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 respect 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.

$$\tau_{gas} = \sum_i \tau_{gas,i} = \sum_i 10^{-6} q_i N_{air} \Delta H \delta_i,$$

where $\tau_{gas,i}$ the optical depth of gas $i$, $\Delta H$ is the thickness (cm) of the layer, $N_{air}$ is the air molecular number density (cm$^{-3}$), $q_i$ and $\delta_i$ 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

$$S_{\tau_{gas}} = \tau_{gas} \frac{\partial S}{\partial \tau_{gas}}.$$
2 Jacobian to gas mixing ratio

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

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

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

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

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

$$ \frac{\partial S}{\partial q_i} = \frac{\tau_{\text{gas}}}{\tau_{\text{gas}}} S_{\tau_{\text{gas}}}. $$  (5)

The units of $\frac{\partial S}{\partial q_i}$ 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 ($n_i(l) = q_i N_{\text{air}} \Delta H$):

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

Jacobian of $S$ to $N_i$ can be calculated by

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

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

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