## Calculation of $\mathrm{O}_{4}$ weighting functions

$\mathrm{SCD}_{\mathrm{O}_{4}}$ resp. $\tau_{\mathrm{O}_{4}}$ at one wavelength $\lambda$ :

$$
\begin{equation*}
\tau_{\mathrm{O}_{4}}=\sigma_{\mathrm{O}_{4}} \mathrm{SCD}_{\mathrm{O}_{4}}=\sigma_{\mathrm{O}_{4}} \sum_{c=1}^{N} l_{c} n_{c}=\sum_{c=1}^{N} l_{c} \beta_{c, \mathrm{O}_{4}} \tag{1}
\end{equation*}
$$

$l_{c}$ sensitivity, $n_{c}$ number concentration of O 4 in the cluster $c$. There are $N$ clusters. $l_{c}$ can be expressed as:

$$
\begin{equation*}
l_{c}=-\frac{d \log (I)}{d \beta_{c, \mathrm{O}_{4}}}=-\frac{1}{I} \frac{d I}{d \beta_{c, \mathrm{O}_{4}}} . \tag{2}
\end{equation*}
$$

$\mathrm{O}_{4}$ weighting functions:

$$
\begin{equation*}
\frac{d \tau_{\mathrm{O}_{4}}}{d x_{c^{\prime}}}=-\frac{d}{d x_{c^{\prime}}} \sum_{c=1}^{N} \frac{\beta_{c, \mathrm{O}_{4}}}{I} \frac{d I}{d \beta_{c, \mathrm{O}_{4}}}=\frac{1}{I^{2}} \sum_{c=1}^{N} \beta_{c, \mathrm{O}_{4}}\left(\frac{d I}{d \beta_{c, \mathrm{O}_{4}}} \frac{d I}{d x_{c^{\prime}}}-I \frac{d^{2} I}{d \beta_{c, \mathrm{O}_{4}} d x_{c^{\prime}}}\right) . \tag{3}
\end{equation*}
$$

Therefore one needs the radiance $I$, the Jacobians $\frac{d I}{d \beta_{c, O_{4}}}$ and $\frac{d I}{d x_{c^{\prime}}}$ and the Hesse matrix elements $\frac{d^{2} I}{d \beta_{c}, \mathrm{O}_{4} d x_{c^{\prime}}}$ for the calculation of $\mathrm{O}_{4}$ weighting functions.

