A Diagnostic Framework for Spectral Biases in Fast Radiative Transfer Models: An HDMR-based Uncertainty Decomposition of RTTOV

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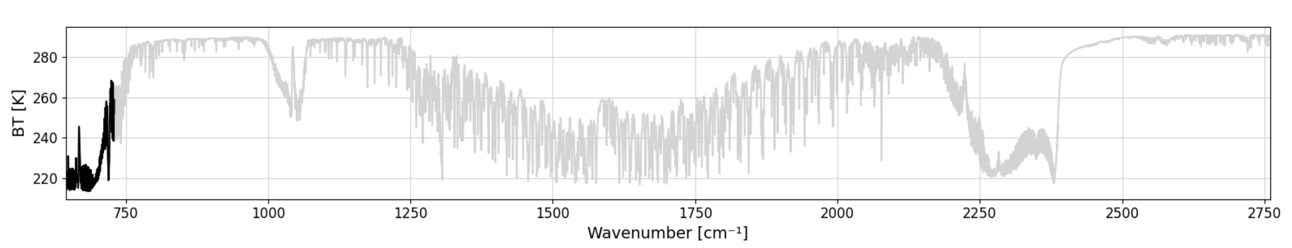
Objectives

- Characterise and attribute error sources in RTTOV simulation
- Quantify the compensation of each error source on RTTOV when compared with IASI observations

RTTOV Simulations

RTTOV is the operational fast RT model used in DA at major NWP centres. In this study, simulations of the CO_2 band of the IASI spectrum are obtained using:

- **Spectroscopy DB:** Aer 3.6
  - Version embedded in LBLRTMv12.8
- **Parametrisation:** Predictors v13
  - The regression coefficients to compute trasmittances are estimated by LBLRTM for a set of 83 training profiles.
- **Input Profiles:** ARSA v2 (Radiousounding + ERA5 + CAMS)
  - 19706 IASI observations colocated with 43-level profiles
  - Conditions: Night / Ocean / Clear-sky / year 2017



Mathematical Framework

Isolating individual error sources in RTTOV requires disentangling coupled effects. In clear-sky conditions and over ocean surface, the main contributors to the output BT errors are: spectroscopy (S), parametrisation (P) and input profiles (F). **Two states are defined for each factor**: the one currently in use (1) and the optimised version (0).

Each model evaluation can be written as:

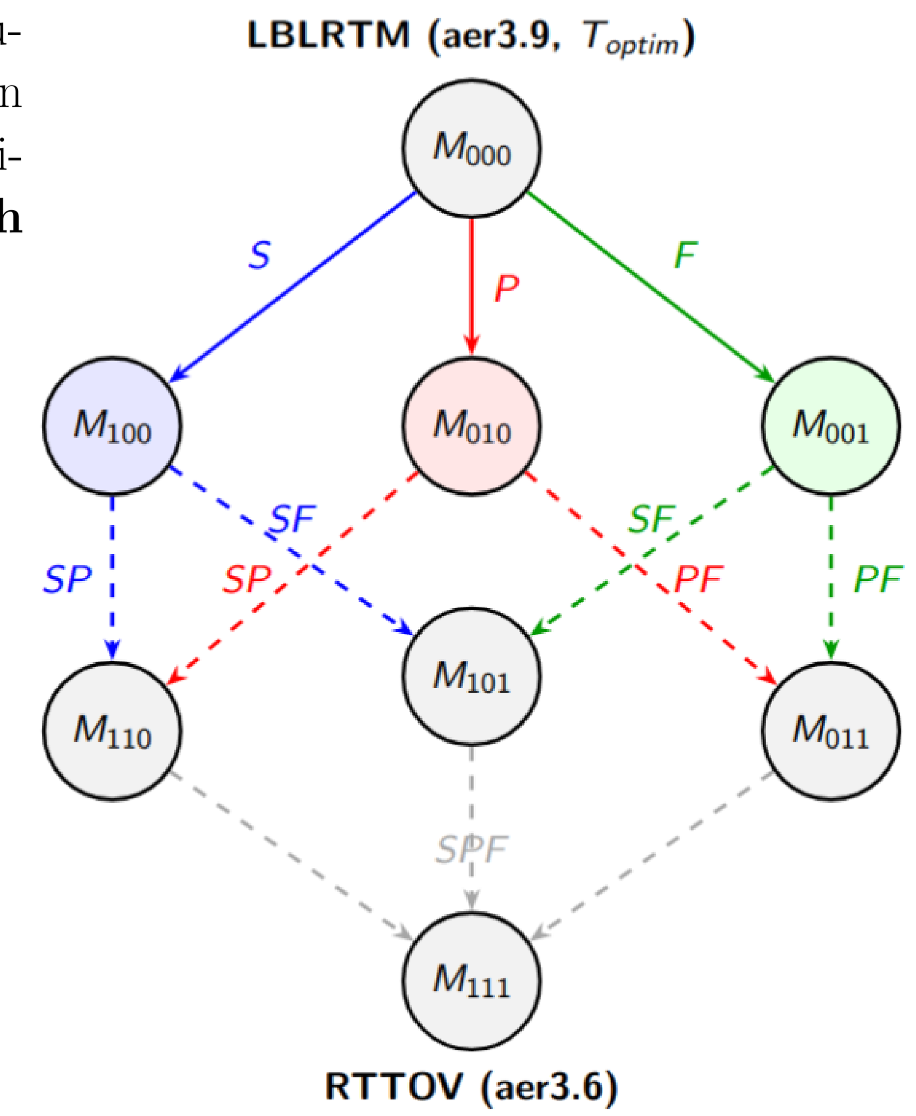
$$M_{ijk} = M(S = i,\ P = j,\ F = k), \qquad i, j, k \in \{0, 1\}$$

⇝ M_{ijk}: BT matrix [#obs, #ch]

⇝ M_{000}: reference case (all factors optimised)

⇝ Changing $0 \to 1$ add the error source

Factor	0 (optimal)	1 (current)
S	aer 3.9	aer 3.6
P	LBLRTM	RTTOV
F	ARSAv2 + T opt.	ARSAv2



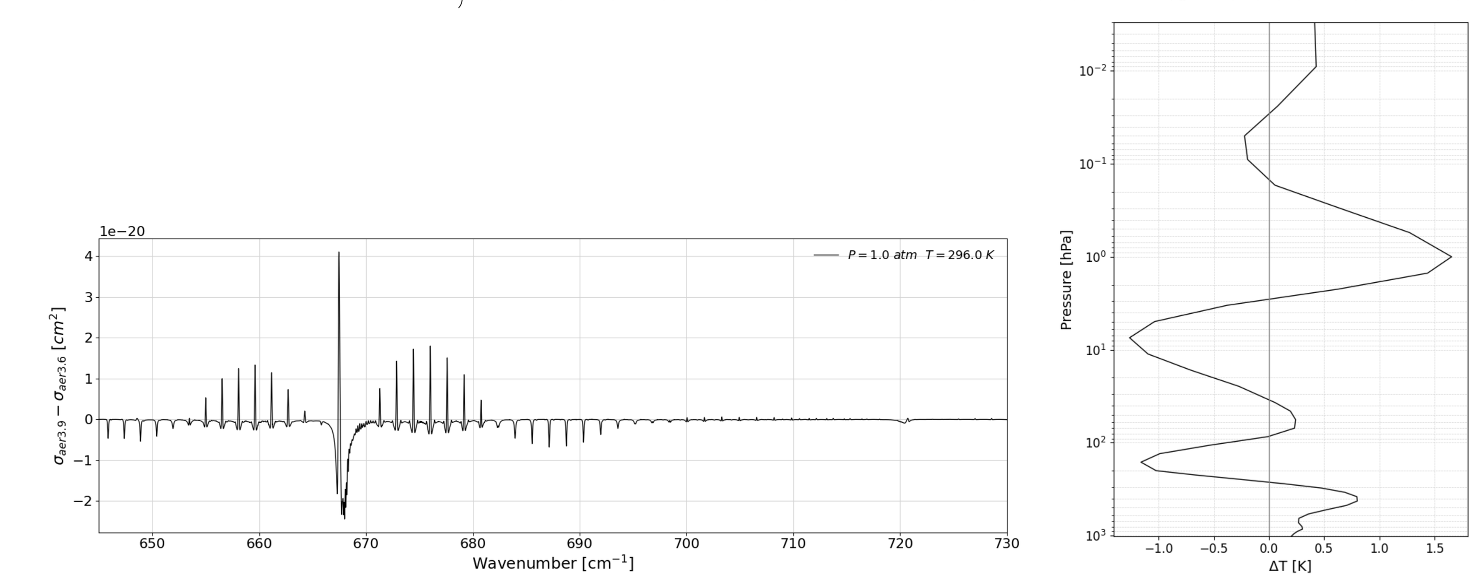
Estimation Optimal Factors

The optimal configuration is defined by replacing each model component with a more accurate or physically complete alternative.

1. For spectroscopy, the most recent version of the **AER database (3.9)** is used, which provides new measurements of line parameters.

2. The effect of parametrisation is assessed by removing the fast RT approximation: RTTOV is replaced with its reference line-by-line model (**LBLRTM**), which explicitly resolves absorption features.

3. For the atmospheric state, the temperature profiles are replaced by **1D-Var retrievals**, which allow a better match with IASI observations.



RTTOV Error Decomposition

High-Dimensional Model Representation (**HDMR**) is used to decompose the RTTOV BTs into contributions from individual error factors and their interactions. This approach provides an efficient way to **approximate complex input–output relationships** in physical models. The general form of the HDMR expansions is (*Rabitz et al, 1998*):

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \dots + f_{12..n}(x_1, x_2, .., x_n)$$

where f_0 is the reference (all factors optimal); $f_i(x_i) = f^i(x_i) - f_0$, with $f^i(x_i)$ being the function where only the "i" variable is changed; finally $f_{ij}(x_i, x_j) = f^{ij}(x_i, x_j) - f_i(x_i) - f_j(x_j) - f_0$. Using the matrix notation M_{ijk}:

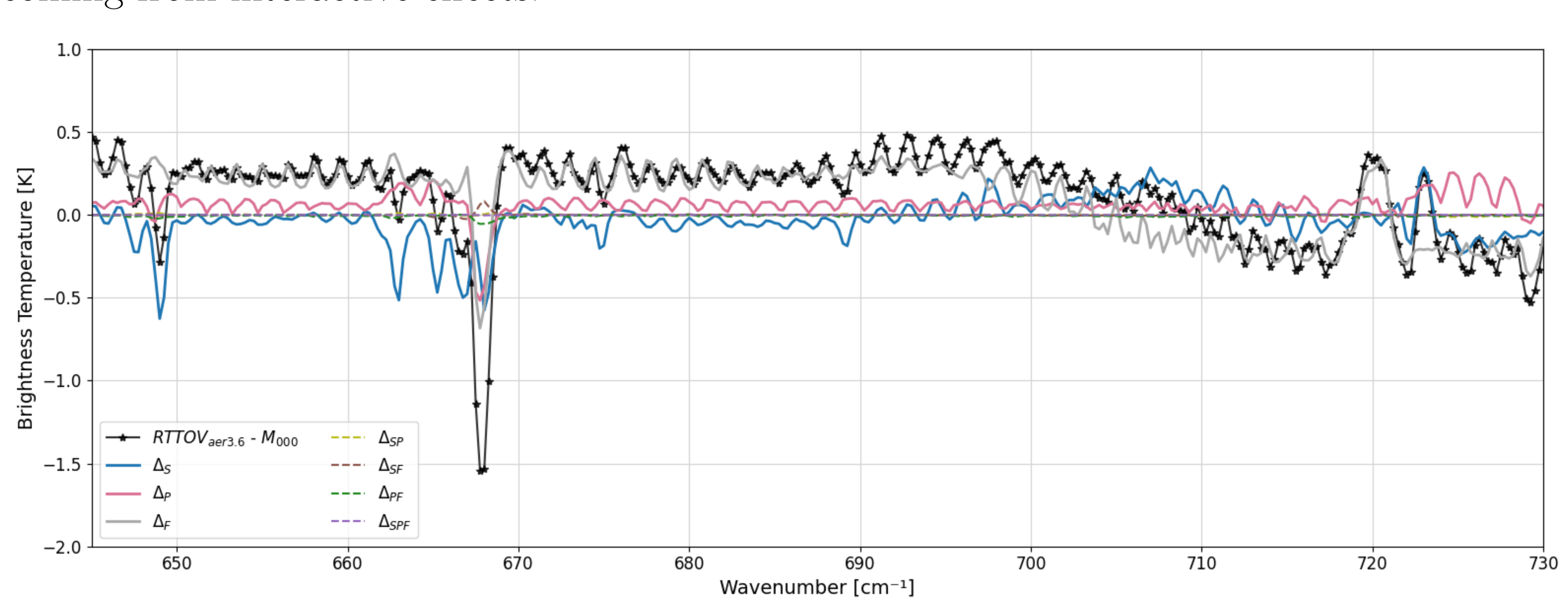
$$f_i(x_i) \equiv \Delta S = M_{100} - M_{000}, \qquad f_{ij}(x_i, x_j) \equiv \Delta SF = M_{101} - M_{100} - M_{001} + M_{000}, \qquad (i = S, j = F)$$

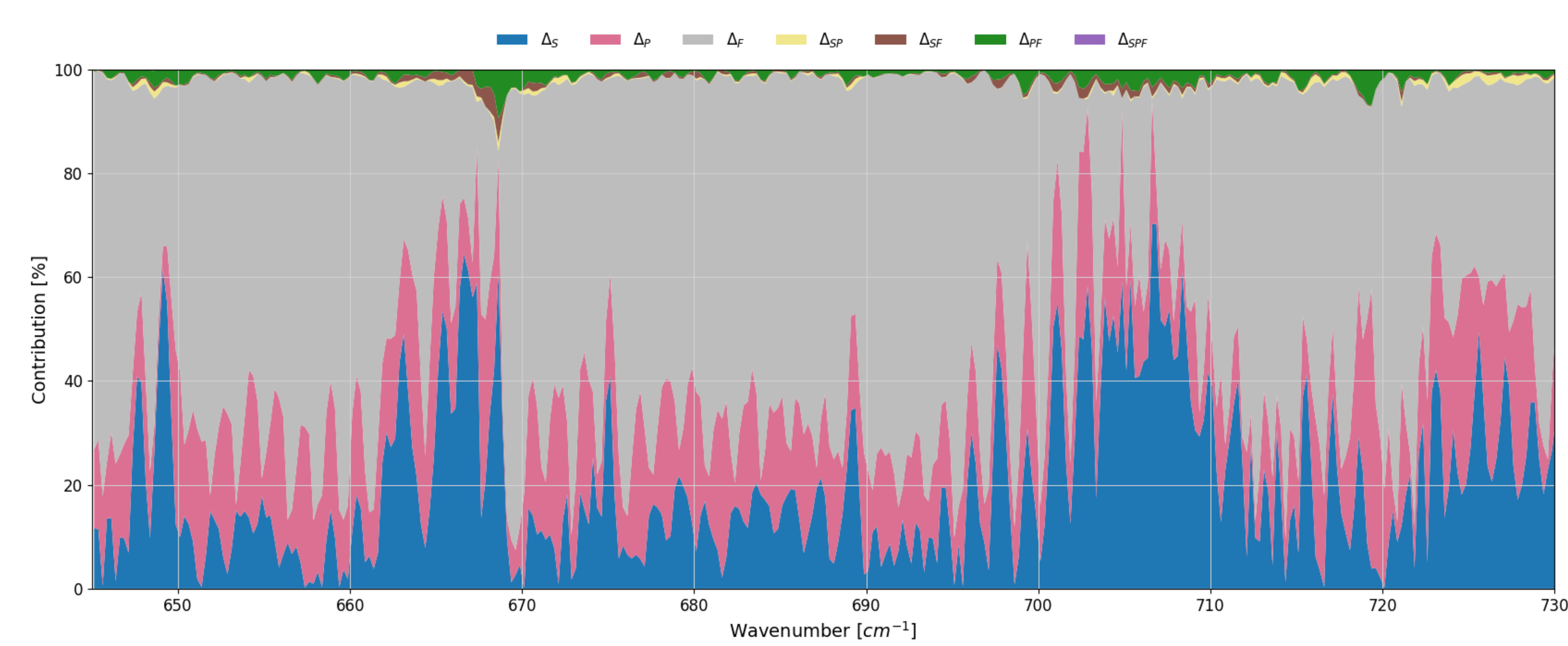
The total RTTOV bias can then be written as:

$$\mathbf{RTTOV_{aer3.6} = M_{000} + \Delta S + \Delta P + \Delta F + \Delta SP + \Delta SF + \Delta PF + \Delta SPF}$$

Interpretation of results, i.e. the centre of the ν_2 band:

⇝ **667.75 cm^{-1}:** RTTOV can be improved by ~1.54K relative to the reference case. Spectroscopy contribution is 18%, parametrisation 35%, profiles 40% and the remaining 7% is coming from interactive effects.





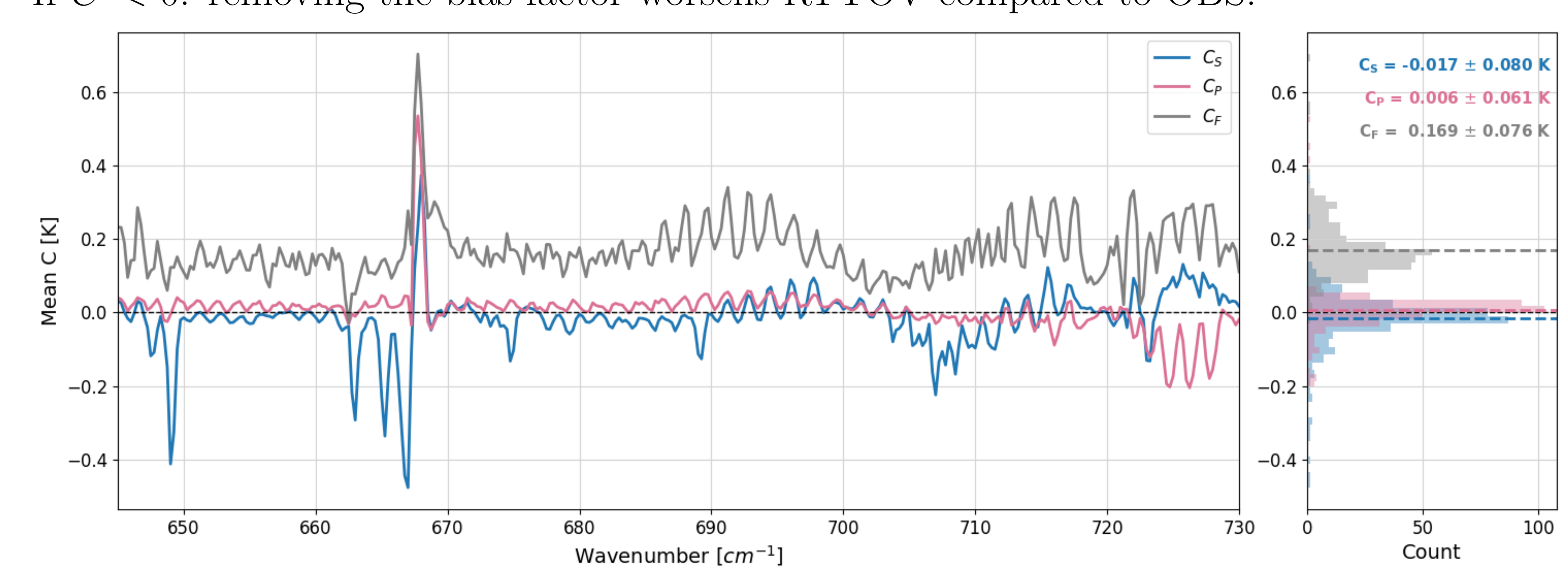
Impact on Observation Bias

To assess how the removal of each RT error source impacts $OBS - RTTOV$ agreement, a new metric called the **C-factor** can be introduced:

$$C_S = |OBS - RTTOV_{aer3.6}| - |OBS - M_{011}|$$
$$C_P = |OBS - RTTOV_{aer3.6}| - |OBS - M_{101}|$$
$$C_F = |OBS - RTTOV_{aer3.6}| - |OBS - M_{110}|$$

If $C > 0$: removing the bias factor improves RTTOV compared to OBS.

If $C < 0$: removing the bias factor worsens RTTOV compared to OBS.



Conclusions

- The HDMR framework is a powerful tool for exploring error sources and their interactions in fast RT modelling.
- Removing a source of bias does not necessarily mean a better agreement with OBS.