampling trial, all five strategies received the same selected subset. Conditional on the fixed wavelength axis, recovery operator, projection setting, and metric definitions, differences among the strategies mainly reflected the fusion strategy rather than changes in preprocessing, spectral recovery, or metric calculation.

2.3. Intensity-Preserving Recovery and Fusion Strategies

For each exposure group or repeated subsampling trial, the current frame index set was written as $\Omega = \{1, 2, \dots, N\}$, where N denotes the number of frames used in that run. The dark corrected interferogram of frame i was denoted by $I_{i(x,y)}$. All five strategies were built on the same recovery operator $R(\cdot)$, so the comparison was tied to the fusion rule rather than to a change in spectral reconstruction.

In this work, $R(\cdot)$ represents a fixed Fourier domain recovery operator. Each dark corrected interferogram was first converted to a double precision array. It was then transformed into the Fourier domain, centered, and projected from the right half positive frequency side along the detector vertical direction to form a one-dimensional spectral sequence. The same Fourier centering, positive side selection, projection direction, and channel indexing were used for every frame, exposure group, and strategy. The analysis was performed on the native detector pixel grid; no pixel snapping, sub pixel registration, or interpolation-based image alignment was applied before spectral recovery. Conditional on this fixed recovery setting, the single frame spectrum was defined as

$$S_{i(\lambda)} = R[I_{i(x,y)}], i \in \Omega \quad (1)$$

The wavelength axis was generated from the instrument parameters listed in Table 1:

$$\lambda(k) = \lambda_0 + k\Delta\lambda, k = 0, 1, \dots, K - 1 \quad (2)$$

where λ_0 is the reference wavelength, $\Delta\lambda$ is the spectral sampling interval, k is the spectral channel index, and K is the number of recovered spectral channels.

Quantitative spectra were retained on the common detector intensity scale after dark correction. Framewise min–max scaling, peak normalization, area normalization, and spectral normalization were not applied. DC or near DC cropping and display contrast adjustment were reserved for visualization only; the full recovered spectra were used for metric extraction.

Four baseline strategies were evaluated under the same input set Ω . For Random Single, one frame r was selected from the current input set, and its recovered spectrum was used without spectral domain fusion:

$$S_{RS(\lambda)} = S_{r(\lambda)}, r \in \Omega \quad (3)$$

For Image Average, dark corrected interferograms were averaged before spectral recovery:

$$I_{avg(x,y)} = \frac{1}{N} \sum_{i \in \Omega} I_{i(x,y)} \quad (4)$$

$$S_{IA(\lambda)} = R[I_{avg(x,y)}] \quad (5)$$

For Spectrum Mean, each frame was recovered independently before averaging in the spectral domain:

$$S_{SM(\lambda)} = \frac{1}{N} \sum_{i \in \Omega} S_{i(\lambda)} \quad (6)$$

For Spectrum Median, the median was calculated pointwise across the independently recovered spectra:

$$S_{SMed(\lambda)} = \text{median}_{i \in \Omega} \{S_{i(\lambda)}\} \quad (7)$$

Image Average and Spectrum Mean were kept as separate strategies because the two operations are not interchangeable. Image Average enters $R(\cdot)$ after interferogram domain

averaging, where frame-to-frame fringe variation may change the effective modulation. Spectrum Mean combines spectra only after each frame has already been recovered. To the extent that frame defects or fringe contrast changes affect the interferogram before Fourier recovery, these two strategies may respond differently.

For SC-QGRF, fusion was performed in the spectral domain with final normalized frame weights:

$$S_{SC-QGRF(\lambda)} = \sum_{i \in \Omega} w_i S_{i(\lambda)}, \quad \sum_{i \in \Omega} w_i = 1 \quad (8)$$

Here, w_i is the final frame weight defined in Section 2.5. With the same input set, wavelength axis, recovery operator, projection setting, and metric definitions, the differences among the five strategies mainly reflect their fusion rules rather than changes in preprocessing, spectral recovery, or metric calculation.

2.4. Repeated Subsampling Protocol

Repeated subsampling was used to examine how each strategy responded to changes in the available frame subset under the same exposure condition. For each potassium and xenon exposure group, 30 trials were carried out. In each trial, 30 frames were drawn without replacement from the 50 valid frames in that exposure group. The subset size and number of trials were determined from the 50 frame valid pool in each exposure group. A 30-frame subset retained most frames while still perturbing the frame composition, and 30 repeated trials provided repeated subset variations for comparing the five strategies under the same sampling protocol. The subsampling index tables were generated before the method comparison and were kept fixed for all five strategies. In a given trial, Random Single, Image Average, Spectrum Mean, Spectrum Median, and SC-QGRF received the same selected subset. Random Single used one frame selected from that subset as the trial output, whereas the other four strategies used all 30 frames.

Each trial produced one recovered spectrum and one set of spectral metrics for each strategy. These trial level metrics were used to evaluate repeatability under frame subset perturbation. Because no external ground-truth spectrum was available for each individual interferogram, frame-level absolute accuracy was not calculated. Instead, repeated subsampling was used to evaluate the stability of recovered spectral metrics under changes in frame composition. For intensity-related metrics, the coefficient of variation was calculated within each exposure group. For wavelength- or position-related metrics, the standard deviation was calculated within each exposure group. The within-exposure statistics were then summarized across exposure groups for each method and metric, so that deterministic exposure-dependent intensity changes were not mixed with variability caused by frame subset changes. This protocol follows a resampling-based stability assessment logic, but uses subsampling without replacement rather than bootstrap resampling.

2.5. Self-Calibrated Quality-Gated Robust Fusion

Figure 3 outlines the SC-QGRF workflow. The method links four steps: single frame spectral recovery, image and spectral quality modelling, quality-guided robust weighting, and final spectral fusion with metric extraction. Its purpose is to estimate frame weights from observable image and spectral evidence while keeping the fused result supported by multiple frames.

$$S_{ref(\lambda)} = \text{median}_{i \in \Omega} \{S_{i(\lambda)}\} \quad (9)$$

This median spectrum was used only to describe within-group spectral consistency. It was not treated as an external ground-truth spectrum, and it was not used to define the final evaluation metrics.

For each frame, image and spectral information were combined into the feature vector

$$f_i = [f_i^{UT}, f_i^{LT}, f_i^{LA}, f_i^{SD}, f_i^{ID}] \quad (10)$$

where *UT*, *LT*, and *LA* denote upper tail anomaly, lower tail anomaly, and local anomaly. The upper tail descriptor targets bright outliers or weak saturation. The lower tail descriptor reflects abnormally dark pixels or local signal loss, and was used to account for local dark regions in the recorded interferograms. The local anomaly descriptor measures small-scale departures from the local median filtered background. Therefore, local dark regions were analyzed as image domain-quality deviations before spectral recovery, rather than as manually segmented regions or independent spectral features. Frames containing stronger local dark anomalies received larger robust standardized scores and consequently lower fusion weights in the SC-QGRF procedure. These descriptors characterize detector plane quality variations only; geospatial or scene-level spatial errors were not estimated because the laboratory data did not contain spatially resolved atmospheric scenes.

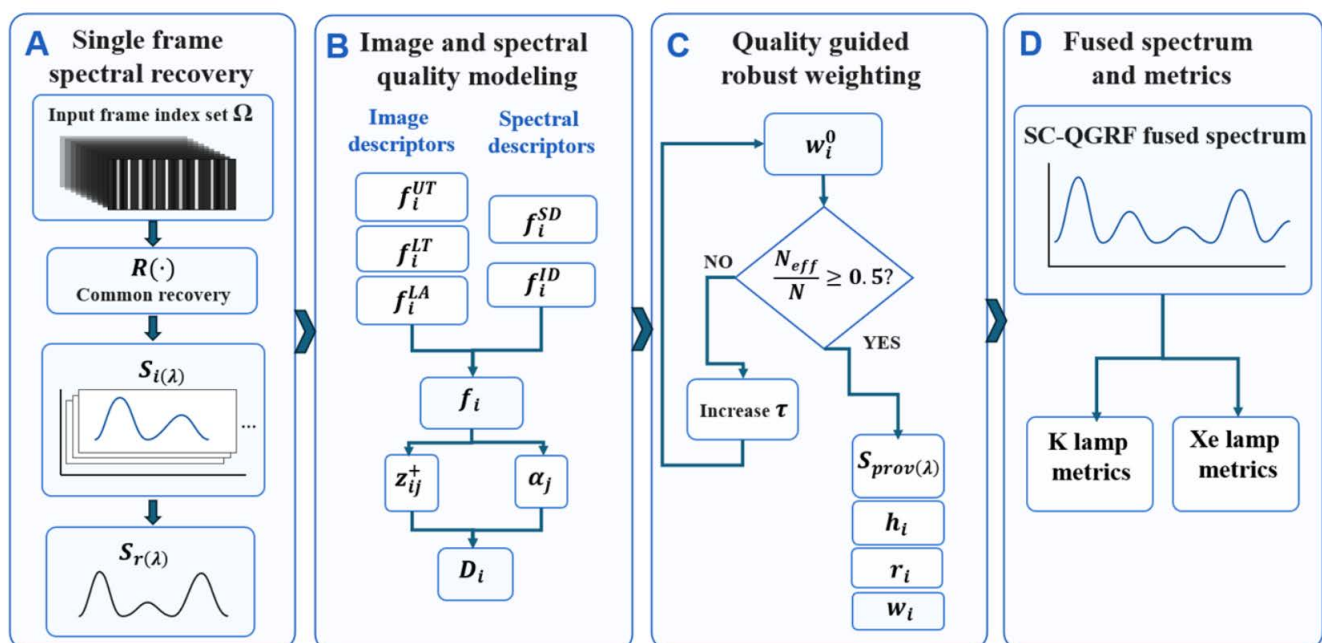


Figure 3. Workflow of the proposed SC-QGRF method.

The three image descriptors were calculated as

$$f_i^{UT} = \frac{[P_{99.9}(I_i) - P_{99}(I_i)]}{[IQR(I_i) + \varepsilon]} \quad (11a)$$

$$f_i^{LT} = \frac{[P_{1}(I_i) - P_{0.1}(I_i)]}{[IQR(I_i) + \varepsilon]} \quad (11b)$$

$$f_i^{LA} = \frac{P_{99}(|I_i - M_i|)}{[IQR(I_i) + \varepsilon]} \quad (11c)$$

where $P_q(\cdot)$ is the q th percentile, $IQR(\cdot)$ is the interquartile range, M_i is the local median filtered image of I_i , and ε prevents division by zero. The median filter setting was fixed before method comparison and remained unchanged for all frames, exposure groups, and lamp sources.

Spectral quality was described by profile consistency and intensity consistency relative to $S_{ref}(\lambda)$:

$$f_i^{SD} = 1 - \text{corr}[S_{i(\lambda)}, S_{ref(\lambda)}] \quad (12a)$$

$$f_i^{ID} = \frac{|A_i - \text{median}_{(m \in \Omega)(A_m)}|}{[\text{median}_{(m \in \Omega)(A_m)} + \varepsilon]} \quad (12b)$$

For potassium spectra, A_i was the sum of the two baseline-corrected peak areas defined in Section 2.6. For xenon spectra, A_i was the band-integrated intensity over the evaluation interval defined in Section 2.6. The correlation in Equation (12a) was calculated over the source-dependent spectral interval used for metric extraction, not over display-cropped spectra.

All five descriptors were defined in the same direction: larger values indicate stronger anomaly or larger spectral inconsistency. Each descriptor was therefore converted into a one-sided robust standardized score:

$$z_{ij}^+ = \max \left\{ 0, \frac{[f_{ij} - \text{median}_{(m \in \Omega)(f_{mj})}]}{[1.4826 \text{MAD}(f_j) + \varepsilon]} \right\} \quad (13)$$

where $\text{MAD}(\cdot)$ is the median absolute deviation of the j th descriptor within the current exposure group. The factor 1.4826 is the standard consistency factor that scales MAD to a standard deviation equivalent estimate under a normal distribution. It was used here only for robust standardization of the quality descriptors.

The contribution of each feature channel was estimated from its within-group variability:

$$v_j = \frac{\text{IQR}(f_j)}{[\text{median}_{i \in \Omega}[f_{ij}] + \varepsilon]}, \alpha_j = \frac{v_j}{\sum_l v_l} \quad (14)$$

The adaptive weights α_j represent the relative variability of the quality descriptors within the current group. They were not optimized using the final spectral metrics. The composite anomaly score for frame i was then given by

$$D_i = \left[\sum_j \alpha_j^2 z_{ij}^+ \right]^{\frac{1}{2}} \quad (15)$$

The anomaly scores were mapped to initial frame weights through a softmax function:

$$w_i^0 = \frac{\exp\left(-\frac{D_i}{\tau}\right)}{\sum_{m \in \Omega} \exp\left(-\frac{D_m}{\tau}\right)} \quad (16)$$

where τ controls weight concentration. Smaller τ produces a more concentrated weight distribution, while larger τ makes the weights closer to equal weighting. To limit implicit best-frame selection, the effective frame number was constrained as

$$N_{eff} = \frac{1}{\sum_{i \in \Omega} (w_i^0)^2}, \frac{N_{eff}}{N} \geq \rho, \rho = 0.5 \quad (17)$$

Here, N_{eff} denotes the equivalent number of equally weighted frames implied by the normalized weights; it is not restricted to integer values. If the constraint was not satisfied, τ was increased and the initial weights were recomputed. The same effective frame ratio threshold and update rule were used for all exposure groups and both lamp sources.

After initial weighting, a provisional fused spectrum was obtained:

$$S_{prov(\lambda)} = \sum_{i \in \Omega} w_i^0 S_{i(\lambda)} \quad (18)$$

The relative residual of each single frame spectrum was calculated as

$$r_i = \frac{\|S_{i(\lambda)} - S_{prov(\lambda)}\|_2}{\left[\|S_{prov(\lambda)}\|_2 + \varepsilon\right]} \quad (19)$$

The residual norm was evaluated over the same source-dependent spectral interval used for spectral consistency assessment. A Huber-type residual factor was then applied to reduce the contribution of spectra that remained inconsistent after initial quality weighting:

$$h_i = \min\left(1, \frac{c}{r_i + \varepsilon}\right) \quad (20)$$

where h_i is the residual correction factor and c is the residual cutoff constant. The cutoff setting was fixed before method comparison and was not tuned separately for a specific exposure group or lamp source. The final normalized frame weight was calculated as

$$w_i = \frac{w_i^0 h_i}{\sum_{m \in \Omega} w_m^0 h_m} \quad (21)$$

The final SC-QGRF spectrum was then calculated using Equation (8). In this framework, image defects, spectral inconsistency, adaptive feature weighting, residual correction, and the effective frame constraint jointly determine the frame weights. The descriptor definitions, robust standardization rule, effective frame ratio threshold, temperature update rule, and residual correction setting were kept fixed across the experiment. SC-QGRF was used as a spectral quality control and fusion step for repeated SHS observations. It reduces unreliable frame contributions while preserving multi-frame support, but it does not replace radiometric calibration, wavelength calibration, or atmospheric forward modelling.

2.6. Spectral Metrics and Stability Evaluation

Spectral metrics were computed from the full recovered spectra, not from spectra cropped for display. All spectral parameters were extracted using the same wavelength axis, analysis intervals, baseline correction rule, and metric definitions for all methods. This setting ensured consistent parameter comparison across methods, but did not constitute absolute wavelength or radiometric calibration. In this laboratory setting, potassium and xenon provided two controlled validation cases: line spectra for potassium and broadband spectra for xenon. They were not interpreted as atmospheric absorption spectra. For potassium spectra, two fixed line windows were centered at 766.48991 nm and 769.89645 nm, with a half width of ± 0.8 nm. After local baseline subtraction, the baseline-corrected positive spectrum was defined as

$$S_{c(\lambda)} = \max[S(\lambda) - B(\lambda), 0] \quad (22)$$

where $B(\lambda)$ denotes the local baseline estimated within the corresponding analysis window, and $S_{c(\lambda)}$ is the positive baseline-corrected spectrum used for subsequent area, FWHM, and centroid calculations.

The area of the p th potassium peak was calculated by numerical integration:

$$A_p = \text{trapz}_{\lambda \in \Lambda_p} S_{c(\lambda)}, \quad p = 1, 2 \quad (23)$$

where Λ_p is the analysis window of the p th peak. The operator *trapz* denotes numerical integration over discrete wavelength samples using the trapezoidal rule. The potassium area ratio was defined as

$$\text{AreaRatio} = \frac{A_2}{A_1} \quad (24)$$

The full width at half maximum of the second potassium peak (FWHM2) was obtained from the second baseline-corrected potassium peak at the half maximum level. Peak separation was calculated from the detected positions of the two potassium peaks.

For xenon spectra, metric extraction used the fixed interval of 760–785 nm. The same baseline-corrected positive-spectrum definition was applied to the broadband case. Band-integrated intensity was calculated as

$$BI = \text{trapz}_{\lambda \in [760, 785]} S_{c(\lambda)} \quad (25)$$

and spectral centroid was calculated as

$$SC = \frac{\text{trapz}_{\lambda \in [760, 785]} \lambda S_{c(\lambda)}}{\text{trapz}_{\lambda \in [760, 785]} S_{c(\lambda)}} \quad (26)$$

For repeated subsampling, metrics summarized by CV were calculated within each exposure group, whereas wavelength or position-related metrics were summarized by standard deviation. Trial-level box plots used within-exposure relative deviations for intensity metrics and absolute deviations from the within-exposure median for position metrics. These statistics describe within-exposure repeatability and frame subset stability, rather than absolute frame-level accuracy against an external reference spectrum. The coefficient of variation (CV) was calculated as the ratio between the standard deviation (STD) and the mean value of the repeated subsampling metric within the same exposure group.

$$CV = 100\% \times \frac{STD(x)}{Mean(x)} \quad (27)$$

For exposure response analysis, a linear model was fitted between exposure time and the selected recovered intensity metric. The fitting quality was reported using the coefficient of determination R^2 , normalized root mean square error (nRMSE), and mean absolute relative error (MARE).

3. Results and Discussion

The results are presented in two evidence categories. Qualitative results are used to examine spectral profile preservation in representative complete frame cases, whereas quantitative and statistical results are used to evaluate exposure response, repeated subsampling stability, and frame weight redistribution.

3.1. Qualitative Complete Frame Spectral Recovery

Before examining exposure response and frame subset stability, the complete frame analysis was used to check whether the main spectral profiles were preserved. Figure 4

presents representative results for the controlled potassium and xenon validation cases. In the potassium 120 ms group, all five strategies retained the main doublet structure, and the weaker long-wavelength peak was still visible in the enlarged region. In the xenon 50 ms group, the broadband profile and a representative local peak were also preserved. Spectrum Mean, Spectrum Median, and SC-QGRF remained close in peak position and overall profile. Under the complete frame condition, this agreement indicates that the quality-guided weighting in SC-QGRF did not introduce visible spectral distortion.

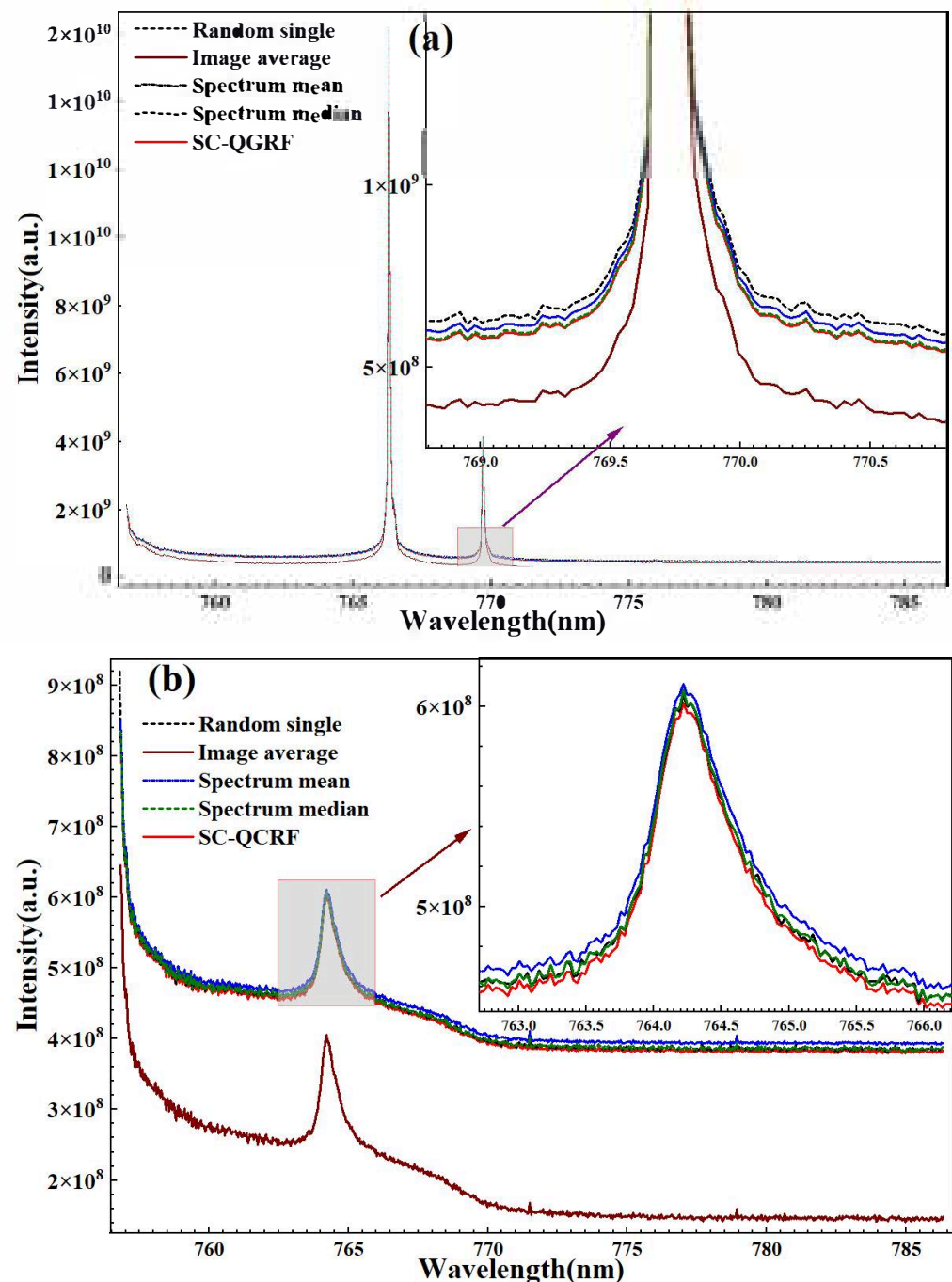


Figure 4. Complete frame spectral recovery for the controlled line and broadband validation cases. Spectra are shown on the recovered intensity scale without framewise normalization. (a) Potassium lamp spectra at 120 ms exposure with an enlarged view of the weak peak region. (b) Xenon lamp spectra at 50 ms exposure with an enlarged view of a representative local spectral peak.

Method-dependent differences were also present. Image Average produced lower recovered intensity for both sources. This behavior is consistent with a possible reduction in effective fringe modulation when interferograms are averaged before spectral recovery, particularly when frame-to-frame fringe contrast, background, or local defect differences are present. Random Single showed stronger local fluctuation and higher background in the enlarged regions, consistent with its reliance on one selected frame. For atmospheric SHS workflows, avoiding artificial profile distortion is relevant to later weak feature extraction, band-integrated analysis, and retrieval preprocessing. The complete frame result therefore serves as a spectral preservation check; exposure response and frame subset sensitivity are examined separately in Sections 3.2 and 3.3.

3.2. Quantitative Exposure-Dependent Spectral Response

The exposure response test examined whether each fusion strategy preserved the relationship between exposure time and recovered intensity metrics. Complete frame results from all exposure levels were used. K-Peak2Area was selected to represent the weak potassium line response, and Xe-BandIntegral was used for the integrated broadband response. For each method and metric, a linear model was fitted between exposure time and the recovered intensity metric; R^2 , nRMSE, and MARE were used to evaluate the fit. In this setting, the test describes the consistency of recovered spectral metrics across exposure time. It should not be interpreted as absolute radiometric calibration.

The fitted responses in Table 2 show clear exposure dependence for all five strategies. For K-Peak2Area, all R^2 values exceeded 0.9997. For Xe-BandIntegral, all R^2 values exceeded 0.998. The fitting errors did not give a uniform method ranking. Image Average produced the lowest fitting errors for the potassium weak peak response, whereas Random Single gave the lowest fitting errors for Xe-BandIntegral in this complete frame exposure test. Linearity and retained intensity magnitude should be considered separately, since Image Average showed low fitting error while giving lower recovered intensity in Figure 4. Within the present laboratory exposure series, SC-QGRF stayed in the same high-linearity range as the baseline strategies and did not show evident exposure-dependent intensity bias.

Table 2. Linear fitting results for exposure-dependent recovered intensity metrics.

Method	K-Peak2Area			Xe-BandIntegral		
	R^2	nRMSE (%)	MARE (%)	R^2	nRMSE (%)	MARE (%)
Random Single	0.999745	0.503	1.510	0.999656	0.569	1.080
Image Average	0.999885	0.338	0.748	0.999312	0.823	1.290
Spectrum Mean	0.999758	0.491	1.492	0.998631	1.149	5.017
Spectrum Median	0.999758	0.491	1.485	0.998906	1.028	4.313
SC-QGRF	0.999771	0.477	1.416	0.998354	1.256	5.438

3.3. Statistical Repeated Subsampling Stability

Repeated subsampling served as the main stability test in this work. Within each trial, the same selected frame subset was supplied to all five strategies, so the distributions in Figure 5 mainly reflect differences in fusion behavior under frame subset perturbation. The box plots pool trial-level results from all exposure groups after within-exposure centering. Metrics summarized by CV are shown as within-exposure relative deviations, whereas Xe-SpectralCentroid is shown as an absolute deviation from the within-exposure median. Random Single produced wider distributions and more outliers, consistent with its dependence on one selected frame. Multi-frame strategies reduced the dispersion to different extents. Among them, SC-QGRF gave the most compact or near-most compact distributions across the four displayed metrics.

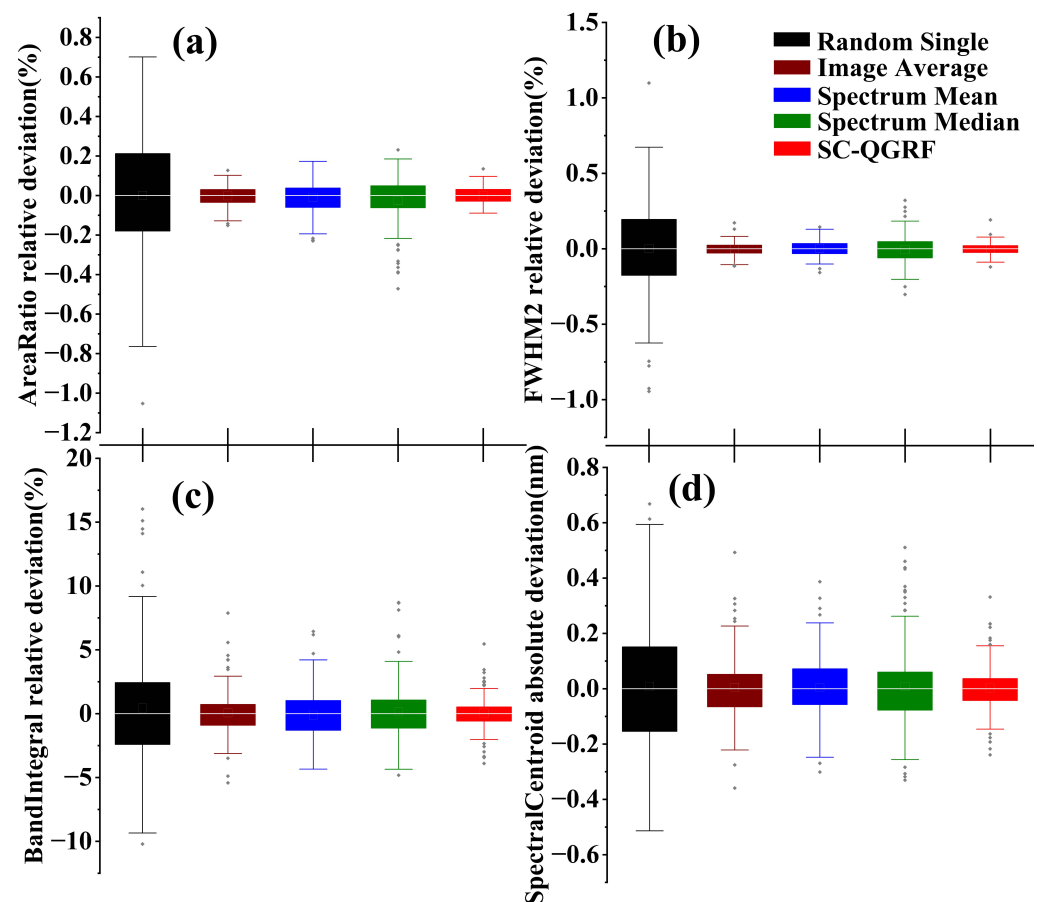


Figure 5. Repeated subsampling stability of core spectral metrics for the controlled line and broadband validation cases. The box plots pool trial-level results from all exposure groups. (a) Potassium AreaRatio relative deviation. (b) Potassium FWHM2 relative deviation. (c) Xenon BandIntegral relative deviation. (d) Xenon SpectralCentroid absolute deviation.

The quantitative summary in Table 3 gives the main evidence for reduced sensitivity to frame subset variation. Under the present repeated subsampling protocol, SC-QGRF achieved the lowest variability in all four core summary metrics: K-AreaRatio CV = 0.0445%, K-FWHM2 CV = 0.0395%, Xe-BandIntegral CV = 1.1770%, and Xe-SpectralCentroid STD = 0.0786 nm. These results are consistent with the intended role of SC-QGRF, namely reducing the influence of low-quality or inconsistent frames without collapsing to a single selected frame. Image Average also showed relatively low dispersion in some potassium metrics, but Figure 4 showed that it gave lower recovered intensity under the complete frame condition. The repeated subsampling result should therefore be interpreted together with the complete frame spectral recovery result. In this laboratory validation setting, SC-QGRF provided a more balanced outcome: it reduced frame subset sensitivity while retaining spectral profiles close to the spectral domain fusion baselines. However, lower subsampling variability should not be interpreted as retrieval-level validation by itself. Quantitative atmospheric retrieval also depends on calibrated Level-1 spectra, radiometric and wavelength calibration, instrumental line-shape characterization, surface reflectance treatment, forward modelling, and uncertainty analysis [1,2,25,26]. Thus, the present result supports the spectral stability role of SC-QGRF, while gas cell and field validation are still required to evaluate retrieval-level improvement.

Table 3. Repeated subsampling variability of the five strategies.

Method	K			Xe	
	AreaRatio CV (%)	FWHM2 CV (%)	BandIntegral CV (%)	SpectralCentroid STD (nm)	
Random Single	0.3371	0.3337	4.6262	0.2499	
Image Average	0.0502	0.0425	1.5366	0.1033	
Spectrum Mean	0.0821	0.0576	1.9855	0.1105	
Spectrum Median	0.1263	0.0989	2.0633	0.1498	
SC-QGRF	0.0445	0.0395	1.1770	0.0786	

3.4. Frame Weight Redistribution Analysis

Frame weight redistribution was examined to trace how SC-QGRF assigned frame contributions after quality modelling and residual correction. Table 4 reports two representative complete frame cases: potassium at 120 ms and xenon at 50 ms. In both cases, the final weights were non-uniform, indicating that frame-level quality differences affected the assigned contributions. The distribution, however, did not collapse toward a single dominant frame. The effective frame numbers were 29.27 and 26.42, with corresponding $\frac{N_{eff}}{N}$ ratios of 0.585 and 0.528. The maximum final weights were 0.0455 and 0.0515, equal to 2.275 and 2.575 times the equal weight baseline. In these representative cases, the weight statistics are consistent with quality-guided redistribution while maintaining multi-frame support.

Table 4. Frame weight statistics for representative complete frame SC-QGRF cases.

Source	Exposure	N	Equal Weight	N_{eff}	N_{eff}/N	Max Final Weight	Max/Equal Ratio
K	120 ms	50	0.02	29.27	0.585	0.0455	2.275
Xe	50 ms	50	0.02	26.42	0.528	0.0515	2.575

A separate xenon 45 ms complete frame group is used in Figure 6 to show the frame-wise weight update. Initial and final weights varied across frames, and frames with larger final weights are marked only for visualization. The final weights remained distributed over multiple frames rather than being reduced to an unreported single-frame selection. For atmospheric SHS workflows, such frame-level traceability is useful because quality control should not silently turn repeated measurements into a single selected-frame output. The weight redistribution analysis therefore supports the interpretability of SC-QGRF; the main stability evidence remains the repeated subsampling result in Section 3.3.

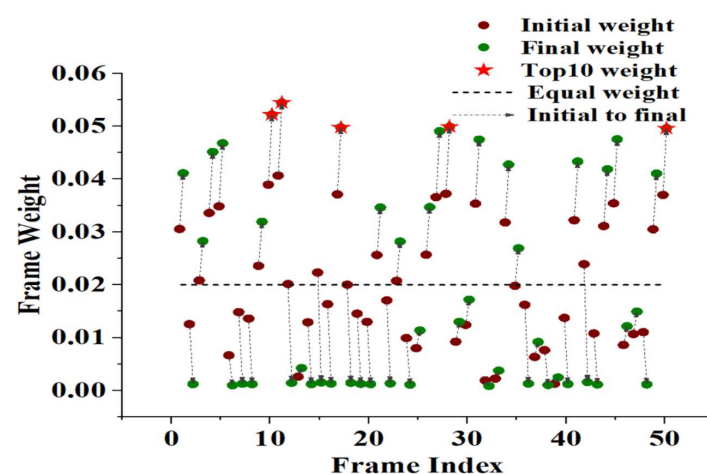


Figure 6. Frame weight redistribution for the representative xenon 45 ms complete frame group. Initial and final weights, the equal weight baseline, and the top 10% final weight frames are shown; dashed arrows indicate the weight update for each frame.

4. Conclusions

This work presented an intensity-preserving framework for multi-frame SHS spectral recovery, using SC-QGRF as the quality-guided fusion strategy. Potassium and xenon lamp measurements served as controlled laboratory cases for line spectrum and broadband spectrum conditions. They were not treated as atmospheric constituents. Random Single, Image Average, Spectrum Mean, Spectrum Median, and the proposed strategy were compared under a common recovery and evaluation setting.

The complete frame analysis retained the main potassium doublet, the weaker potassium peak, and the xenon broadband profile for the spectral domain fusion strategies and the proposed strategy. Within the present laboratory exposure series, the method stayed in the same high-linearity range as the baseline strategies and showed no evident exposure-dependent intensity bias. The repeated subsampling test provided the main stability evidence. Under this protocol, SC-QGRF gave the lowest variability among the tested strategies in all four core metrics: K-AreaRatio CV = 0.0445%, K-FWHM2 CV = 0.0395%, Xe-BandIntegral CV = 1.1770%, and Xe-SpectralCentroid STD = 0.0786 nm. Frame weight analysis also indicated non collapsed multi-frame contribution, supporting the interpretability of the weighting process rather than an implicit best-frame selection.

For atmospheric SHS workflows, the proposed strategy can be used as a spectral quality control and fusion step before retrieval. It reduces the contribution of unreliable or inconsistent frames while preserving the recovered intensity scale and keeping the fused result supported by multiple frames. The present evidence should therefore be interpreted as spectral-level stability improvement, rather than as direct proof of improved trace-gas retrieval accuracy, concentration estimation, or retrieval uncertainty. The method does not replace radiometric calibration, wavelength calibration, instrumental line-shape characterization, spatial error assessment, or atmospheric forward modelling. The current validation remains limited to two controlled lamp sources obtained from a single laboratory SHS setup; it does not include gas cell absorption tests, field atmospheric observations, independent instruments, public SHS datasets, machine learning benchmarks, processing time assessment, or systematic sensitivity analysis of key weighting parameters. Future work should extend the validation from controlled lamp measurements to gas cell experiments with known path length and gas concentration, and then to field measurements. In these retrieval-level tests, external uncertainties such as calibration errors, instrumental line-shape variation, spatial registration or mapping errors, surface effects, and environmental variability should be included in the uncertainty analysis. Further work should also evaluate broader SHS datasets, parameter sensitivity, computational performance, and possible comparisons with learning-based denoising or fusion methods.

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References

- McGarraugh, G.R.; O'Dell, C.W.; Crowell, S.M.R.; Somkuti, P.; Burgh, E.B.; Moore, B., III. The GeoCarb greenhouse gas retrieval algorithm: Simulations and sensitivity to sources of uncertainty. *Atmos. Meas. Tech.* **2024**, *17*, 1091–1121. [\[CrossRef\]](#)
- Conway, E.K.; Souri, A.H.; Benmergui, J.; Sun, K.; Liu, X.; Staebell, C.; Chan Miller, C.; Franklin, J.; Samra, J.; Wilzewski, J.; et al. Level0 to Level1B processor for MethaneAIR. *Atmos. Meas. Tech. Discuss.* **2024**, *17*, 1347–1362. [\[CrossRef\]](#)
- Chan Miller, C.; Roche, S.; Wilzewski, J.S.; Liu, X.; Chance, K.; Souri, A.H.; Conway, E.; Luo, B.; Samra, J.; Hawthorne, J.; et al. Methane retrieval from MethaneAIR using the CO₂ proxy approach: A demonstration for the upcoming MethaneSAT mission. *Atmos. Meas. Tech.* **2024**, *17*, 5429–5454. [\[CrossRef\]](#)
- Schneising, O.; Buchwitz, M.; Hachmeister, J.; Vanselow, S.; Reuter, M.; Buschmann, M.; Bovensmann, H.; Burrows, J.P. Advances in retrieving XCH₄ and XCO from Sentinel-5 Precursor: Improvements in the scientific TROPOMI/WFMD algorithm. *Atmos. Meas. Tech.* **2023**, *16*, 669–694. [\[CrossRef\]](#)
- Lorente, A.; Borsdorff, T.; Martinez-Velarte, M.C.; Landgraf, J. Accounting for surface reflectance spectral features in TROPOMI methane retrievals. *Atmos. Meas. Tech.* **2023**, *16*, 1597–1608. [\[CrossRef\]](#)
- Jacob, D.J.; Turner, A.J.; Maasakkers, J.D.; Sheng, J.; Sun, K.; Liu, X.; Chance, K.; Aben, I.; McKeever, J.; Frankenberg, C. Satellite observations of atmospheric methane and their value for quantifying methane emissions. *Atmos. Chem. Phys.* **2016**, *16*, 14371–14396. [\[CrossRef\]](#)
- Zhang, Y.; Gautam, R.; Pandey, S.; Omara, M.; Maasakkers, J.D.; Sadavarte, P.; Lyon, D.; Nesser, H.; Sulprizio, M.P.; Varon, D.J.; et al. Quantifying methane emissions from the largest oil-producing basin in the United States from space. *Sci. Adv.* **2020**, *6*, eaaz5120. [\[CrossRef\]](#) [\[PubMed\]](#)
- Humpage, N.; Boesch, H.; Okello, W.; Chen, J.; Dietrich, F.; Lunt, M.F.; Feng, L.; Palmer, P.I.; Hase, F. Greenhouse gas column observations from a portable spectrometer in Uganda. *Atmos. Meas. Tech.* **2024**, *17*, 5679–5707. [\[CrossRef\]](#)
- Müller, A.; Tanimoto, H.; Sugita, T.; Patra, P.K.; Nakaoka, S.; Machida, T.; Morino, I.; Butz, A.; Shiomi, K. Ship- and aircraft-based XCH₄ over oceans as a new tool for satellite validation. *Atmos. Meas. Tech.* **2024**, *17*, 1297–1316. [\[CrossRef\]](#)
- Irakulis-Loitxate, I.; Guanter, L.; Liu, Y.N.; Varon, D.J.; Maasakkers, J.D.; Zhang, Y.; Chulakadabba, A.; Wofsy, S.C.; Thorpe, A.K.; Duren, R.M.; et al. Satellite-based survey of extreme methane emissions in the Permian basin. *Sci. Adv.* **2021**, *7*, eabf4507. [\[CrossRef\]](#) [\[PubMed\]](#)
- Duren, R.M.; Thorpe, A.K.; Foster, K.T.; Rafiq, T.; Hopkins, F.M.; Yadav, V.; Bue, B.D.; Thompson, D.R.; Conley, S.; Colombi, N.K.; et al. California's methane super-emitters. *Nature* **2019**, *575*, 180–184. [\[CrossRef\]](#) [\[PubMed\]](#)
- Valjarević, A.; Popovici, C.; Djekić, T.; Morar, C.; Filipović, D.; Lukić, T. Long-term monitoring of high optical imagery of the stratospheric clouds and their properties new approaches and conclusions. *Egypt. J. Remote Sens. Space Sci.* **2022**, *25*, 1037–1043. [\[CrossRef\]](#)
- Luo, H.; Li, Z.; Wu, Y.; Qiu, Z.; Shi, H.; Wang, Q.; Xiong, W. Greenhouse Gases Monitoring Instrument on GaoFen-5 Satellite-II: Optical Design and Evaluation. *Remote Sens.* **2023**, *15*, 1105. [\[CrossRef\]](#)
- Han, Y.; Shi, H.; Li, Z.; Luo, H.; Ding, Y.; Xiong, W.; Hu, Z. Greenhouse gas monitoring instrument on the GF-5 satellite-II: On-orbit spectral calibration. *Appl. Opt.* **2023**, *62*, 5839–5849. [\[CrossRef\]](#) [\[PubMed\]](#)
- Wang, Q.; Luo, H.; Li, Z.; Shi, H.; Han, Y.; Xiong, W. Greenhouse gases monitoring instrument on a GF-5 satellite-II: Correction of spatial and frequency-dependent phase distortion. *Opt. Express* **2023**, *31*, 3028–3045. [\[CrossRef\]](#) [\[PubMed\]](#)
- Han, Y.; Shi, H.; Luo, H.; Li, Z.; Ye, H.; Li, C.; Ding, Y.; Wu, S.; Wang, X.; Xiong, W.; et al. Research on Calculation Method of On-Orbit Instrumental Line Shape Function for the Greenhouse Gases Monitoring Instrument on the GaoFen-5B Satellite. *Remote Sens.* **2024**, *16*, 2171. [\[CrossRef\]](#)
- Guo, Y.; Gong, C.; Hu, Y.; Zheng, F.; Liu, Y. On-Orbit Wavelength Calibration Error Analysis of the Spaceborne Hyperspectral Greenhouse Gas Monitoring Instrument Using the Solar Fraunhofer Lines. *Remote Sens.* **2024**, *16*, 3367. [\[CrossRef\]](#)
- Wu, X.; Tan, Y.; Yi, Y.; Zhang, Y.; Yi, F. Two-dimensional spatial heterodyne spectrometer for atmospheric nitrogen dioxide observations. *Opt. Express* **2019**, *27*, 20942–20957. [\[CrossRef\]](#) [\[PubMed\]](#)
- Sahoo, A.; Mathew, J.; Battisti, A.; Tucker, B. Compact Spatial Heterodyne Spectrographs for Future Space-Based Observations: Instrument Modeling and Applications. *Sensors* **2024**, *24*, 4709. [\[CrossRef\]](#) [\[PubMed\]](#)
- Zhang, W.L.; Liu, Z.Y.; Liang, K.; Wang, Y.; Chen, K.F.; Sun, Y.W.; Wang, S. Experimental realization of visible gas sensing technology based on spatial heterodyne spectroscopy. *Sci. Rep.* **2022**, *12*, 1423. [\[CrossRef\]](#) [\[PubMed\]](#)
- Wang, Q.; Luo, H.; Li, Z.; Ding, Y.; Xiong, W. High dynamic range spatial heterodyne one-dimensional imaging spectroscopy based on a digital micromirror device. *Opt. Express* **2024**, *32*, 22067–22077. [\[CrossRef\]](#) [\[PubMed\]](#)
- Wang, Q.; Luo, H.; Li, Z.; Ding, Y.; Xiong, W. Analysis of signal-to-noise ratio of spatial heterodyne spectroscopy. *Measurement* **2024**, *237*, 115180. [\[CrossRef\]](#)
- Zhang, W.L.; Liu, Z.Y.; Wang, H.; Chen, Y.; Wang, Y.; Zhao, Z.Z.; Sun, T. Research status of spatial heterodyne spectroscopy—A review. *Microchem. J.* **2021**, *166*, 106228. [\[CrossRef\]](#)

24. Li, X.; Riedel, J.; You, Y. Practical high-resolution spectroscopy with a spatial heterodyne spectrometer: Determination of instrumental function for lineshape recovery. *Spectrochim. Acta Part B At. Spectrosc.* **2024**, *221*, 107053. [[CrossRef](#)]
25. Roesler, F.L.; Harlander, J.M. Spatial heterodyne spectroscopy: Interferometric performance at any wavelength without scanning. *Proc. SPIE* **1990**, *1318*, 234–243. [[CrossRef](#)]
26. Liu, D.; Huang, Y.; Cao, Z.; Lu, X.; Liu, X. The Influence of Instrumental Line Shape Degradation on Gas Retrievals and Observation of Greenhouse Gases in Maoming, China. *Atmosphere* **2021**, *12*, 863. [[CrossRef](#)]
27. Veefkind, J.P.; Aben, I.; McMullan, K.; Förster, H.; de Vries, J.; Otter, G.; Claas, J.; Eskes, H.J.; de Haan, J.F.; Kleipool, Q.; et al. TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. *Remote Sens. Environ.* **2012**, *120*, 70–83. [[CrossRef](#)]
28. Wunch, D.; Toon, G.C.; Blavier, J.F.L.; Washenfelder, R.A.; Notholt, J.; Connor, B.J.; Griffith, D.W.T.; Sherlock, V.; Wennberg, P.O. The Total Carbon Column Observing Network. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.* **2011**, *369*, 2087–2112. [[CrossRef](#)]
29. Rinnan, Å.; van den Berg, F.; Engelsen, S.B. Review of the most common pre-processing techniques for near-infrared spectra. *TrAC Trends Anal. Chem.* **2009**, *28*, 1201–1222. [[CrossRef](#)]
30. Burger, J.; Gowen, A. Data handling in hyperspectral image analysis. *Chemom. Intell. Lab. Syst.* **2011**, *108*, 13–22. [[CrossRef](#)]
31. Rousseeuw, P.J.; Croux, C. Alternatives to the median absolute deviation. *J. Am. Stat. Assoc.* **1993**, *88*, 1273–1283. [[CrossRef](#)]
32. Huber, P.J. Robust estimation of a location parameter. *Ann. Math. Stat.* **1964**, *35*, 73–101. [[CrossRef](#)]

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