Jean-François Smekens
Fall, 2025

Measuring Trace Gases and Aerosols in the Atmosphere

Week #5: September 24, 2025

I. Guest Lecture

- Dr. Jean-Francois Smekens
  - *Assistant Research Professor, Northern Arizona University*

- some concepts introduced here will be explained in detail later in the regular class lecture, so do not feel overwhelmed by the topic
- try to focus on the important points and summary slides

II. Gases and Aerosols in Volcanic Plumes

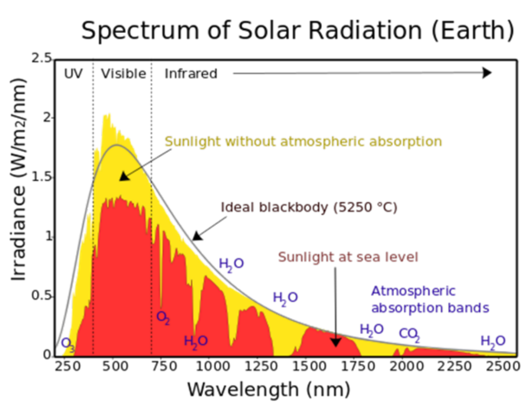
- composition
  - Gases: H_2O, CO_2, SO_2, H_2S, HF, HBr
  - Aerosols: sulfates (H_2SO_4), halogens (Cl-, F-, Br-, etc.)
  - Vehicle for trace metals (e.g., Cu, Zn, Hg, As, Pb)
  - Silicate ash

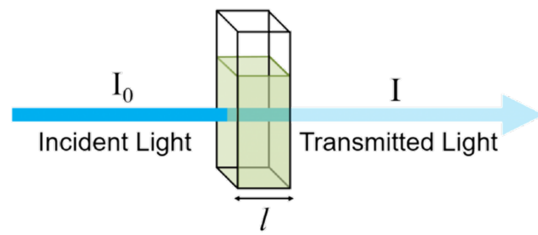
- Atmospheric impacts
  - Tropospheric: health hazards on local and regional scales
  - Stratospheric: Radiative forcing

- Physical volcanology
  - Reflect conditions in the subsurface

- Measurement techniques
  - Remote sensing (mature plumes): e.g., satellite (IR, UV, VIS), weather radars
  - Direct sampling (near-source): e.g., filter packs, particle counters

III. Principles: Absorption Spectroscopy





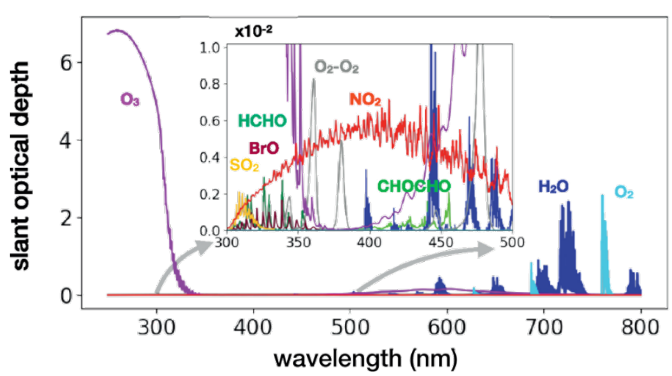
- Beer-Lambert law

$$A = \varepsilon c l = -ln\frac{I(\lambda)}{I_0(\lambda)}$$

  - A = absorbance
  - ε = molar absorptivity
  - c = concentration
  - l = pathlength
  - $I(\lambda)$ = radiation intensity at wavelength λ

- Source of radiation: backscattered/reflected sunlight
  - Important factors:
    - ➢ Incident radiation (solar zenith angle)
    - ➢ Surface reflectance
    - ➢ Vertical distribution of target gas

  - Features: electronic transitions



- Source of radiation: emitted directly from ground
  - Important factors:
    - ➢ Surface Temperature
    - ➢ Surface Emissivity
    - ➢ Vertical distribution of target gas

  - Features: vibrational/rotational modes

IV. Satellite Instruments: A synoptic view

- Large spatial scale datasets:
  - Provide context to interpret ground-based localized measurements
  - Identify sources and sinks and estimate fluxes

- Contrast conditions in separate geographical areas
- This enables crucial capabilities
  - Establish global and regional long-term trends (temporal and/or spatial)
  - Monitor evolution of large-scale events during times of crisis
  - Provide initial bounding conditions for forecast models

- Earth Observing fleet: Meteosat Third Generation (MTG)
  - Infrared Sounding Spectrometer (IRS)
    - First IR sounding instrument in GEO orbit
    - Full disc sounding every hour

  - Sentinel 4: UV-VIS-NIR spectrometer
    - 8x8 km^2 spatial resolution
    - 0.5 nm (UV-VIS) and 0.12 nm (NIR) spectral resolution
    - Designed to monitor tropospheric pollutants (e.g., O_3, NO_2, SO_2, HCHO)

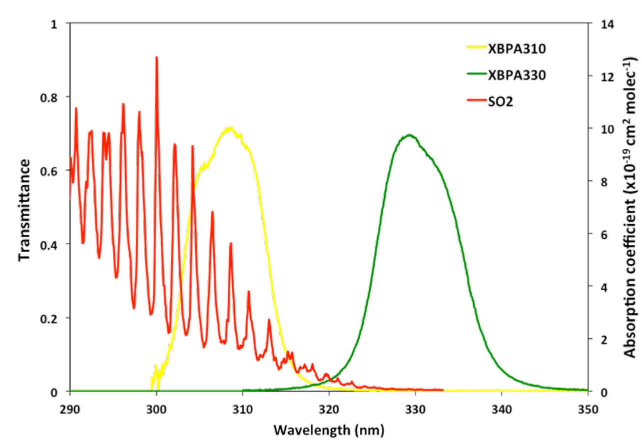
  - Flexible Combined Imager (FCI)
    - VNIR imager (1 km pixel at nadir, 8 channels)
    - IR imager (2 km at nadir, 8 channels)
    - Full disc coverage every 10 mins
    - Europe RSS: 2.5 mins

  - Sounding instruments in GEO orbit will enable:
    - Hourly maps of pollutants retrieved with high accuracy
    - More representative global daily/monthly average maps, accounting for daily variability
    - Increasing the likelihood of capturing cloud-free scenes

V. Ground-based methods: imagers

- Low spectral resolution (multispectral filter imagers)
- Increased sampling frequency from static viewpoint
- Provides valuable contextual information
- Determination of plume velocity from time series
- Capture rapid variations of the emission rate close to the source

  - The SO_2-camera
    - 2 synchronized cameras
    - Detector: CCD / CMOS
    - 2 Bandpass filters: 310 & 330 nm
    - Image capture at < 1 Hz
    - Calibration using gas cells or co-located spectrometer



- Semeru, Indonesia example
    - Notes:

- The SO_2-camera: validation of orbital data
    - Ground-based measurements are often more sporadic
        - Limited in temporal extent
        - Irregular sampling (instrument failure, maintenance)

    - They provide metrics that satellite data cannot:
        - High spatial resolution
        - High sampling rate
        - Emissions at the source

    - Finding appropriate metrics for validation
        - Integrating emission rates towards point measurements
        - Deriving emission rates from point measurements
        - Look at trends (e.g., fluxes) rather than instantaneous values

- **The SO_2-camera: summary**
    - Quantitative retrieval of gas emission rates
        - SO_2 as a tracer of volcanic gases
        - Wind speed derived from images

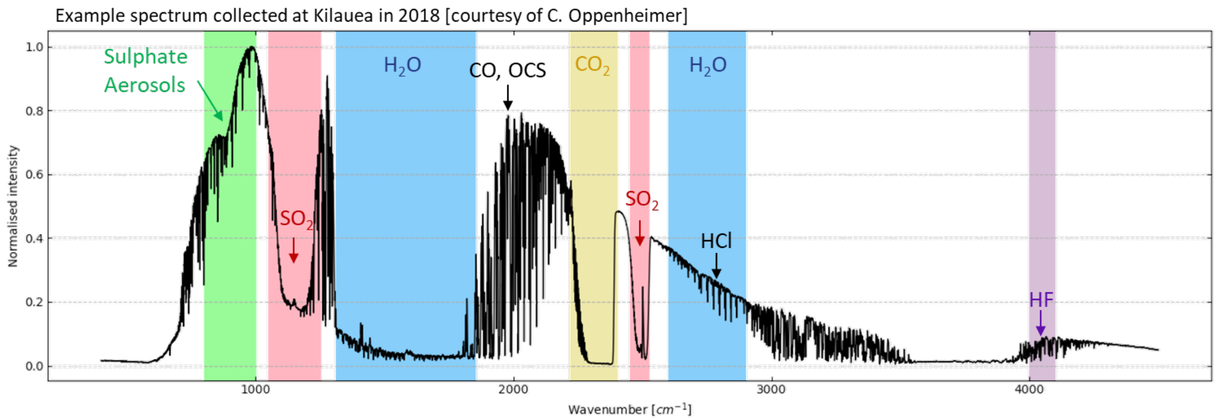
    - Disadvantages
        - Low spectral resolution → Errors from ash and/or aerosols
        - Needs good weather conditions

    - Gradual changes in degassing magnitude over short periods (< 30 mins)
    - Ideal for eruption monitoring
        - Provides hourly measures of degassing rates
        - Adaptable (partly) to changes in wind direction
        - 2-D data provides context for interpretation (e.g., ash/aerosols in the plume)

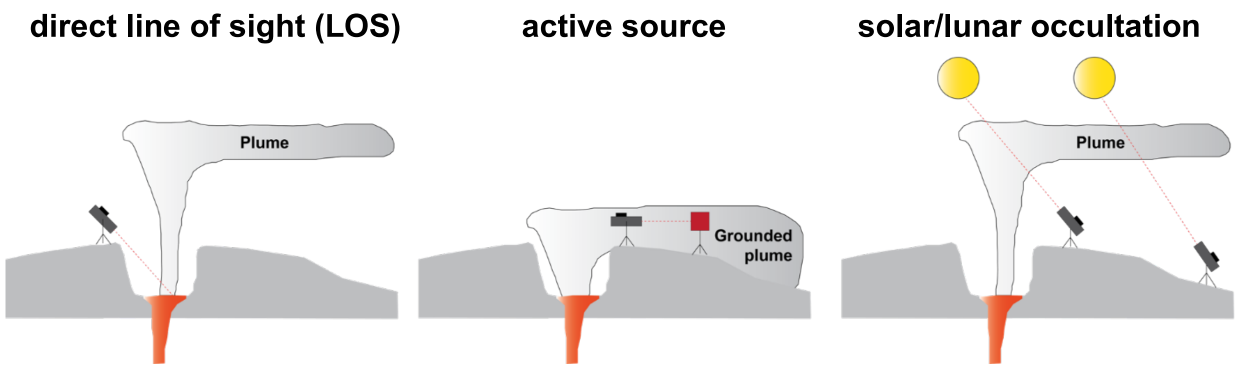
VI. Ground-based methods: point spectrometers

- High spectral resolution for precision retrieval
- Narrow field of view (single pixel spot)
- OP-FTIR: Composition of gases at the source
- UV DOAS: Cross-section (traverse) as plume passes overhead
- *Sporadic monitoring of small to moderate emissions*

- OP-FTIR
  - Fourier Transform Infrared (FTIR) spectrometers measure the intensity of radiation at wavelengths 1-50 μm
  - Strong source of IR radiation (lamp, sun, lava!!)
  - Wide range of target gases
  - Gas composition (gas ratios) rather than fluxes



  - Wide range of target gases



- Reykjanes peninsula, Iceland example
  - Notes:

- **OP-FTIR: summary**
    - Quantitative retrieval of plume composition
        - Many individual gases
        - Detailed thermal properties of the gas
    - Direct observation of primary aerosol formation
        - SO_2/SO_4^{2-} ratio controlled by plume temperature / explosivity at the vent
        - Rapid condensation of H2O aerosols
    - Gradual changes in plume characteristics over short periods (< 30 mins)
    - Ideal for eruption monitoring
        - Measure of aerosol input at the source (SO_2/SO_4^{2-}) for atmospheric dispersion models
        - Linking changes in gas composition to other monitoring signals with similar sampling rates (e.g., seismic, deformation, thermal flux, etc.)