UNL-VRTM Notes 5
Jacobians to Gas Mixing Ratio

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Abstract

This note discusses the calculation of Jacobian with respect to gaseous mixing ratio from the VLIDORT output of profile Jacobian with recpect total gaseous absorbing optical depth.

1 Gas absorption and its Jacobian

UNL-VRTM considers up to 22 gas species. The gas absorption are computed using HITRAN spectroscopic database and gas profiles from various standard atmospheres and/or user-specified profile.

At any atmospheric layer, the gaseous absorbing optical depth is the summation of the absorbing optical depths of all gases.

$$\tau_{\text{gas}} = \sum_i \tau_{\text{gas}_i} = \sum_i 10^{-6} q_i N_{\text{air}} \Delta H \delta_i, \tag{1}$$

where τ_{gas_i} the optical depth of gas i, ΔH is the thickness (cm) of the layer, N_{air} is the air molecular number density (cm^{-3}), q_i and δ_i are the mixing ratio (ppm) and absorption cross-section (cm^2) of the gas i.

If turned on, the Jacobian of Stokes S with respect to gas absorption of each layer will be calculated by UNL-VRTM, which is defined by

$$\text{S}_{\tau_{\text{gas}}} = \tau_{\text{gas}} \frac{\partial \text{S}}{\partial \tau_{\text{gas}}}. \tag{2}$$

2 Jacobian to gas mixing ratio

Now, we want to caluclate the Jacobian of Stokes S with respect to the mixing ratio q_i of given gas i, the $q_i \frac{\partial \mathrm{S}}{\partial q_i}$, of any atmospheric layer. According to the chain rule,

$$q_i \frac{\partial \mathrm{S}}{\partial q_i} = q_i \frac{\partial \mathrm{S}}{\partial \tau_{\text{gas}}} \frac{\partial \tau_{\text{gas}}}{\partial \tau_{\text{gas}_i}} \frac{\partial \tau_{\text{gas}_i}}{\partial q_i}. \quad (3)$$

It is straightforward that $\frac{\partial \tau_{\text{gas}}}{\partial \tau_{\text{gas}_i}} = 1$ and $\frac{\partial \tau_{\text{gas}_i}}{\partial q_i} = \Delta H 10^{-6} N_{\text{air}} \delta_i$. So the equation (3) becomes

$$q_i \frac{\partial \mathrm{S}}{\partial q_i} = q_i \frac{\partial \mathrm{S}}{\partial \tau_{\text{gas}}} \Delta H 10^{-6} N_{\text{air}} \delta_i = \tau_{\text{gas}_i} \frac{\partial \mathrm{S}}{\partial \tau_{\text{gas}}} = \frac{\tau_{\text{gas}_i}}{\tau_{\text{gas}}} \mathrm{S}_{\tau_{\text{gas}}}. \quad (4)$$

Finally, the derivative of S to gas mixing ratio q_i can be calculated by

$$\frac{\partial \mathrm{S}}{\partial q_i} = \frac{\tau_{\text{gas}_i}}{\tau_{\text{gas}} q_i} \mathrm{S}_{\tau_{\text{gas}}}. \quad (5)$$

The units of $\frac{\partial \mathrm{S}}{\partial q_i}$ is radiance units divided by the units of q_i.

3 Jacobian to columnar density of any gas

Sometimes, one wants to calculate the Jacobian of Stokes S with respect to the columnar density (concentration) of any given gas i. The columnar density (N_i) is the sum of columnar density at each atmospheric layer($n_i(l) = q_i N_{air} \Delta H$):

$$N_i = \sum_l n_i(l) = \sum_l q_i N_{air} \Delta H \quad (6)$$

Jacobian of S to N_i can be caculated by

$$N_i \frac{\partial \mathrm{S}}{\partial N_i} = \sum_l \left[n_i(l) \frac{\partial \mathrm{S}}{\partial n_i(l)} \right] \quad (7)$$

Replace $n_i(l)$ in above equation, we get

$$N_i \frac{\partial \mathrm{S}}{\partial N_i} = \sum_l \left[q_i(l) \frac{\partial \mathrm{S}}{\partial q_i(l)} \right] \quad (8)$$