

Calculate the measured optical density $D_{\text{CE,meas}}(\lambda) = \ln[I_0(\lambda)/I(\lambda)]$.

Calculate Rayleigh extinction coefficient α_{ray} for the measurement. Set all initial trace gas concentrations to zero $c_i^{(0)} = 0$.

Start with the first iteration: $n = 1$.

- Estimate the true optical density

$$D_{\text{CE}}^{(n)}(\lambda) = \ln \left[1 + \bar{L}_0(\lambda) \left(\sum_i \sigma_i(\lambda) \cdot c_i^{(n-1)} + \sigma_{\text{ray}}(\lambda) \cdot c_{\text{air}} \right) \right]$$

- Estimate the effective path length

$$\bar{L}_{\text{eff}}^{(n)}(\lambda) = \bar{L}_0(\lambda) \cdot K^{(n)}(\lambda) = \bar{L}_0(\lambda) \cdot \frac{D_{\text{CE}}^{(n)}(\lambda)}{e^{D_{\text{CE}}^{(n)}(\lambda)} - 1}.$$

- Compute the effective fit references

$$\Theta_i^{(n)}(\lambda) = H(\lambda) \otimes \left(\bar{L}_{\text{eff}}^{(n)}(\lambda) \cdot \sigma_i(\lambda) \right).$$

- DOAS fit with $\Theta_i^{(n)}(\lambda)$ to $D_{\text{CE,meas}}(\lambda)$ to get improved estimates for the trace gas concentrations $c_i^{(n)}$.

Did the iterative procedure converge?

no

$n = n + 1$

yes

Finished with trace gas concentrations c_i .