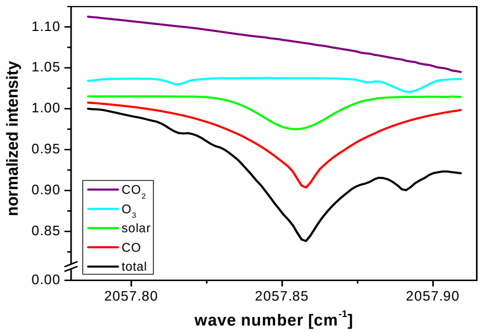
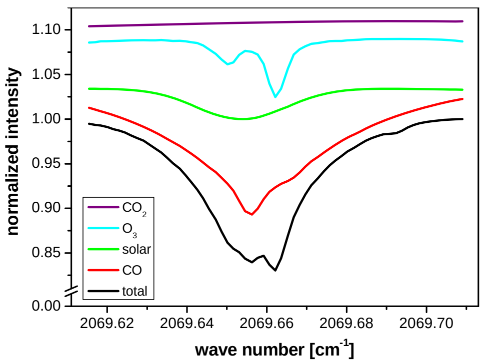
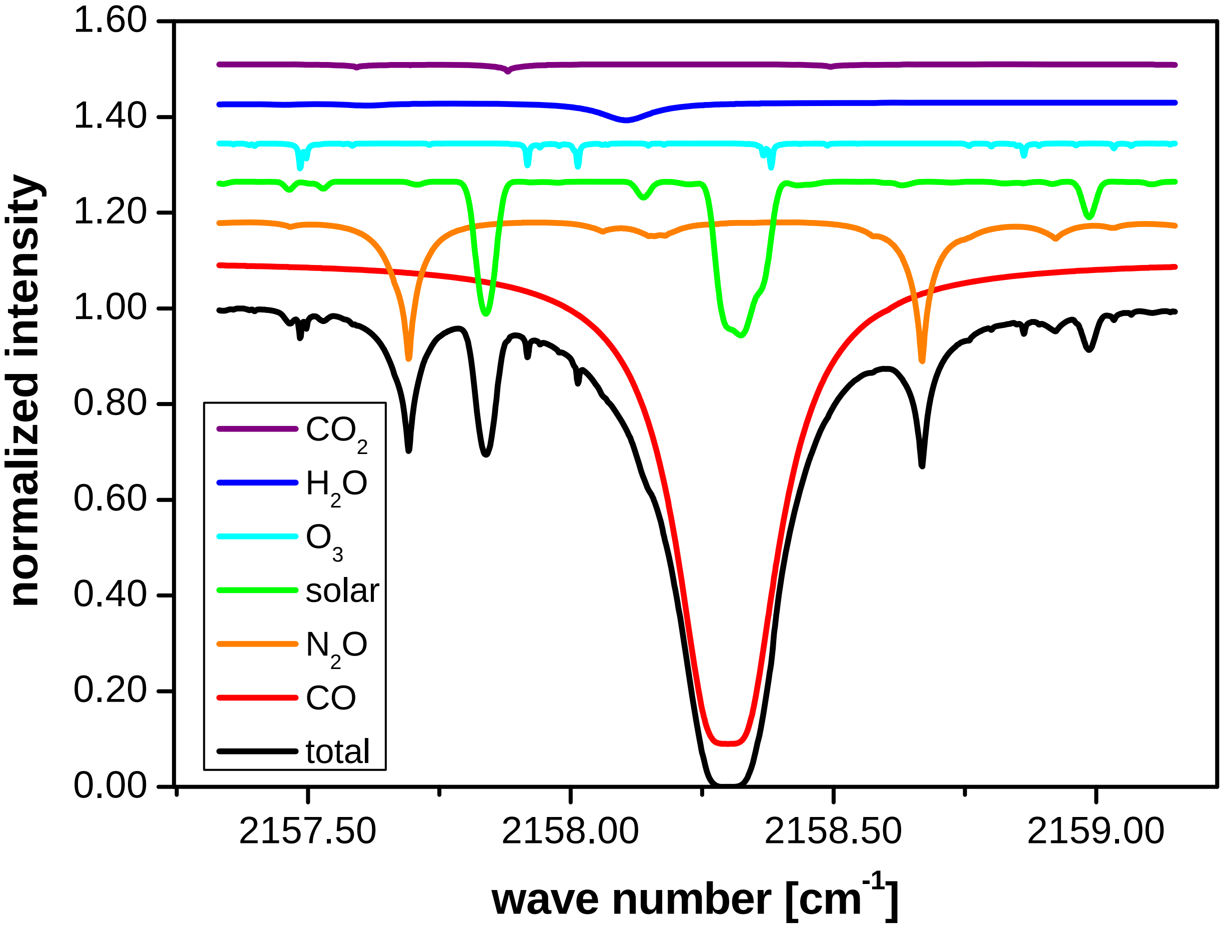
Interference errors in infrared remote sounding: I) General formulation

Spectroscopic orgin: overlap of vibration-rotation lines of different species







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Ralf Sussmann and Tobias Borsdorff: *Interference errors, Atmos. Chem. Phys., 7, 3537-3557,2007*

What is the origin of interference errors in terms of retrieval-theory ?

“interference error” refers to all errors that originate from any type of soft or hard constraint imposed on the retrieval of the profile of an interfering species;

this causes spectral residuals around the spectral signature of the interfering species;

in consequence, the profile retrieval of the target species tends to compensate for this, meaning that an artifact is introduced into the retrieved target profile.

In other words:

Interference errors originate from the smoothing error of the interfering species and its error propagation upon the retrieval of the target profile.

Can we describe interference errors by Rodgers (2000, equation 3.16) ?

profile of target species only

$$
\begin{aligned}
\hat{\boldsymbol{x}} - \boldsymbol{x} \quad = \quad & (\mathbf{A} - \mathbf{I})(\boldsymbol{x} - \boldsymbol{x}_a) && \ldots \textit{smoothing error} \\
& + \mathbf{G}_y \mathbf{K}_b (\boldsymbol{b} - \hat{\boldsymbol{b}}) && \ldots \textit{model parameter error} \\
& + \mathbf{G}_y \Delta \mathbf{f}(\boldsymbol{x}, \boldsymbol{b}, \boldsymbol{b}') && \ldots \textit{forward model error} \qquad (0) \\
& + \mathbf{G}_y \boldsymbol{\varepsilon} && \cdots \textit{retrieval noise}
\end{aligned}
$$

where $\mathbf{A} = \partial \hat{\boldsymbol{x}} / \partial \boldsymbol{x}$, $\mathbf{G}_y = \partial \hat{\boldsymbol{x}} / \partial \boldsymbol{y}$, $\mathbf{K}_b = \partial \mathbf{F} / \partial \boldsymbol{b}$

⇒ No, not in general.

Only the special case of unretrieved interfering species can be treated via model parameter errors

⇒ Idea: include interfering species into a generalized state vector

$$\boldsymbol{x} := \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \\ v_{11} \\ \vdots \\ v_{1n} \\ v_{21} \\ \vdots \\ v_{2n} \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix} \in \Re^l \qquad (1)$$

Since

… a <u>classical smoothing error covariance</u> contains off diagonals that describe errors of the target species at a certain altitude resulting from true variability at another altitude …

… the <u>generalized smoothing error covariance</u> should contain off diagonals that describe errors for the target species at a certain altitude resulting from variability of an intefering species at another altitude

Avoid a serious error: don´t treat VMR-profile scaling retrievals as scalars

$$\boldsymbol{x} := \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \\ v_{11} \\ \vdots \\ v_{1n} \\ v_{21} \\ \vdots \\ v_{2n} \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix}$$

Even if an interfering species is retrieved via one profile scaling parameter - must always <u>implement a full profile entry</u> in the state vector!

<u>don´t implement just a simple scalar</u> if the interfering quantity is in reality a profile vector

Why?

- interference errors on the target species are due to the smoothing error of the interfering species

sqrt $[(\boldsymbol{a}_{\text{totcol}} - \boldsymbol{a}_{\text{ideal}})^T \mathbf{S}_a (\boldsymbol{a}_{\text{totcol}} - \boldsymbol{a}_{\text{ideal}})]$

which is <u>driven by the true fine structure profile- type variability</u> and not at all by pure VMR-profile scaling type variability.

- interference errors from jointly retrieved true physical scalars should be $\equiv$0 if there is enough spectral info (dofs $\geq$1).

Avoid a less serious error: don´t use soft constraints for retrieval of scalars

e.g., don´t use a limited a priori uncertainty of 100 % for profile scaling retrieval of water

```
detail
pbpfile
../input/solarlines/041123_S.dat
statevec
eap.dat
eph.dat
sainv_combi
hallo
summary
../input/cfgl/
 5 0
 CH4
   66    5    1.000E+04        0.000       100.000
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 H2O
    1    0    1.0000E+04        0.000       100.000
   1.0  1.0
```

(circled: 1.0) → **better increase to very large number, e.g., 10 000.0!**

… since there is in most cases sufficient spectral information (dofs ≥1) and it unnecessarily increases smoothing errors, or interference errors.

Case I: Quantification for fine-grid profile retrieval of interfering species

$$\boldsymbol{x} := \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{v}_1 \\ \boldsymbol{v}_2 \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} t_1 \\ \vdots \\ t_n \\ v_{11} \\ \vdots \\ v_{1n} \\ v_{21} \\ \vdots \\ v_{2n} \\ \vdots \\ s_1 \\ s_2 \\ \vdots \end{pmatrix} \qquad (1)$$

Reformulate Rodgers eq 3.16:

$$\hat{\boldsymbol{x}} - \boldsymbol{x}_a = \mathbf{A}(\boldsymbol{x} - \boldsymbol{x}_\alpha) + \boldsymbol{\varepsilon}_x \qquad (2)$$

$$\mathbf{A} = (\mathbf{K}_{\boldsymbol{x}}^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_{\boldsymbol{x}} + \mathbf{R})^{-1} \mathbf{K}_{\boldsymbol{x}}^T \mathbf{S}_\varepsilon^{-1} \mathbf{K}_{\boldsymbol{x}} \qquad (3)$$

with $\mathbf{K}_{\boldsymbol{x}} = \partial \mathbf{F} / \partial \boldsymbol{x}$, $\mathbf{R} = \mathbf{S}_R^{-1}$

A denotes in our case a generalized averaging kernel matrix: inserting Eq.(1) into Eq.(2) yields …

Case I: Quantification for fine-grid profile retrieval of interfering species

This generalized averaging kernel matrix $\mathbf{A}$ comprises sub-matrices $\mathbf{A}_{ij}$, (column) vectors $\boldsymbol{a}_{ij}$, row vectors $\boldsymbol{a}_{ji}^T$, as well as scalars a_{ii}. Note that $\mathbf{A}_{tt}$ is what is usually called the "averaging kernel matrix":

$$\hat{\boldsymbol{x}} - \boldsymbol{x}_a = \begin{pmatrix} \hat{\boldsymbol{t}} - \boldsymbol{t}_a \\ \hat{\boldsymbol{v}}_1 - \boldsymbol{v}_{1a} \\ \hat{\boldsymbol{v}}_2 - \boldsymbol{v}_{2a} \\ \vdots \\ \hat{s}_1 - s_{1a} \\ \hat{s}_2 - s_{2a} \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{tt} & \mathbf{A}_{tv1} & \mathbf{A}_{tv2} & \cdots & \boldsymbol{a}_{ts1}^T & \boldsymbol{a}_{ts2}^T & \cdots \\ \mathbf{A}_{v1t} & \mathbf{A}_{v1v1} & \mathbf{A}_{v1v2} & \cdots & \boldsymbol{a}_{v1s1}^T & \boldsymbol{a}_{v1s2}^T & \ddots \\ \mathbf{A}_{v2t} & \mathbf{A}_{v2v1} & \mathbf{A}_{v2v2} & \cdots & \boldsymbol{a}_{v2s1}^T & \boldsymbol{a}_{v2s2}^T & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \boldsymbol{a}_{s1t} & \boldsymbol{a}_{s1v1} & \boldsymbol{a}_{s1v2} & \ddots & a_{s1s1} & a_{s1s2} & \ddots \\ \boldsymbol{a}_{s2t} & \boldsymbol{a}_{s2v1} & \boldsymbol{a}_{s2v2} & \ddots & a_{s2s1} & a_{s2s2} & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \boldsymbol{t} - \boldsymbol{t}_a \\ \boldsymbol{v}_1 - \boldsymbol{v}_{1a} \\ \boldsymbol{v}_2 - \boldsymbol{v}_{2a} \\ \vdots \\ s_1 - s_{1a} \\ s_2 - s_{2a} \\ \vdots \end{pmatrix} + \begin{pmatrix} \boldsymbol{\varepsilon}_t \\ \boldsymbol{\varepsilon}_{v1} \\ \boldsymbol{\varepsilon}_{v2} \\ \vdots \\ \varepsilon_{s1} \\ \varepsilon_{s2} \\ \vdots \end{pmatrix} . \qquad (4)$$

If the retrieved auxiliary scalar parameters *s1*, *s*2, … describe true physical scalar-type quantities (*i.e.*, they are not scalar approximations to a vector-type physical quantity), and they are not correlated, then the retrieval of these scalars can and should be performed without any regularization. In this case Eq.(4) simplifies to …

Case I: Quantification for fine-grid profile retrieval of interfering species

$$\hat{\boldsymbol{x}} - \boldsymbol{x}_a = \begin{pmatrix} \hat{\boldsymbol{t}} - \boldsymbol{t}_a \\ \hat{\boldsymbol{v}}_1 - \boldsymbol{v}_{1a} \\ \hat{\boldsymbol{v}}_2 - \boldsymbol{v}_{2a} \\ \vdots \\ \hat{s}_1 - s_{1a} \\ \hat{s}_2 - s_{2a} \\ \vdots \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{tt} & \mathbf{A}_{tv1} & \mathbf{A}_{tv2} & \cdots & 0 & 0 & \cdots \\ \mathbf{A}_{v1t} & \mathbf{A}_{v1v1} & \mathbf{A}_{v1v2} & \cdots & 0 & 0 & \ddots \\ \mathbf{A}_{v2t} & \mathbf{A}_{v2v1} & \mathbf{A}_{v2v2} & \cdots & 0 & 0 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & \ddots & 1 & 0 & \ddots \\ 0 & 0 & 0 & \ddots & 0 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \boldsymbol{t} - \boldsymbol{t}_a \\ \boldsymbol{v}_1 - \boldsymbol{v}_{1a} \\ \boldsymbol{v}_2 - \boldsymbol{v}_{2a} \\ \vdots \\ s_1 - s_{1a} \\ s_2 - s_{2a} \\ \vdots \end{pmatrix} + \begin{pmatrix} \boldsymbol{\varepsilon}_t \\ \boldsymbol{\varepsilon}_{v1} \\ \boldsymbol{\varepsilon}_{v2} \\ \vdots \\ \varepsilon_{s1} \\ \varepsilon_{s2} \\ \vdots \end{pmatrix} \quad . \qquad (5)$$

We then obtain the following relation between $\hat{\boldsymbol{t}}$, $\boldsymbol{t}_a$, and $\boldsymbol{t}$

$$\hat{\boldsymbol{t}} - \boldsymbol{t}_a = \mathbf{A}_{tt}(\boldsymbol{t} - \boldsymbol{t}_\alpha) + \mathbf{A}_{tv1}(\boldsymbol{v}_1 - \boldsymbol{v}_{1a}) + \mathbf{A}_{tv2}(\boldsymbol{v}_2 - \boldsymbol{v}_{2a}) + \ldots + \boldsymbol{\varepsilon}_t \quad , \qquad (6)$$

which can be rearranged …

Case I: Quantification for fine-grid profile retrieval of interfering species

$$\hat{\boldsymbol{t}} - \boldsymbol{t} = (\mathbf{A}_{tt} - \mathbf{I})(\boldsymbol{t} - \boldsymbol{t}_{\alpha}) \quad \ldots \textit{smoothing error}$$

$$\boxed{+ \mathbf{A}_{tv1}(\boldsymbol{v}_1 - \boldsymbol{v}_{1a}) + \mathbf{A}_{tv2}(\boldsymbol{v}_2 - \boldsymbol{v}_{2a}) + \ldots \quad \ldots \textit{interference error}} \tag{7}$$

$$+ \boldsymbol{\varepsilon}_t \quad .$$

We call $\mathbf{A}_{tv1}$, $\mathbf{A}_{tv2}$, ... interference kernel matrices.

The statistics of the smoothing error is described by the error covariance

$$\mathbf{S}_{tt} = (\mathbf{A}_{tt} - \mathbf{I})\, \mathbf{S}_t\, (\mathbf{A}_{tt} - \mathbf{I})^T \tag{8}$$

where $\mathbf{S}_t$ is a best estimate of the true *a priori* covariance of the target profiles $\boldsymbol{t}$.

The statistics of the interference errors are described by the error covariance matrices

$$\boxed{\begin{aligned} \mathbf{S}_{tv1} &= \mathbf{A}_{tv1}\, \mathbf{S}_{v1}\, \mathbf{A}_{tv1}^T \\ \mathbf{S}_{tv2} &= \mathbf{A}_{tv2}\, \mathbf{S}_{v2}\, \mathbf{A}_{tv2}^T \\ &\vdots \end{aligned}} \tag{9}$$

where $\mathbf{S}_{v1}$, $\mathbf{S}_{v2}$, … are best estimates of the true *a priori* covariances of the profiles $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, … of the interfering species (and retrieved auxiliary profile-type quantities, *e.g.*, temperature).

Case II: Quantification in case of coarse-grid retrieval of interfering species

in case of a simple unconstrained VMR-profile scaling retrieval of the interfering species, the (erroneous) application of Eqs.(3,4,9) on this coarse (1-layer) grid would lead to the interference error be (scalar) zero.

Of course this is not true.

The reason for is the implicitly made erroneous assumption that the true atmospheric variability of the interfering species is only of profile-scaling type, which means there would be no changes in profile shape (which is wrong, of course).

The algorithmic effect leading to the error is then the well known fact, that an unconstrained VMR-profile scaling/shifting retrieval is always able to perfectly retrieve any profile-scaling/shifting type difference relative to the a priori profile. Therefore, the retrieval of the interfering species would not lead to any residual under this assumption and, in consequence, there would be no interference effect on the target species.

In a similar way, direct application of Eq.(3,4,9) to all other coarse-grid retrievals of interfering species (dividing their vertical profiles into 2, 3, … layers) will always lead to a serious underestimate of the true interference errors.

Case II: Quantification in case of coarse-grid retrieval of interfering species

In order to overcome this difficulty, we have to implement a sufficiently fine retrieval grid for the interfering species and emulate their coarse-grid retrieval (namely that of the operational algorithm to be characterized). This can be achieved by using an appropriate soft constraint $\mathbf{R} = \mathbf{S}_R^{-1}$ for the interfering species.

An unconstrained retrieval of the interfering species on a (coarse) 1-layer grid (e.g., VMR-profile shifting) can be emulated on a n-layer fine grid using the Tikhonov-type first order regularization matrix for the interfering species

$$\mathbf{R}_{one\ \ block} = \alpha \times \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 2 & -1 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix} \in \Re^{n \times n} \qquad (10)$$

with a very high regularization strength, i.e., $\alpha \to \infty$.

Case II: Quantification in case of coarse-grid retrieval of interfering species

The emulation of other (2, 3, …-layer) coarse-grid retrievals of the interfering species on a *n*-layer fine grid is straightforward if we use the following multi-block-Tikhonov regularization

$$\mathbf{R}_{multi\ block} = \alpha \times \left(\begin{array}{ccccc:ccccc:c} 1 & -1 & 0 & \cdots & 0 & 0 & & \cdots & & 0 & \\ -1 & 2 & \ddots & \ddots & \vdots & & & & & & \\ 0 & \ddots & \ddots & \ddots & 0 & \vdots & & \ddots & & \vdots & \cdots \\ \vdots & \ddots & \ddots & 2 & -1 & & & & & & \\ 0 & \cdots & 0 & -1 & 1 & 0 & & \cdots & & 0 & \\ \hdashline 0 & & \cdots & & 0 & 1 & -1 & 0 & \cdots & 0 & \\ & & & & & -1 & 2 & \ddots & \ddots & \vdots & \\ \vdots & & \ddots & & \vdots & 0 & \ddots & \ddots & \ddots & 0 & \ddots \\ & & & & & \vdots & \ddots & \ddots & 2 & -1 & \\ 0 & & \cdots & & 0 & 0 & \cdots & 0 & -1 & 1 & \\ \hdashline & & \vdots & & & & & \ddots & & & \ddots \end{array}\right) \in \Re^{n \times n} \qquad (11)$$

for the interfering species, again with $\alpha \rightarrow \infty$.

Case II: Quantification in case of coarse-grid retrieval of interfering species

Finally …

After having emulated the coarse-grid retrieval of the interfering species on a fine grid, the quantification of interference errors can be performed by straightforward application of Eq.(9) on the fine grid.

Case III: Quantification in the case of unretrieved interfering species

Case III is the only subgroup of interference errors that could be quantified by classical error analysis, i.e, the concept of model parameter errors, as defined in Rodgers (2000, equation 3.16, second term).

$$
\begin{aligned}
\hat{\boldsymbol{x}} - \boldsymbol{x} \quad = \quad & (\mathbf{A} - \mathbf{I})(\boldsymbol{x} - \boldsymbol{x}_a) && \ldots \textit{smoothing error} \\
& \boxed{+\mathbf{G}_y \mathbf{K}_b (\boldsymbol{b} - \hat{\boldsymbol{b}}) \quad \ldots \textit{model parameter error}} \\
& +\mathbf{G}_y \Delta \mathbf{f}(\boldsymbol{x}, \boldsymbol{b}, \boldsymbol{b}') && \ldots \textit{forward model error} \\
& +\mathbf{G}_y \boldsymbol{\varepsilon} && \cdots \textit{retrieval noise}
\end{aligned}
$$

where $\mathbf{A} = \partial \hat{\boldsymbol{x}} / \partial \boldsymbol{x}$, $\mathbf{G}_y = \partial \hat{\boldsymbol{x}} / \partial \boldsymbol{y}$, $\mathbf{K}_b = \partial \mathbf{F} / \partial \boldsymbol{b}$

Implementation of this approach is somewhat laborious since the climatological covariance of the interfering species has to be transferred to measurement space (via Jacobian $\mathbf{K}_b$, which has to be calculated) and then mapped back to state space (via $\mathbf{G}_y$) to quantify the impact upon the target species retrieval. This has been performed before (e.g., von Clarmann and Echle, 1998; Echle et al., 2000; Dudhia et al. 2002).

Case III: Quantification in the case of unretrieved interfering species

We suggest here a simple alternative way to characterize the errors from unretrieved interfering species directly in state space: in case of algorithms (like SFIT2) where the interfering species are readily implemented on a fine grid within the state vector, Eqs.(3,4,9) can be directly applied (using $\mathbf{K}_x$ which is readily available) by formally retrieving the interfering species, but using a simple "dead regularization" of the (L_0) form

$$\mathbf{R}_{dead} = \beta \times \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} \in \Re^{n \times n}$$

with $\beta \to \infty$. This emulates a non-retrieval of the interfering species while preserving their fine-grid entry to the state vector, which allows the correct application of Eqs.(3,4,9). This alternative approach may be used, e.g., for a quick test of the effect of non-retrieving versus retrieving a certain interfering species.

Summary (I): General Formulation for Quantification of Interference Errors

covered:

Case I: Quantification in case of fine-grid profile retrieval of interfering species

Case II: Quantification in case of coarse-grid retrieval of interfering species

Case III: Quantification in the case of unretrieved interfering species

pointed to easy-to-be made errors:

- **don´t treat VMR-profile scaling retrievals of interfering species as scalars within the state vector for the purpose of interference error estimation**

- **don´t use soft constraints for joint retrieval of scalars**