I thank the reviewers for the useful comments. In the following, I answer the specific comments (included in "**boldface**" for clarity) and, whenever required, I describe the related changes implemented in the revised manuscript. Page and line numbers indicated refer to the original version of the Comment published on AMTD.

### Anonymous Referee #1

This Comment on "Synergetic use of IASI and TROPOMI space borne sensors for generating a tropospheric methane profile product by Schneider et al. (2021)" is necessary to compliment the original paper in terms of comparison/reference of existing data fusion methods. If Schneider et al. (2021) had properly referenced Warner et al. (2014) and Ceccherini et al. (2015) with good understanding of the similarities and differences, this Comment would not have been necessary. This Comment clearly and thoroughly compared the Schneider et al. (2021) approach, which was published by Warner et al. (2014) for a different data set, and that of Ceccherini et al. (2015) via derivation of equations. The Comment also reiterated the similarity of the above approaches to that of Ceccherini et al. (2009), which was discussed by Schneider et al. (2021). This reviewer recommends the publication of this Comment.

The referee recommends the publication of the Comment as it is.

### **Anonymous Referee #2**

The main purpose of this paper was to prove the equivalency of two methods in previous literature, Schneider et al. (2021) and Ceccherini et al. (2015). Overall, this work does a good job in doing this and the mathematical derivation in Section 2 is sound. The manuscript could use additional information that would be useful for the reader - the background and conclusions can be slightly extended to better express why this study is significant. I provide some suggestions below that would be beneficial to implement in the paper. However for the most part, the quality of the pre-print is good, and with a few minor edits I would recommend it for publication.

I will provide a revised version of the Comment with implemented the suggestions of the referee.

### **Specific comments:**

Introduction: It would be helpful to more clearly state the significance and motivation behind proving the equivalence of the two methods. I understand this is mostly a technical study but it would good for the reader to know the scientific implications of the derivation.

In the revised version of the Comment, I added a few sentences at the end of the introduction that clarify the significance and the motivation behind proving the equivalence of the two methods.

Introduction: A few sentences that summarize the retrieval techniques and how they work would be useful to set the background behind this study.

In the revised version of the Comment, I added a few sentences at the beginning of the introduction that summarize the retrieval techniques and how they work.

## Section 2: Define $F_1$ and $F_2$ and $F_i$ in the equation (Eq 5 and 6). Was not completely clear to me what the relationship between those variables are. Also a sentence describing the physical meaning behind the key equations would be helpful (for example Eq 1, 5 and 15).

In the revised version of the Comment, I slightly modified the sentence that defines  $\mathbf{F}_1$  and  $\mathbf{F}_2$  and I added a sentence describing the physical meaning of these matrices. Furthermore, I added sentences at the end of the paragraphs including Eq. (1), Eq. (5, 6) and Eq. (15) describing the physical meaning of these equations.

# Conclusions: The main point of the paper was proving the equivalence of the two methods which shows the similarities between them. Is there any fundamental difference between them? If possible, it would be useful to also mention some advantages of using one method over the other when performing satellite retrievals.

I have identified a significant difference of implementation in the case that we have to combine more than two measurements. In this case, the CDF has an advantage with respect to the Kalman filter method that I have described at the end of the conclusions in the revised version of the Comment.

### **Technical corrections:**

Line 14 and Line 17: Spell out the names of the sensors where abbreviations are used for the first time. i.e. TROPOMI, IASI, MLS...

In the revised version of the Comment, I spelled out the names of the sensors.

### Line 60-62: The sentence "However, the original CDF formula..." is a bit long. It can potentially be split into two sentences.

In the revised version of the Comment, I split the sentence into two sentences.

### Line 64-65: The sentence "Case that corresponds to having singular matrices" was a bit confusing. Consider rewording this part.

In the revised version of the Comment, I deleted this sentence.

### Comment on "Synergetic use of IASI and TROPOMI space borne sensors for generating a tropospheric methane profile product"

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Abstract. A great interest is growing about methods that combine measurements from two or more instruments that observe the same species either in different spectral regions or with different geometries. Recently, a method based on the Kalman filter has been proposed to combine IASI (Infrared Atmospheric Sounding Interferometer) and TROPOMI (TROPOspheric Monitoring Instrument) methane products. We show that this method is equivalent to the Complete Data Fusion method. Therefore, the choice between these two methods is driven only by the advantages of the different implementations. From the comparison of the two methods a generalization of the Complete Data Fusion formula, which is valid also in the case that the noise error covariance matrices of the fused products are singular, is derived.

### **1** Introduction

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- 15 Remote atmospheric measurements are obtained with retrieval techniques (Rodgers, 2000) that determine the distribution of an atmospheric parameter by fitting forward model simulations to the available observations. Generally, the fitting procedure consists in the minimization of a cost function made of the summation of two terms. The first term is the square of the differences between observations and simulations, weighted with the inverse covariance matrix (CM) of the observations and the second term is a constraint that reflects our a priori knowledge of the distribution of the atmospheric parameter. When
- 20 two or more instruments sound the same portion of atmosphere and observe the same atmospheric parameter either in different spectral regions or with different geometries, the problem arises to identify the best strategy to combine the different measurements in order to exploit all the information that is provided by the observations in presence of the retrieval constraints.

Recently, Schneider et al. (2021) presented a method for the combined use of the individual retrieval products of IASI

- 25 (Infrared Atmospheric Sounding Interferometer) and TROPOMI (TROPOspheric Monitoring Instrument). The method is based on the Kalman filter (Rodgers, 2000) and, as stated by the authors, is largely equivalent to using the spectra of the different sensors together in a single retrieval procedure (simultaneous retrieval). This method was already presented in Warner et al. (2014) and used to combine CO products of AIRS (Atmospheric InfraRed Sounder) and TES (Tropospheric Emission Spectrometer) as well of AIRS and MLS (Microwave Limb Sounder).
- 30 The purpose of this comment is to study the relationship between the method presented in Schneider et al. (2021) and the Complete Data Fusion (CDF) method presented in Ceccherini et al. (2015). CDF too uses the output of the individual retrievals and, in the case that the linear approximation holds in the range of the retrieved products, provides products equivalent to those of the simultaneous retrieval.

The formulas of the two methods are algebraically different but the connection of both methods with the simultaneous

35 retrieval suggests a close relationship between them. It is important to understand whether the two methods are equivalent (that is they provide the same results) and otherwise to identify the reasons of the differences, because this analysis allows to highlight the advantages of using one method or the other. In effect, in Sections 2 we prove the equivalence between the two methods and in Section 3 we draw the conclusions. Given the similarities between the two methods, it is reasonable to expect a close relationship between them and in effect in Section 2 we prove their equivalence. Conclusions are drawn in Section 3.

#### 40 2 Equivalence between data fusion with Kalman filter and CDF

In this Section, we prove the equivalence of the method proposed in Schneider et al. (2021) and the CDF method proposed in Ceccherini et al. (2015).

We start from Eq. (A9) of Schneider et al. (2021):

$$\hat{\mathbf{x}}^{a} = \hat{\mathbf{x}}^{b} + \mathbf{M} \Big[ \hat{\mathbf{x}}^{o} - \mathbf{H} \hat{\mathbf{x}}^{b} \Big], \tag{1}$$

where  $\hat{\mathbf{x}}^{a}$  is the analysis state,  $\hat{\mathbf{x}}^{b}$  is the background state,  $\hat{\mathbf{x}}^{o}$  is the new observation, **M** is the Kalman gain matrix and **H** is the measurement forward operator. In our case, this equation determines the product of the fusion of two measurements (the analysis state) by combining the first measurement (the background state) with the information provided by the second measurement (the new observation).

We substitute in Eq. (1) the different quantities as given in Appendix A2.3 of Schneider et al. (2021). From Eq. (A14), (A15) and (A13) we have, respectively:

$$\hat{\mathbf{x}}^b = \hat{\mathbf{x}}_1 - \mathbf{x}_a \,, \tag{2}$$

(3)

$$\hat{\mathbf{x}}^o = \hat{\mathbf{x}}_2 - \mathbf{x}_a$$

and

$$\mathbf{H} = \mathbf{A}_2,\tag{4}$$

50 where  $\hat{\mathbf{x}}_1$  and  $\hat{\mathbf{x}}_2$  are the two individual retrieval products,  $\mathbf{x}_a$  is the a priori state vector and  $\mathbf{A}_2$  is the averaging kernel matrix of  $\hat{\mathbf{x}}_2$ . The Kalman gain matrix **M** is given by Eq. (A17) that using Eq. (A4) becomes:

$$\mathbf{M} = \left(\mathbf{F}_1 + \mathbf{F}_2 + \mathbf{S}_a^{-1}\right)^{-1} \left(\mathbf{F}_2 + \mathbf{S}_a^{-1}\right),\tag{5}$$

where  $\mathbf{S}_a$  is the a priori <del>covariance matrix (CM)</del> and we have introduced the Fisher information matrices (Fisher, 1935; Ceccherini et al., 2012)  $\mathbf{F}_1$  and  $\mathbf{F}_2$ , which are given by:

$$\mathbf{F}_{i} = \mathbf{K}_{i}^{T} \mathbf{S}_{\mathbf{y}_{i},\mathbf{n}}^{-1} \mathbf{K}_{i} = \mathbf{A}_{i}^{T} \mathbf{S}_{\hat{\mathbf{x}}_{i},\mathbf{n}}^{-1} \mathbf{A}_{i} = \mathbf{S}_{\hat{\mathbf{x}}_{i}}^{-1} \mathbf{A}_{i} \qquad i = 1, 2,$$

$$(6)$$

 $\mathbf{K}_i$  being the Jacobian matrices of the forward models,  $\mathbf{S}_{\mathbf{y}_i,\mathbf{n}}$  the CMs for noise on the measured radiances  $\mathbf{y}_i$ ,  $\mathbf{S}_{\hat{\mathbf{x}}_i,\mathbf{n}}$  the noise error CMs of the retrieved states and  $\mathbf{S}_{\hat{\mathbf{x}}_i}$  the a posteriori CMs. The Fisher information matrices are useful quantities that fully describe the information provided by the observations on the state vectors and are easily obtained using either the quantities that characterise the observations or those that characterise the measurements. In the case that the matrices  $\mathbf{S}_{\hat{\mathbf{x}}_i,\mathbf{n}}$ are singular, Eq. (6) is still valid replacing the matrices  $\mathbf{S}_{\hat{\mathbf{x}}_i,\mathbf{n}}^{-1}$  with the generalized inverse matrices (Kalman, 1976)  $\mathbf{S}_{\hat{\mathbf{x}}_i,\mathbf{n}}^{\#}$ , as shown in the appendix of Ceccherini et al. (2012). Eqs. (5, 6) show that the Kalman gain matrix takes into account the uncertainties of both measurements as well of the a priori state vector when we combine them using Eq. (1).

In analogy with Eqs. (2) and (3), we introduce the quantity  $\hat{\mathbf{x}}_f$  such as the analysis state  $\hat{\mathbf{x}}^a$  is the difference between  $\hat{\mathbf{x}}_f$  and  $\mathbf{x}_a$ :

$$\hat{\mathbf{x}}^a = \hat{\mathbf{x}}_f - \mathbf{x}_a \,. \tag{7}$$

Substituting Eqs. (2-5) and (7) in Eq. (1), we obtain:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \hat{\mathbf{x}}_{1} - \mathbf{x}_{a} + \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) \left[\hat{\mathbf{x}}_{2} - \mathbf{x}_{a} - \mathbf{A}_{2}\left(\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}\right)\right].$$
(8)

Using Eqs. (A2-A3) of Schneider et al. (2021) and Eq. (6), we have:

$$\mathbf{A}_{i} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{i} \qquad i = 1, 2,$$
(9)

65 therefore, Eq. (8) can be written as:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \left[\mathbf{I} - \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{2}\right] (\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}) + \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{2} - \mathbf{x}_{a}) = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[ \left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{1} - \mathbf{x}_{a}) + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right) (\hat{\mathbf{x}}_{2} - \mathbf{x}_{a}) \right]$$
(10)

Consistently with Eq. (3) of Ceccherini et al. (2015), we introduce the  $\alpha_i$  quantities, such as:

$$\hat{\mathbf{x}}_i - \mathbf{x}_a = \mathbf{a}_i - \mathbf{A}_i \mathbf{x}_a \qquad i = 1, 2 \tag{11}$$

and Eq. (10) becomes:

$$\hat{\mathbf{x}}_{f} - \mathbf{x}_{a} = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right)\left(\boldsymbol{\alpha}_{1} - \mathbf{A}_{1}\mathbf{x}_{a}\right) + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)\left(\boldsymbol{\alpha}_{2} - \mathbf{A}_{2}\mathbf{x}_{a}\right)\right] = \\ = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right)\boldsymbol{\alpha}_{1} + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)\boldsymbol{\alpha}_{2} - \mathbf{F}_{1}\mathbf{x}_{a} - \mathbf{F}_{2}\mathbf{x}_{a}\right] = \\ = \left(\mathbf{F}_{1} + \mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\left(\mathbf{F}_{1} + \mathbf{S}_{a}^{-1}\right)\boldsymbol{\alpha}_{1} + \left(\mathbf{F}_{2} + \mathbf{S}_{a}^{-1}\right)\boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a}\right] - \mathbf{x}_{a}$$
(12)

where we have used Eq. (9).

Using Eqs (A2) and (A5) of Schneider et al. (2021), we can write the noise error CMs as:

$$\mathbf{S}_{\hat{\mathbf{x}}_{i,n}} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \mathbf{F}_{i} \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right)^{-1} \qquad i = 1, 2.$$

$$(13)$$

70 In the case that  $S_{\hat{x}_{i,n}}$  are not singular matrices, from Eq. (9) it results:

$$\mathbf{A}_{i}^{T} \mathbf{S}_{\hat{\mathbf{x}}_{i},\mathbf{n}}^{-1} = \left(\mathbf{F}_{i} + \mathbf{S}_{a}^{-1}\right) \qquad i = 1, 2$$

$$(14)$$

and, using Eqs. (6) and (14), from Eq. (12) we obtain:

$$\hat{\mathbf{x}}_{f} = \left(\mathbf{A}_{1}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{1},n}^{-1}\mathbf{A}_{1} + \mathbf{A}_{2}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{2},n}^{-1}\mathbf{A}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\mathbf{A}_{1}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{1},n}^{-1}\boldsymbol{\alpha}_{1} + \mathbf{A}_{2}^{T}\mathbf{S}_{\hat{\mathbf{x}}_{2},n}^{-1}\boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a}\right],$$
(15)

which is the equation of the CDF reported in Eq. (5) of Ceccherini et al. (2015), proving the equivalence of the Kalman filter method reported in Schneider et al. (2021) with the CDF method reported in Ceccherini et al. (2015). The form of Eq. (15) highlights that the combination of the two measurements is a generalization of the weighted mean, where in the weights not only the CMs, but also the averaging kernel matrices are taken into account. The expression coincides with the weighted mean in the case that the averaging kernel matrices are equal to the identity matrices.

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In the case that  $\mathbf{S}_{\hat{\mathbf{x}}_{i},n}$  are singular matrices, we cannot write Eq. (15). However, using Eq. (A4) of Schneider et al. (2021) and Eq. (6), from Eq. (12) we obtain:

$$\hat{\mathbf{x}}_{f} = \left(\mathbf{S}_{\hat{\mathbf{x}}_{1}}^{-1}\mathbf{A}_{1} + \mathbf{S}_{\hat{\mathbf{x}}_{2}}^{-1}\mathbf{A}_{2} + \mathbf{S}_{a}^{-1}\right)^{-1} \left[\mathbf{S}_{\hat{\mathbf{x}}_{1}}^{-1}\boldsymbol{\alpha}_{1} + \mathbf{S}_{\hat{\mathbf{x}}_{2}}^{-1}\boldsymbol{\alpha}_{2} + \mathbf{S}_{a}^{-1}\mathbf{x}_{a}\right].$$
(16)

Eq. (16) is valid also when  $\mathbf{S}_{\hat{\mathbf{x}}_{i,n}}$  are singular matrices and fully maintains the equivalence with the method proposed in 80 Schneider et al (2021), furthermore, it is equivalent to Eq. (15) when  $\mathbf{S}_{\hat{\mathbf{x}}_{i,n}}$  are not singular matrices. Therefore, Eq. (16) is more general than Eq. (15) proposed for the CDF in Ceccherini et al. (2015).

### **3** Conclusions

The equivalence between the method for the synergetic use of data acquired by different instruments proposed in Schneider et al. (2021) and the CDF method proposed in Ceccherini et al. (2015) has been proved. However, the original CDF formula can only be used in the case that the noise error CMs of the fused products are not singular. and tThe full equivalence of the

two methods exists only in the case of the revised CDF formula that has been here derived, and given in Eq. (16).

The CDF method was also proved (Ceccherini, 2016) to be equivalent to the measurement space solution data fusion method (Ceccherini et al., 2009) that explicitly considered the case of measurements made in an incomplete space. Case that corresponds to having singular matrices. Therefore, the three methods are equivalent among themselves and, for linear and

- 90 moderately nonlinear problems, they are all equivalent to the simultaneous retrieval. Consequently, we expect that the choice of which among these three methods can be more efficiently used in an operational data fusion depends only on the implementation advantages. Studies that assess the implementation convenience of the three methods for different data fusion problems would be very useful. A significant difference in the implementation between the method proposed in Schneider et al. (2021) and the other two methods occurs when we have to combine more than two measurements. In this
- 95 <u>case</u>, while the Kalman filter method requires a sequential approach in which we add one measurement at a time, the CDF and the measurement space solution data fusion methods have the advantage that can be implemented fusing all the available measurements in a single step.
- 100 Competing interests. The author declares that he has no conflict of interest.

Acknowledgments. The author is grateful to Bruno Carli for useful discussions.

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