HTHH Retrieval Package User’s Guide

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1. Introduction

This document is a user guide for Hunga Tonga–Hunga Haʻapai (HTHH) package, which was developed in Spurr et al. (2025). The tool retrieves stratospheric aerosol optical depth (AOD) and aerosol peak height (Z_p > 20 km), and SO_2 column density by fitting the hyperspectral solar backscattered ultraviolet (BUV) radiation using on-line Vector Linearized Discrete Ordinate Radiative Transfer (VLIDORT) model version 2.8 combined with the polydisperse Mie calculations.

Although the authors in Spurr et al. (2025) used BUV radiance data from TROPOspheric Monitoring Instrument (TROPOMI) and ozone profiles from M2-SCREAM reanalysis data (MERRA-2 Stratospheric Composition Reanalysis of Aura Microwave Limb Sounder (MLS) produced by NASA's Global Modelling and Assimilation Office) for the Hunga-Tonga volcanic eruption on January 17, 2022. This package can also be applied to other volcanic eruption events using data from various hyperspectral instruments that cover ultraviolet wavelength regions (e.g., OMPS, OMI, and TOMS).

The Hunga tool was originally designed to support a 3-parameter retrieval of AOD, Z_p, and SO_2. Spurr et al. (2025) demonstrated that a reliable 2-parameter retrieval (AOD and Z_p) can be achieved using a 289–296 nm fitting window. Building on this work, the tool is being continuously updated to enable stable SO_2 retrievals by extending the fitting window. This also includes accounting for the effect of tropospheric clouds introduced by the extended window, by considering the impact of cloud albedo in both plume and background (Rayleigh) scenarios.

Therefore, this user guide is designed to assist users interested in aerosol and SO_2 retrievals during volcanic eruptions by providing a straightforward way to use the HTHH package. The guide includes a brief introduction to the HTHH retrieval algorithm, an overview of the package structure, and instructions on modifying the code or shell scripts for practical application. This information will be valuable for users intending to apply this package to other volcanic events or using data from different instruments.

2. Structure of HTHH Package and How to Run

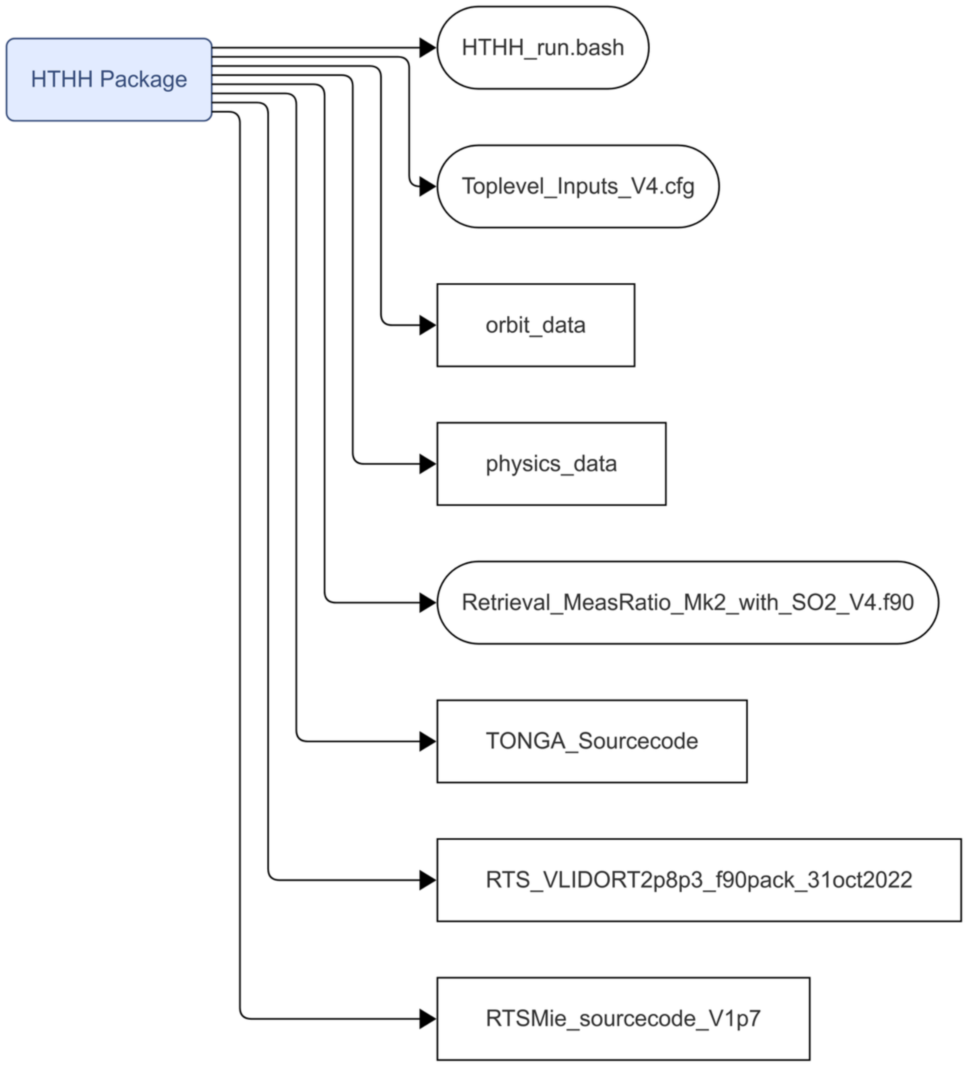

Figure 1. Structure of the HTHH Package

Each directory serves a specific purpose:

- **HTHH_run.bash**: Main shell script file to execute the HTHH package.
- **Toplevel_Inputs_V4.cfg**: Main configuration file for the package (see Section 3.5).
- **orbit_data/physics_data**: Directory containing input files (BUV radiance, pressure, temperature, ozone profiles, Mie parameters, absorption cross sections; see Section 3.1–3.4).

- **Retrieval_MeasRatio_Mk2_with_SO2_V4.f90**: Main Fortran retrieval code for the HTHH workflow.
- **TONGA_Sourcecode:** Directory containing HTHH internal source modules.
- **RTS_VLIDORT2p8p3_f90pack_31oct2022:** Directory containing VLIDORT radiative transfer model source code.
- **RTSMie_sourcecode_V1p7:** Directory containing Mie source code.

**Our package supports the OpenMP option. Please use the files marked with "_OMP" for running with OpenMP (e.g., HTHH_run_OMP.bash, Retrieval_MeasRatio_Mk2_with_SO2_V4_OMP.f90, and Toplevel_Inputs_V4_OMP.cfg).*

To run the HTHH package, follow these steps:

1. **Set Up Configuration Files:**
   - Open the Toplevel_Inputs_V4.cfg file in the package and adjust any necessary settings according to your desired output.
2. **Prepare Input Data:**
   - Place the required input files in the orbit_data (atmospheric profiles and BUV radiance) and physical_data (absorption cross sections) directory. Ensure that files are formatted and named correctly as specified in the package instructions.
3. **Run the HTHH Package:**
   - By running the HTHH_run.bash file, you can execute the HTHH tool.
   - *MIE calculation:* Set "T" for "Performs Mie calcs and dumps Mie results to file ONLY" in the configuration file. MIE parameters are calculated using the wavelength grid of the input BUV radiance data.
   - *Main retrieval:* Set "T" for "Uses Mie file data if TRUE" in the configuration file.

     For the retrieval of aerosols and SO2 (TBD), the calculated MIE parameters must be located in the orbit_data/mie directory.
4. **View the Output:**
   - After running, the results will be saved in the **main** directory. Check the output files to verify that the data retrieval was successful. See Section 4 for the details of the output files.

3. Guidelines for inputs

The HTHH package requires specific input parameters, formatted and structured precisely. The input data type and format for the HTHH package can be summarized in Table 1. 'Mandatory change files' refer to files that need to be changed for each pixel during the retrieval of AOD, aerosol layer height, and SO_2. 'Fixed or customizable files' refer to files that can be adjusted or replaced if necessary. All files are in ASCII format, and the file names and the number of columns/lines in the files *must be* matched with the input data. Detailed information for each input data is described in Section 3.1 to 3.5.

Table 1. List of input data

	Input	Directory	Notes
Mandatory Change Files	Atmospheric profiles* (Section 3.1)	/orbit_data/atmos	Atmospheric pressure, temperature, and ozone profiles for background and plume pixels
	Level 1 B data* (Section 3.2)	/orbit_dara/rad	Measurement geometries, BUV radiance, and signal to noise ratio for background and plume pixels
	Mie coefficients (Section 3.3)	/orbit_data/mie	MIE parameters
Fixed or Customizable Files	Absorption cross sections (Section 3.4)	/orbit_data/physics_data	Temperature-dependent SO_2 and O_3 absorption cross sections
	Configure file (Section 3.5)	/	Configuration for spectral fitting window, plume control, and aerosol scattering control

** Those files are required for both "background" and "volcanic plume" scenarios.*

3.1 Vertical profiles of height, pressure, temperature, and ozone (H/P/T/O3)

- **Directory**: /orbit_data/atmos
- **Filename**:
  - **Background pixel**: make_063_HPTZ_22085_2071_03.dat
  - **Plume pixel**: make_063_HPTZ_22086_2071_03.dat

This file contains vertical profiles with 72 layers and 6 columns, including layer number, altitude, pressure, temperature, O_3 column density, and O_3 volume mixing ratio (VMR). These profiles can be sourced from the MLS M2-SCREAM product or other atmospheric data sources, as long as they follow this exact format.

3.2 Radiance

- **Directory**: /orbit_data/rad
- **Filename**:
  - **Background pixel**: TROPOMI_03_BD1_22085_2071_03, TROPOMI_21_BD2_22085_2071_03
  - **Plime pixel**: TROPOMI_03_BD1_22086_2071_03, TROPOMI_21_BD2_22086_2071_03

In Spurr et al. (2025), the HTHH tool was designed to read two separate TROPOMI radiance files — BD1 (~300 nm) and BD2 (above 300 nm) — to cover the extended fitting window from 289 nm to 310 nm. Therefore, the tool reads radiance information for both bands separately for background and plume pixels.

Each radiance file includes a two-line header followed by five columns:

Headers

- **1st Header**: Number of wavelengths
- **2nd Header**: Coordinates and measurement geometries, including latitude, longitude, Solar Zenith Angle (SZA), Viewing Zenith Angle (VZA), Solar Azimuth Angle (SAA), and Viewing Azimuth Angle (VAA).

Columns

- **1st column:** Wavelength
- **2nd column:** BUV radiance
- **3rd column:** Spectral signal-to-noise ratio (used as error covariance matrix; see Spurr et al., 2025)

3.3 MIE Coefficients

- **Directory**: /orbit_data/mie
- **Filename**: MIE_22086_2071_03_TROPOMI_2Band

The MIE coefficients are essential for the main retrieval process and are generated by executing the HTHH_run.bash file. This step must be completed prior to running the main retrieval code. The MIE coefficients are specifically calculated based on the wavelength details from the Level 1B radiance data.

3.4 Absorption Cross Sections

- **Directory**: /physics_data
- **Files**:
  - **SO_2**: Bogumil_so2_xsec_tmp_270_400nm.dat
  - **O_3**: o3abs_brion_195_660_vacfinal.dat

The HTHH package allows for the use of customized absorption cross-sections. If the users want to use their own user-defined cross-section data, the files must retain the above names to ensure compatibility. This is because the package is configured to read only from files with specific names for absorption cross sections.

3.5 Configuration File

- **Directory**: /
- **Filename**: Toplevel_Inputs_V4.cfg

This configuration file allows users to customize various retrieval settings to make the HTHH package useful for different atmospheric scenarios and volcanic events. By adjusting these settings, users can adapt the retrieval process for various environmental conditions. Users can change main settings include the fitting window, plume shape, and aerosol properties, which help the retrieval process match specific needs in the analysis.

For example, adjusting the fitting window helps users focus on the desired wavelength range, allowing them to concentrate on the most relevant wavelengths and reflect the characteristics of the L1B data being used. Additionally, changing the plume shape settings can better capture the structure of volcanic plumes in different conditions. Users can also set aerosol properties that match the expected types of aerosols. By default, the aerosol properties in this file are based on scattering aerosols (sulfate) measured from AERONET at the Lucinda site on Jan 17, 2022, but users can adjust these settings as needed to reflect other environments.

Table 2. Details of Configuration Parameters for the HTHH Package

Category	**Parameter**
Parallel Computing Control *(OpenMP only)*	Number of processor cores Retrieval & Forward model timing
Retrieval Scene Pre-screening	Wavelength Index (lower limit) for pre-screening Wavelength index (upper limit) for pre-screening Radiance Ratio threshold for pre-screening
RT Control	Number of stokes vector elements Half of the RT streams Find layer control for FOCORR_OUTGOING in VLIDORT No multiple scatters in VLIDORT
Wavelength Limits	Lower wavelength limit for the fitting window [nm] Upper wavelength limit for the fitting window [nm]

Plume Control	Upper limit of plume [km] Lower limit of plume [km] Halfwidth half maximum of plume [km] Flag for retrieving plume fwhm Reference wavelength [nm] First-guess value of AOD First-guess value of Peak Height [km]
SO_2 Control	Flag for including SO_2 Source file of SO_2 cross section First-guess value of total column SO_2 (DU) Flag for retrieving SO_2
Aerosol Scattering Control (parameterized values for aerosol; default: sulfate)	Flag for retrieving refractive index (real part) (TBD) Flag for retrieving refractive index (imaginary part) (TBD) Bimodal number fraction *Fine mode* refractive index (real part) *Fine mode* refractive index (imaginary part) *Fine mode* radius *Fine mode* shape parameter *Coarse mode* refractive index (real part) *Coarse mode* refractive index (imaginary part) *Coarse mode* radius *Coarse mode* shape parameter Flag for doing initial Mie calculations (Performs desired Mie calculations and dumps Mie results to file only) Flag for use initial Mie calculations (Uses dumped Mie data directly if TRUE)

4. Outputs

The output from running the HTHH package is saved in the main directory. The final retrieved values for AOD, Hgt, and SO_2 column density are saved in the DAT file, while retrieval logs are stored in the LOG file, and the PLT file contains wavelength-specific fitting results and errors. Detailed descriptions are provided in Sections 5.1 through 5.3.

The output file name is determined according to user-defined settings in the configuration file, including the number of retrieval parameters (par), fine mode fraction (Bf), fine mode radius (Rg), fine mode shape parameter (Sg), the real (Nr) and imaginary (Ni) parts of the refractive index, the lower (WLo) and upper (WHi) limits of the fitting window, and the flag for including SO_2 ($IncSO_2$). For example:

- 2-parameter retrieval
  RetRes_2par_AOD_PKHT_{Bf}_{Rg}_{Sg}_{Nr}_{Ni}_{WLo}_{WHi}_{IncSO2}_22086_2071_03_RType5.{DAT, LOG, or PLT}_nt4
- 3-parameter retrieval
  RetRes_3par_AOD_PKHT_SO2_{Bf}_{Rg}_{Sg}_{Nr}_{Ni}_{WLo}_{WHi}_{IncSO2}_22086_2071_03_RType5.{DAT, LOG, or PLT}_nt4

4.1 Retrieval Output (DAT)

- **Filename (3-paramter retrieval example)**: RetRes_3par_AOD_PKHT_SO2_{Bf}_{Rg}_{Sg}_{Nr}_{Ni}_{WLo}_{WHi}_{IncSO2}_22086_2071_03_RType5.**DAT**_nt4

The first line of the DAT file contains the chi-square (CHISQ) value, ALAMBDA, final AOD, Hgt, and SO_2 values along with their respective errors from the last iteration, where CHISQ is minimized after multiple iterations in the HTHH package. The second line is blank, and lines 3 to 5 present the cross-correlation matrix among AOD, Hgt, and SO_2 (Figure 2).

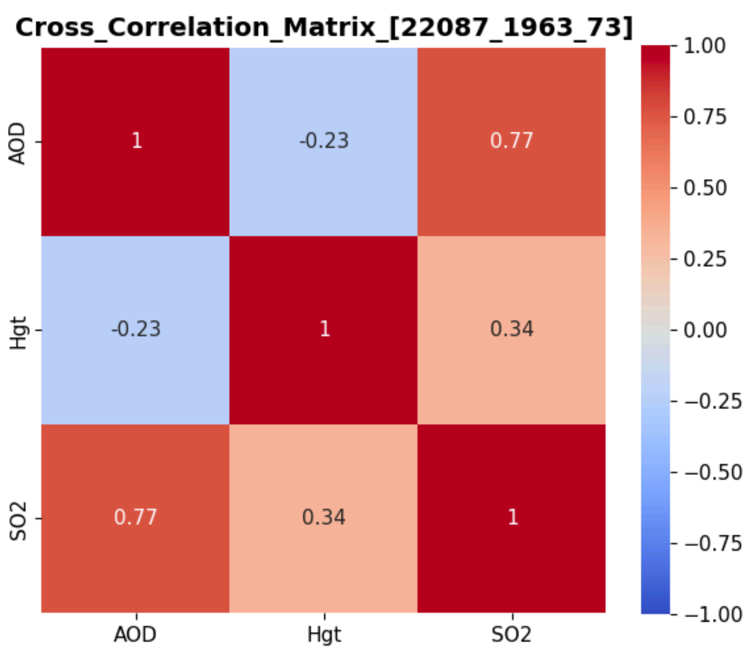

Figure 2. Cross Correlation Matrix from 3-parameter retrieval (NOrbit: 22087; NTime: 1963; NScan: 73)

4.2 Retrieval Log (LOG)

- **Filename (3-paramter retrieval example)**: RetRes_3par_AOD_PKHT_SO2_{Bf}_{Rg}_{Sg}_{Nr}_{Ni}_{WLo}_{WHi}_{IncSO2}_22086_2071_03_RType5.**LOG**_nt4

The LOG file records the changes in CHISQ across each iteration until convergence, as well as the values of CHISQ, ALAMBDA, retrieved AOD, Hgt, and SO_2 column density for each iteration (Figure 3).

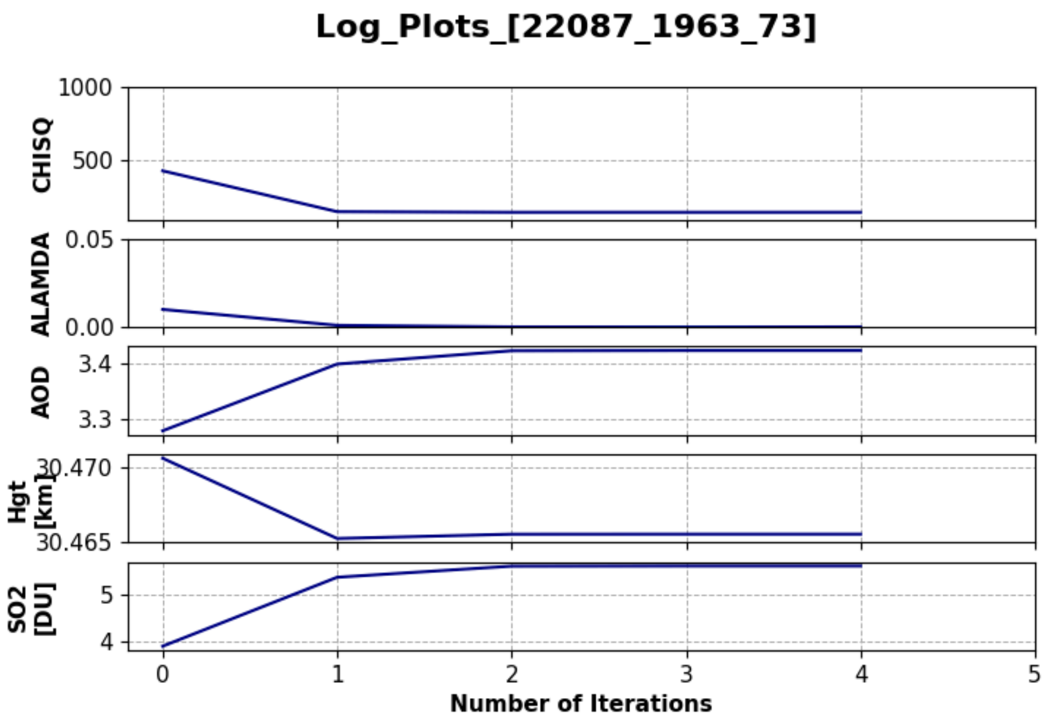

Figure 3. Log Plots for CHISQ, Alambda, AOD, Hgt, and SO_2 from 3-parameter retrieval (NOrbit: 22087; NTime: 1963; NScan: 73)

4.3 Information for Retrieval Process (PLT)

- **Filename (3-paramter retrieval example):**
  RetRes_3par_AOD_PKHT_SO2_{Bf}_{Rg}_{Sg}_{Nr}_{Ni}_{WLo}_{WHi}_{IncSO2}_22086_2071_03_RType5.**PLT**_nt4

The PLT file includes details from the final converged iteration, showing measured radiance, simulated radiance, Jacobians for each retrieved parameter, radiance errors, and forward model errors (Figure 4). Additionally, the tool provides SO_2 air mass factors (AMFs) for 3-parameter retrieval across the fitting window. The labels for each column retrieval are as follows:

3-parameter retrieval (AOD, Hgt, and SO_2)

- **Column 1**: Wavelength
- **Column 2**: Measured radiance ratio
- **Column 3**: Simulated radiance ratio
- **Columns 4-6**: Simulated Jacobian for each parameter (AOD, Hgt, SO_2)
- **Column 7**: Standard deviation of radiance ratio noise (sigs_orig)
- **Column 8**: Standard deviation of forward model error (sigF)
- **Column 9**: Combined error (sigs_orig + sigF)
- **Column 10**: Forward model error (epsF)
- **Column 11**: SO_2 AMF

2-parameter retrieval (AOD and Hgt)

- **Column 1**: Wavelength
- **Column 2**: Measured radiance ratio
- **Column 3**: Simulated radiance ratio
- **Columns 4-5**: Simulated Jacobian for each parameter (AOD and Hgt)
- **Column 6**: Standard deviation of radiance ratio noise (sigs_orig)
- **Column 7**: Standard deviation of forward model error (sigF)
- **Column 8**: Combined error (sigs_orig + sigF)
- **Column 9**: Forward model error (epsF)

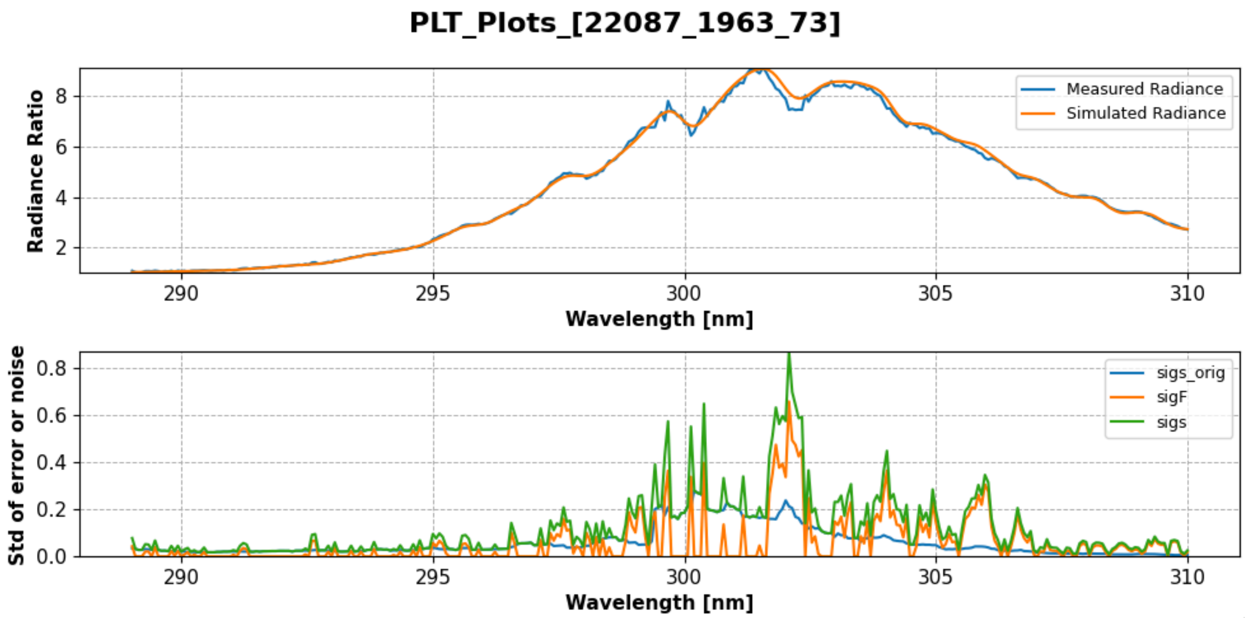

Figure 4. PLT plots for radiance ratios and errors from 3-parameter retrieval (NOrbit: 22087; NTime: 1963; NScan: 73)

References

Spurr, R. J. D., Christi, M., Krotkov, N. A., Choi, W.-E., Carn, S., Li, C., Kramarova, N., Haffner, D., Yang, E.-S., Gorkavyi, N., Vasilkov, A., Wargan, K., Torres, O., Loyola, D., Di Pede, S., Veefkind, J. P., and Bhartia, P. K.: Solar Backscatter Ultraviolet (BUV) Retrievals of Mid-Stratospheric Aerosols from the 2022 Hunga Eruption, EGUsphere [preprint], https://doi.org/10.5194/egusphere-2025-2938, 2025.