Building an efficient gaseous absorption database for the Eradiate open-source 3D radiative transfer model.

Eradiate: new open-source 3D radiative transfer model for cal/val applications.

Yvan Nollet, Vincent Leroy, Yves Govaerts // Rayference

Gas absorption coefficient spectra

Absorption coefficient database

Example: atmospheric profile influence on top-of-atmosphere reflectance



Extinction spectrum representative of desert aerosol dust particles versus absorption spectrum of a $H_2O + CO_2 + O_3 + O_2$ gas mixture at T = 296 K and p = 101325 Pa.

- Gas molecules absorption lines are narrow
- Within satellite radiometers' spectral bands, thousands of lines to resolve
- Modelling gaseous absorption accurately improves the quality of aerosol retrievals

The line-by-line-method



Workflow



Workflow to build the absorption coefficient database in a range of air pressure, air temperature and molecules mole fraction values representative of the Earth's atmosphere. Monochromatic absorption spectra are computed with RADIS vesion 0.14 (Pannier and Laux, 2019) and HITRAN2020 (Gordon et al, 2021).

2 Datasets format

Coordinates

- Spectral interval
- quantile (g-points)
- ♦ air pressure
- air temperature
- \bullet molecules (H₂O, CO₂, . . .) mole fractions
- Data variables:

Atmospheric profile



Dotted: water vapour mole fraction (left) and temperature (right) profile in the Midlatitude Summer atmosphere model by Anderson et al (1986). Solid: water vapour mole fraction (left) and temperature (right) profile from the Copernicus Atmospheric Monitoring Serive (CAMS) reanalysis datasets on 2020-07-01 at 12:00 over the Lybia-4 PICS. **Dashed**: rescaled Midlatitude Summer water vapour mole fraction profile so that the total column amount matches the CAMS profile.



In Sentinel-2A MSI band 5



Superposition of the atmosphere transmittance spectrum (w.r.t. absorption) and the spectral response function of the band 5 of the MSI instrument onboard Sentinel-2A, illustrating the spectral resolution required to resolve each individual absorption line.

Unbiased approach Prohibitive computational (and memory) cost

The correlated-*k* **distribution (CKD) method**

Features and assumption

Band method (see Goody et al, 1989 for a review)

Spectral mapping transformation: $\lambda \rightarrow g$

Assumes a linear relationship (correlation) between spectra

Radiative transfer with the CKD method



Absorption coefficient

Relative error on average atmosphere transmittance

O Usage within Eradiate

- Supports (almost) any atmospheric profile
- Adapts to the spectral interval (variable molecules number)
- Freedom to choose the g-quadrature type and parameters
 - Configure for speed or accuracy
 - Find optimized number of *g*-points (tradeoff)



Relative error on the average atmosphere transmittance (w.r.t absorption) as a function of the number of Gauss-Legendre quadrature points in the spectral interval from 694.45 nm to 699.30 nm. The reference average atmosphere transmittance value is obtained by integrating monochromatic computations. The atmospheric profile is set to the U.S. Standard model by Anderson et al (1986).

References

Top: Top-of-atmosphere bidirectional reflectance factors (BRF) for the three selected atmospheric profiles in the spectral region 694 nm to 715 nm corresponding to Sentinel-2A MSI instrument band 5 (average atmosphere transmittance \approx 97%). **Bottom**: Relative difference when the reflectance spectrum obtained with the CAMS profile is used as reference.

In [715, 735] nm



Illustration of the spectral mapping transformation $\lambda \rightarrow g$. Left: absorption coefficient

spectrum of the gas mixture. Right: corresponding quantile function.

Compute the quantile function of the absorption coefficient

Compute radiative transfer at each quantile (g) point

Retrieve the integrated spectral quantities by computing the quadrature in g-space

Limitations

- Provides access to integrated spectral quantities only Correlation assumption is not strictly satisfied
- Impossible to predict/enforce an arbitrary accuracy

• Anderson, G. P., Clough, S. A., Kneizys, F. X., Chetwynd, J. H. Shettle, E. P. AFGL atmospheric constituent profiles (0.120km). AFGL-TR-0208 Environemental Research papers (1986).

- Goody, R., West, R., Chen, L. Crisp, D. The correlated-k method for radiation calculations in nonhomogeneous atmospheres. Journal of Quantitative Spectroscopy and Radiative Transfer 42, 539-550 (1989).
- Pannier, E. Laux, C. O. RADIS: A nonequilibrium line-by-line radiative code for CO2 and HITRAN-like database species. Journal of Quantitative Spectroscopy and Radiative Transfer 222-223, 12-25 (2019).
- van den Bekerom, D. C. M. Pannier, E. A discrete integral transform for rapid spectral synthesis. Journal of Quantitative Spectroscopy and Radiative Transfer 261, 107476 (2021).
- Gordon, I. E. et al. The HITRAN2020 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer 277, 107949 (2022).

Same as figure above but in the spectral region from 715 nm to 735 nm corresponding to stronger water vapour absorption (average atmosphere transmittance \approx 88%).

Acknowledgments

The development of Eradiate was initiated during the MetEOC-3 project (EMPIR grant 16ENV03). The two first development phases are funded by the European Space Agency (contract no 40000127201/19/I-BG).







