

Title: Fast Atmospheric Line-by-line Code with Aerosol and Cloud Scattering (FALCAS): application to TROPOMI Total Column Water Vapour Retrievals in the SWIR band

Fast radiative transfer models are essential for the efficient processing of hyperspectral satellite remote sensing data in trace gas retrievals. Accurate simulation of high-spectral-resolution measurements with full multi-stream radiative transfer models is computationally demanding, especially when accounting for multiple scattering effects caused by aerosols, clouds and Rayleigh scattering. In this regard, acceleration techniques for radiative transfer solvers are required to process the data from the new generation of atmospheric composition sensors, such as Sentinel 4 and Sentinel 5.

We introduce a surrogate forward model, FALCAS (Fast Atmospheric Line-by-line Code with Aerosol and Cloud Scattering), which adopts the FOCAL multiple-scattering approximation based on a virtual isotropic scattering layer. It is implemented using Py4CAtS line-by-line radiative transfer modules. This approach retains much of the accuracy of full multi-stream calculations while enabling rapid simulations. The trace gas concentrations together with auxiliary model parameters are retrieved by minimizing spectral residuals between FALCAS spectra and measurements using a quasi-Newton BFGS inversion algorithm combined with a multistart strategy.

We assess the accuracy of FALCAS using synthetic spectra from the discrete ordinate line-by-line model PYDOME in the near-infrared spectral range considering various aerosol and geometric conditions. The error in retrieved concentrations is about 1.0 % and slightly increases with the aerosol optical thickness. The computation time of FALCAS is 1000 times smaller than that of PYDOME.

We also apply FALCAS to real measurements from the TROPOspheric Monitoring Instrument (TROPOMI) for total column water vapour (TCWV) retrieval in the shortwave infrared band around 2.3 μm , and the retrievals are compared to the TROPOMI Level-2 TCWV from the CH₄ product. A total of 67,713 valid retrieval pixels across 13 regions covering the major continents are analyzed. The FALCAS results are correlated with TROPOMI Level-2 TCWV data with a Pearson correlation coefficient greater than 0.99. After bias correction, the mean relative difference between the FALCAS retrievals and the operational product is reduced to below 4%, with a standard deviation under 4%. This demonstrates that FALCAS can be directly applied to real hyperspectral measurements with minimal loss of accuracy compared to operational algorithms offering substantial computational advantages for large-scale processing.