General comments:

This review represents my response to points made in the Author's Response uploaded on Oct 8th, primarily concerning issues raised by the reviewers that were in no way addressed by the authors. I recommend the paper for further revision.

Each time I saw a response of “I could not see this comment in Revision 2”, I had a desire to reject this paper completely as the authors appear to be arguing in bad faith. You submitted a major revision and there was over a year between our reviews. We brought fresh eyes the second time. Just because a comment wasn't brought up in the previous round doesn't mean you can ignore it now.

(Editor’s note: the reviewer’s comment about fresh eyes is important to bear in mind. I do not believe that the reviewers were bringing up new comments maliciously. Having discussed with them, we agree that it is important to bring up only new points of substance, in order to avoid dragging out reviews unduly, and I feel that the points raised are valid.)

I am aware that this was not the kindest series of reviews. We think that your method is conceptually interesting but see little evidence that it is worthwhile from the evidence you present here or in Part II. You provide no evidence that the use of discrete aerosol classes produces a worse product – merely a conceptual argument that continuous variation is more rigorous. Though I agree with you on a technical level, your critique of existing retrievals uses unduly aggressive language and, to a native speaker, comes across as a personal attack. Your continual refusal to tone down your language implies you genuinely wish to insult the entire field. I shall stop requesting changes there and simply wish you luck.

(Editor’s note: Please consider these comments about the tone of the work. As we are an international community, certain words can seem quite loaded to readers. There are some wording suggestions below, but please contact me if something seems uncertain.)

Your title remains misleading. I have asked several of my colleagues, including those outside of atmospheric science. The phrase “continuous variation of the state variables in solution space” was interpreted to mean “our state vector and prior information were cast in terms of surface reflectance and aerosol properties”. You definitively do not do that for aerosol properties. You defined some representative aerosol models, which you refer to as vertices, and retrieve a linear combination of those, from which the SSA and asymmetry parameter are derived. To be clear – there is nothing wrong with that idea. However, you title should represent the work you did. It should mention that your method uses the linear combination of idealised aerosol models (or words to that effect).

(Editor’s note: perhaps “Joint retrieval of surface reflectance and aerosol properties through linear combinations of aerosol absorption and asymmetry vertices, Part 1: theoretical concept” or “Joint retrieval of surface reflectance and aerosol properties through linear combinations of aerosol optical vertices, Part 1: theoretical concept” or similar would be a more suitable title? I understand that you want to emphasise that these optical parameters vary continuously rather than discretely, but I am not sure of a natural way to include the word “continuous” in the title here. Note this comment would of course be relevant to Part II as well.)

I passed your query along to the reviewer and had a follow-up discussion with them about it this morning. Below is a summary of our conversation about that review comment, edited into a more coherent form:

The reviewer's understanding is that CISAR behaves as follows for SSA retrieval:

retrieved_SSA = a_1 * SSA_1 + a_2 * SSA_2 + a_3 * SSA_3 + a_4 * SSA_4,

where retrieved_SSA is the single scatter albedo the retrieval reports, SSA_n is the single scatter albedo of the nth aerosol vertex, and the constants (retrieved weights) a_n are a complicated function of satellite observations and meteorology determined by the retrieval. In many of the experiments, certain a values are explicitly forced to equal zero, removing those vertices from the equation.

The retriever believes the title implies CISAR does this:

retrieved_SSA = f(satellite_observations, meteorology, other_assumptions),

where f is some complicated function. The first equation is a particular (linear) case of the second.

The reviewer sees the distinction, and the problem with the current title/terminology "continuous", that though the variables are varied continuously, they do so within a particular space defined by the vertices. For example, it isn't possible to retrieve an SSA smaller than the SSA of any vertex used. That choice to describe state space as a linear combination of aerosol vertices is the interesting and (mostly) unique choice made by this algorithm. Thus, the reviewer feels that aspect should be conveyed by the title.

All statistical retrievals permit the continuous variation of state variables. They merely define different state variables, such as AOD and fine mode fraction, while keeping other model parameters constant (e.g. ancillary meteorology) or discrete (e.g. aerosol optical models as in MODIS). As the authors argue, the choice of which variables vary continuously matters. A feature of CISAR as well as a few other aerosol approaches is taking aerosol "type" out of the discrete model space and putting it in this continuous but bounded vertex space.

The statement "All statistical retrievals permit the continuous variation of state variables. They merely define different state variables, such as AOD and fine mode fraction, while keeping other model parameters constant (e.g. ancillary meteorology) or discrete (e.g. aerosol optical models as in MODIS). As the authors argue, the choice of which variables vary continuously matters." is pretty inaccurate with respect to these basics principles. Additionally, the model parameters and not constant parameters but vary in space and time.

As a result, the reviewer suggests a title such as:

"Joint retrieval of surface reflectance and aerosol properties in a continuous state space by the linear combination of representative aerosol types"

This manuscript addresses the deficiencies of our 2010 JGR paper as clearly stated in Section 2. It is clearly not our intension here to blame the concept of aerosol models. Following the JGR 2010 publication, I had intense discussion with Oleg Dubovik who was critical about mixing discrete and continuous state variables. A proceedings[1] has been published following these discussions where we announced future improvements of the 2010 algorithm: "These improvements include: (1) an hourly retrieval of the aerosol concentration; (2) a continuous variation of the state variables in the solution space; …

To make it short, the major critic was not on the use of aerosol models which is a convenient concept for many applications but on the mathematical inconsistency resulting from mixing discrete and continuous variables in the state vector within an OE framework.

Oleg Dubovik proposed the GRASP algorithm and we developed CISAR, the theory of which is presented in this manuscript. Our original idea was to present it as a stand-alone paper focusing on radiation transfer theory and inverse modelling.

The need for continuity of the state vector can be found in any good textbooks about optimization but also on Wikipedia. We summarise here the main concepts :

1. Observation and solution space. The formalism used here is based on a function F, , with y = F(x) + e with y representing the observations, x the state variables and e the uncertainty
2. The function F here is a radiative transfer model (FASTRE) that solves the radiative transfer equation at the equilibrium. In this equation the atmospheric scattering properties are represented with a set of single scattering properties, namely the phase function, the single scattering albedo and the optical thickness. Mathematically speaking, there is no justification to have one variable continuous and the other one discrete.
3. Solving the inverse x = F-1(y) implies to find the set of values x so that F-1(y) fits the observation within the solution space R. To my knowledge, this space is always bounded by the physical range of the variables, e.g. the single scattering albedo $\in$[0,1], the asymmetry parameter $\in$ [-1,1], … The same reasoning also holds for the surface parameters. The values of x should be defined in any points of the "bounded" solution space. Finding the value of x that represents the observations y means therefore that both x and their second partial derivative are defined everywhere in R. These two conditions impose the continuity of x $\in$R, R being by definition continuous, neglecting the quantum physic theory effects. In the present case, the (g,w_0) space is bounded in a more restrictive way than its physical bound not to let the algorithm search for solution in pretty unlikely possible places.

The point is to have the state variables that vary continuously, not the space itself on which we have no control. The concept of "continuous solution space" missed therefore the point.

The following changes have been made to the text:

1. Reference to the proceedings has been added to the following sentence of Section 2 "However, this Land Daily Aerosol (LDA) algorithm suffers from two major limitations: (*i*) the use of pre-defined aerosol classes and, (*ii*) the algorithm delivers

[1] Govaerts, Y. M., S. Wagner, and Dubovik, O. "Enhanced Retrieval of Loading and Detailed Micro-Physics of Atmospheric Aerosol from MTG/FCI Observations." In *EUMETSAT Meteorological User Conference*. Córdoba, Spain, 2010. (Available on www.eumetsat.int web page)

only one mean aerosol value per day when applied on MSG/SEVIRI data (Govaerts et al. 2010a)."

2. The sentences "*Retrieval methods based on OE applied only to a limited number of aerosol models as in Govaerts et al. (2010b) represent a major drawback as it does not permit a continuous variation of the state variables in the solution space. The new method presented in this paper specifically addresses this issue, allowing continuous variations of the aerosol single scattering properties in the solution space without the aerosol micro-physical properties explicitly appearing as state variables*." read now "*The limitations due to a combined used of discrete and continuous state variables in retrieval methods based on OE as in Govaerts et al. (2010b) are discussed in Section (2). The new method presented in this paper specifically addresses these limitations, allowing continuous variations of the aerosol single scattering properties in the solution space without the aerosol micro-physical properties explicitly appearing as state variables*."

Specific comments:

Specific points, in the order I encountered them, follow. Line numbers below refer to those given in the Author's Response.

- I considered the SSA and asymmetry parameter to be microphysical properties but, looking into it, I see that is not a common opinion. My apologies for offering inappropriate terminology for your title.

(Editor's comment: the reviewer is agreeing with you here, no change needed.)

Good

- "Why decouple the papers when there's only one forward model?" Apologies for my poor phrasing. I meant, "Why have a single forward model to retrieve aerosol and surface reflectance but describe the manner of their retrieval in two independent papers separated by 8 years?" Yes, you didn't change the surface forward model and, yes, surface reflectance is less visible in the current research climate, but I would have liked to see a discussion and presentation of the non-linear interactions of these two coupled variables that are evaluated separately everywhere else. You're experts in both fields – a rare combination; I would have liked to hear what you had to say.

The 8 years between the 2 papers was due to issues beyond our control. I agree with the reviewer on the surface-atmosphere radiative coupling importance. It is however not main topic of this paper (see Section 2). Following Wagner et al. 2010 publication, we consider this aspect of the retrieval not innovative enough in the current manuscript.

- Your example of a merged Figs. 6-9 is another case where the authors appear to be arguing in bad faith. They merge Figs. 5-12, which is indeed difficult to read. Showing only the three (5, 6-9, and 10-12, making three total images) we asked for will also be messy, but that can be alleviated by (a) setting the error bars to have a transparency (using the alpha keyword in matplotlib) and using additional colours to distinguish the three curves. The Brewer colour table, "tab10" in Python, has 11 colours designed to be distinguishable in different light levels and by people with various sight problems, which should be sufficient. (As this journal is not physical published, except on demand, the generation of solely colour images should not be a concern.)

(Editor's comment: please consider some merging.)

Sorry, the merging suggestion was not well understood. The left and right side of these figures go together. It might be possible to merge the left side, but the right side might just become too busy. The merged figures 5-9 and 10-12 (without uncertainties and including only the left panel) are now available in the supplement.

L20) You described the lower layer of your conceptual radiative transfer scheme as "soil/vegetation strata", which the reviewer disagreed with. When retrieving surface reflectance, one may use multiple "layers" within the vegetation layer. When retrieving atmospheric properties, the surface is typically a boundary condition on the system (as opposed to an active component). If your retrieval actually has layers in both the atmosphere and surface, keep your current sentence but replace "bottom" with "lower" as the former word implies a singular element. If not, try splitting the sentence and briefly describing the problem in both (i.e. in the atmosphere, layers represent temperature, ozone, the free troposphere vs boundary layer, etc. while near the surface, layers represent the canopy, under-canopy, brush, etc.).

This sentence does not describe the FASTRE model but is part of the introduction where the concept of the coupled radiative problem that needs to be solved is explained. FASTRE is described in Section 4.

L20) The comment was asking you to say "can be further complicated" rather than "is further complicated".

The sentence has been modified accordingly.

L50) I can understand why the reviewer asked to use "models" instead of "classes", as the latter can describe a collection of the former. You may have difficulty in future work if you maintain the current terminology, but that's your choice to make.

"Aerosol class" has been replaced by "aerosol model" everywhere in the manuscript.

L59) Try "approaches under-perform compared to methods" to reduce the ambiguity here.

The sentence has been modified accordingly.

L61-65) The reviewer meant that these lines repeat a sentiment you made twice already in the introduction. The second sentence, in particular, seems redundant. However, I see why you wanted to make a summary of the paper's intent here. As an alternative, a brief statement of what you do that is unique (e.g. calculating SSA and g from the linear combination of aerosol models) would be useful for a reader that skips directly to the conclusions.

It exactly what is written just below these lines: "The proposed method expresses the single scattering albedo and phase function values as a linear mixture of basic aerosol models. The sentence

"*This new method takes advantage of the lessons learned from past attempts to retrieve simultaneously surface reflectance and aerosol properties*."
has been deleted.

L90) While VIS0.6 is the official name of the bands, most of your readers aren't going to know that. I note that this disagreement arises repeatedly throughout the paper, so I'm going to assume you want to us the engineering terminology of "bands". I leave it to the Editor to decide if that is appropriate for the audience of this journal.

(Editor's note: yes, it would be good to show spectral response functions and/or report central wavelengths here, for broader understanding. Then you can state the shorthand names adopted for these channeles.)

The purpose of this theoretical paper is not to describe any specific radiometer. The sentence reads now : "*The GSA algorithm has been further improved for the processing of SEVIRI data on-board MSG for the retrieval of the total column AOT from observations acquired in three solar bands centred at 0.6 μm, 0.8 μm and 1.6 μm (Govaerts et al., 2010b; Wagner et al., 2010)*"

L93) "smallest cost" would be more accurate than "best fit" as the latter doesn't have a single, objective meaning.

The sentence has been modified accordingly.

L100) "a continuous variations" is not valid English. "the continuous variation" would be grammatically correct but, as the reviewers have complained in two successive reviews, isn't likely to be understood by most of your readers. You appear to have no intention of changing it, presumably because the recent ESA ITT requested "continuous variation of the aerosol optical properties" and you have a box to tick.

(Editor's note: this, and the two comments below, are important points relating to the perceived harshness of your current wording.)

The sentence reads now "a continuous variation"
Please refer to our response to the general comment on the use of "continuous variation of the state variables", a common phrasing in the inverse problem solving (e.g. Sinha, S. C., N. R. Senthilnathan, and R. Pandiyan. "A New Numerical Technique for the Analysis of Parametrically Excited Nonlinear Systems." Nonlinear Dynamics 4, no. 5 (October 1, 1993): 483–98. https://doi.org/10.1007/BF00053692.).

L101) It would be nice if you said "preferred" rather than "required".

Please refer to our response on the general comment concerning the continuity. The sentence

The former issue prevents a continuous variations of the state variables characterizing the aerosol single scattering properties as required by an OE approach (Rodgers, 2000).

reads now

The former issue prevents a continuous variation of the state variables characterizing the aerosol single scattering properties as required to find the minimum of the cost function.

L103) Your response to the comment here is good. Writing “but uncertainties cannot be assigned to this choice in a straightforward manner” would be useful.

The sentence

A consistent implementation of such approach is not straightforward since aerosol classes are defined as prior knowledge of the observed medium but no uncertainties are assigned to this information.

read now:

A consistent implementation of such approach is not straightforward since aerosol models are defined as prior knowledge of the observed medium but uncertainties cannot be easily assigned to this choice.

L105) Try “information and its associated uncertainties” to improve clarity.

The sentence

Consequently, the estimated retrieval uncertainty is inconsistent as it does not account for the use of prior information and associated uncertainties.

Reads now

Consequently, the estimated retrieval uncertainty is inconsistent as it does not account for the use of prior information and its associated uncertainties.

L116) Probably remove “or planned” as both 3MI and PACE intend to offer multi-angular observations and, to different extents, polarisation.

The sentence has been modified accordingly.

L119) Replace the comma with “by” and I think you address the reviewer's comment.

The sentence has been modified accordingly.

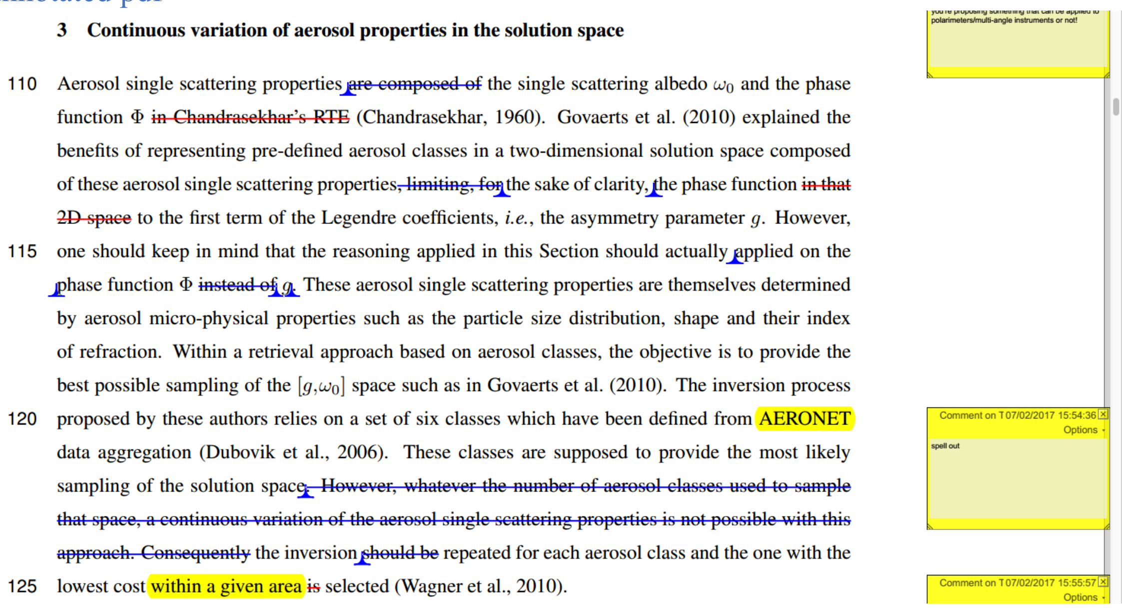
L127) You've made the response “No comment were made on this paragraph in revision 2” repeatedly. What, exactly do you mean by this? I've checked the files stored online, and these comments are all present there. If you mean “you didn't complain about it the first time, so why should I fix it now,” that is the height of arrogance. I will give you the benefit of the doubt and assume what you meant is “we don't know why this paragraph is confusing to you.” I empathise that comments like “Please reword” aren't very useful as you will have tried your best to write to be understood. In this case, I would recommend,
Putting a comma between “properties” and “such” on L128.
Confusing sentences can be simplified by moving interrupting statements into the main sentence. An alternative to the sentence starting at L129 is, “The objective of retrievals that

assume aerosol classes is to provide a reasonable sampling of the [g, w0] space. Omitting areas of that space may produced biased retrievals, as discussed in Govaerts et al. (2010)." Try "in this paper" rather than "by these authors" as the latter could be thought to refer to the authors of the 2010 paper.
For the sentence on L133, perhaps, "That choice of classes was intended to provide a sampling of solution space representative of real-world conditions. The inversion is repeated for each aerosol class and the result with the best fit is reported (rather than vary the aerosol properties continuously, as would be preferable)."

(Editor's note: Please pay attention to the above – let me know if something is unclear.)

I am now pretty confused with all these different versions, so I included some print screen to try to make sure we are talking about the same versions. In the first annotated pdf we received, the first paragraph of Section 3 contains a list of editorial comments that we implemented. The second annotated pdf indicates that the paragraph is now disjoint and should be reworded. I do appreciate the reviewer's efforts to improve our manuscript clarity, but it should not lead into an endless round of review processes.

First annotated pdf



3 Continuous variation of aerosol properties in the solution space

Aerosol single scattering properties ~~are composed of~~ the single scattering albedo ω_0 and the phase function Φ ~~in Chandrasekhar's RTE~~ (Chandrasekhar, 1960). Govaerts et al. (2010) explained the benefits of representing pre-defined aerosol classes in a two-dimensional solution space composed of these aerosol single scattering properties~~, limiting, for~~ the sake of clarity, the phase function ~~in that 2D space~~ to the first term of the Legendre coefficients, *i.e.*, the asymmetry parameter g. However, one should keep in mind that the reasoning applied in this Section should actually applied on the phase function Φ ~~instead of~~ g. These aerosol single scattering properties are themselves determined by aerosol micro-physical properties such as the particle size distribution, shape and their index of refraction. Within a retrieval approach based on aerosol classes, the objective is to provide the best possible sampling of the $[g, \omega_0]$ space such as in Govaerts et al. (2010). The inversion process proposed by these authors relies on a set of six classes which have been defined from AERONET data aggregation (Dubovik et al., 2006). These classes are supposed to provide the most likely sampling of the solution space~~. However, whatever the number of aerosol classes used to sample that space, a continuous variation of the aerosol single scattering properties is not possible with this approach. Consequently~~ the inversion ~~should be~~ repeated for each aerosol class and the one with the lowest cost within a given area ~~is~~ selected (Wagner et al., 2010).

Second annotated pdf

3 Continuous variation of aerosol properties in the solution space

Aerosol single scattering properties include the single scattering albedo ω_0 and the phase function Φ in RTE. Govaerts et al. (2010) explained the benefits of representing pre-defined aerosol classes in a two-dimensional solution space composed of these aerosol single scattering properties. For the sake of clarity, they limited the phase function in that 2D space to the first term of the Legendre coefficients, *i.e.*, the asymmetry parameter g. However, one should keep in mind that the reasoning applied in this Section should be applied on the entire phase function Φ. These aerosol single scattering properties are themselves determined by aerosol micro-physical properties such as the particle size distribution, shape and their complex index of refraction. Within a retrieval approach based on aerosol classes, the objective is to provide the best possible sampling of the $[g,\omega_0]$ space such as in Govaerts et al. (2010). The inversion process proposed by these authors relies on a set of six classes which have been defined from AErosol RObotic NETwork (AERONET) data aggregation (Dubovik et al., 2006). These classes are supposed to provide the most likely sampling of the solution space but, since the scattering properties are not continuously varied, the inversion is typically repeated for each aerosol class and the one with the best fit is selected (Wagner et al., 2010).

Highlight 12/08/2018 00:49:27
Options
this sentence sounds out of place here

Highlight 18/08/2018 03:58:20
Options
This entire part is very disjointed. What is the point it is trying to make? Consider rewording

We have implemented the latest comments concerning this paragraph. These lines read now:

These aerosol single scattering properties are themselves determined by aerosol micro-physical properties, such as the particle size distribution, shape and their complex index of refraction. The objective of retrievals that assume aerosol models is to provide a reasonable sampling of the (g,ω0) space. Omitting areas of that space may produce biased retrievals, as discussed in Govaerts et al. (2010). The inversion process proposed by in this paper relies on a set of six models which have been defined from Aerosol RObotic NETwork (AERONET) data aggregation (Dubovik et al., 2006). That choice of models was intended to provide a sampling of solution space representative of real-world conditions. The inversion is repeated for each aerosol class and the result with the best fit is reported, rather than vary the aerosol properties continuously, as would be preferable.

L138) The reviewer makes an interesting comment. Looking into it, your use of braces {} to denote the set {g, w0} is accurate. I'm less certain of using square brackets to denote the solution space. Definitions of linear vector spaces appear to use braces (and using {} everywhere would look nicer), but I think this is a matter for the typesetter.

The use of the square brackets to define the space have been replaced by braces.

Fig.2) If you're using LaTeX, I will point out the existence of \textmu, which can be used outside math mode for a non-italic character.

The legend of figure 2 has been corrected to remove the unnecessary italic word.

L144) Your web reference for these definitions could be a good footnote.
The reference has been added as a footnote

L146) The copy editor will need to add commas to this sentence.

The comma has been added

L154) "relatively" would be better than "almost".

The sentence has been modified accordingly

L177) Try “This work” rather than “The present study”.

The sentence has been modified accordingly

Fig.4) Add “gas” before “absorption”.

The legend of Fig. 4 has been modified accordingly

L201) Yes, the gases depend on the wavelength but, if someone is going to replicate your work from this paper (the ideal we aspire to), they need to know which of the major species you accounted for. You don't need to be specific as to where they're used, as that would take too long, but the different aerosol groups vary in what gases they consider and Patadia et al. (2018, doi:10.5194/amt-2018-7) showed that that choice matters.

(Editor’s note: I encourage you to provide this information, the reviewer is correct that it can be important, particularly when considering systematic contributions to errors.)

The main gas species accounted for are H_2O, O_3, O_2, CO_2, CH_4, N_2O and CO. However, some species like CH_4 are present only in specific spectral regions not processed in these test experiments. We do not want to dive into these kind of details not to distract the reader from the manuscript main objective. Additionally, the estimations of this gaseous transmittance is pretty straightforward and not at all the topic of this manuscript. The coupling between gaseous transmittance and scattering is expressed in Eq. 7.

L207) Move the \Phi to after “parameter” to be clear what it stands for.

The \Theta parameters have been moved.

L222) How about “in the Fourier space for all illumination and...”?

The sentence has been modified accordingly

L225) The reviewer meant you should define the general meaning of the word Jacobian. Some members of our field were not educated in the physical sciences as undergraduates and it's friendly to not assume they know what all our terms mean.

The Jacobian matrix is the matrix of all first-order partial derivatives of a vector-valued function. When the matrix is a square matrix, both the matrix and its determinant are referred to as “the Jacobian”. I personally feel very uncomfortable to add such basic definition in this manuscript as the value of K_x is clearly expressed as a partial derivative in the text.

In the Introduction, the sentence

The forward radiative transfer model that includes the Jacobians computation is described in Section (4).

reads now

The forward radiative transfer model that includes the Jacobians, i.e. the partial derivative, computation is described in Section (4).

S4.4L1) Perhaps “principal” rather than “most important”?

The sentence has been modified accordingly

L237) You don't need “As can be seen”. It's the sort of thing we say out loud to give us time to remember what to say next but just wastes time when written.

The sentence has been modified accordingly

L238) “Another” is one word.

The sentence has been modified accordingly

L239) The copy editor is going to ask you to define PROBA-V. You can omit the word here if you want to wait to define it till later.

The acronym has been defined.

L299) By your notation, its obvious that \Delta \tau_a is a change in \tau_a. Explaining it simply made me stop and think about things to work out what you meant.

The sentence reads now : Hence, during the iterative optimisation process, when the change \Delta\tau_a between iteration j and j+1 is small …

L7 after 295) Try “in two successive iterations” rather than “twice consecutively”.

The sentence has been modified accordingly

L303) Maybe “chosen” rather than “delineated”.

The sentence has been modified accordingly

L303) Add 's after CISAR.

The sentence has been modified accordingly

Tab.2) I believe the reviewer's sarcastic remark was attempting to point out that you can give values to X significant figures rather than Y decimal places. However, if you actually used these precise figures, leave them in so that we may all judge your undue precision.

The number of digits has been set to 3.

L309) The reviewer appears to have misunderstood what you meant by “assumed that the surface parameters are known a priori”. Perhaps this sentence could read, “In these experiments, to concentrate on the retrieval of aerosol properties, the surface parameters are set to the true values used in simulation (Table 2) and are ascribed a small uncertainty of 0.03 (though they remain part of the retrieved state vector).”

(Editor’s note: I can see how the other reviewer’s confusion has arisen, and agree with a rewording similar to the above suggestion.)

The proposed rewording is also somewhat misleading as the first guess in not set equal to the prior value. The sentence reads now:

In these experiments, to concentrate on the retrieval of aerosol properties, the surface parameters prior values are set to the true values used in simulation (Table 5) with an ascribed uncertainty of 0.03. The first guess values are randomly chosen within this uncertainty interval.

Tab.4) The first “experiment” should be plural and the second singular.

The caption has been modified accordingly.

Fig.5) There is always uncertainty. You just might have reason to believe it's really small.

The caption reads now:

The forward aerosol properties are shown in black and the retrieved ones in red. Vertical and horizontal red bars indicate the uncertainty of the retrieved values.

Tab.6) The plus/minus notation is a good idea. The fact it didn't occur until now isn't justification to not do it.

Table 6 has been modified accordingly and merged with Table 5.

Tab.7) I suspect the typesetter will have opinions about where the % sign should go.

Table 7 (now Table 6) has been clarified.

L383) Perhaps “at” rather than “in”.

The sentence has been corrected accordingly.

L385) “The CISAR algorithm retrieves total AODs consistent with the truth.” would be a better sentence.

The sentence has been corrected accordingly.

L387) Technically, the vertex is not a degree of freedom but that is the phrase that would be used in the scientific vernacular. Maybe put quote marks around it?

The sentence has been corrected accordingly.

L389-401) I can understand why the reviewer responded strongly to this paragraph. Intuitively, it feels like adding more variation should produce a better retrieval. What I

suspect is happening is that the fourth vertex can be closely mimicked by some combination of the other three vertex together (in the terminology of linear algebra, it is almost linearly dependent on the other three). The increase in uncertainty represents a flattening of the cost function because changing the input of vertex CS is similar to changing the others.
A more detailed discussion of this would be interesting, replacing "is therefore not straightforward". The word "overconstrained" would likely appear.

The reported uncertainty represents only the diagonal terms of the error covariance matrix and is the quadratic sum of the uncertainty associated to optical thickness of each vertex. Adding vertices increases therefore the uncertainty. It is therefore not necessarily due to a flattening of the cost function at the solution. A complete uncertainty analysis would require to analyse the entire error covariance matrix as in Wagner et al. (2010). We do not believe that experiment F13 is "overconstrainted" as no new constraints, i.e. more observations or prior information, have been added. It is the opposite, i.e., the extent of the solution space has been increased.

The sentence

The actual benefit of adding this fourth vertex is therefore not straightforward, and should be noted that increasing the number of vertices impacts the computational time.

reads now

The actual benefit of adding this fourth vertex, i.e. expanding the solution space, is therefore not straightforward, and should be noted that increasing the number of vertices impacts the computational time.

L389) I don't believe you can state that the use of *any* two coarse mode vertices is worthless. Perhaps replace "adding two coarse mode vertices" with "using these two coarse mode vertices". (I'd hope you did some work to eliminate any obvious pairings and, if you did, "using any obvious pair of coarse mode vertices" would be appropriate.)

The sentence has been corrected accordingly.

L392) Further to that point, could you add make this sentence, "This series of experiments has shown that, of the four considered, the use of the FN, FA and CL vertices provides the highest quality retrieval of aerosol class F1." We wouldn't want someone to cite this paper as proof that only these three vertices are necessary to retrieve any aerosol.

The sentence

This series of experiments has shown that the use of the FN, FA and CL vertices provides the best combination for the retrieval of the properties of aerosol model F1.

reads now

This series of experiments has shown that, of the four considered, the use of the FN, FA and CL vertices provides the best combination for the retrieval of aerosol model F1.

L444) Could you mention that experiments with noise perturbation are included in the supplement?

(Editor's note: yes, the Supplement should be mentioned and discussed as appropriate in the text, even if just in a few summary sentences. Otherwise it is unlikely that readers will see it.)

The following text has been added to the manuscript

8 Supplement

Includes the plots of case F22 adding a 3% Gaussian noise to the simulated TOA BRF for AOT = 0.05 (Fig. S1), AOT = 0.2 (Fig. S2), AOT = 0.4 (Fig. S3) and AOT = 0.8 (Fig. S4). Fig. S5 shows the merged results in the {g,ω0} space of experiments F11, F12 and F13. Fig. S6 shows the merged 455 results in the {g,ω0} space of experiments F21, F22 and F23.

Manuscript prepared for Atmos. Meas. Tech.
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Joint retrieval of surface reflectance and aerosol properties with continuous variation of the state variables in the solution space: Part 1: theoretical concept

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Abstract. This paper presents a new algorithm for the joint retrieval of surface reflectance and aerosol properties with continuous variations of the state variables in the solution space. This algorithm, named CISAR (Combined Inversion of Surface and AeRosol), relies on a simple atmospheric vertical structure composed of two layers and an underlying surface. Surface anisotropic reflectance effects are taken into account and radiatively coupled with atmospheric scattering. For this purpose, a fast radiative transfer model has been explicitly developed, which includes acceleration techniques to solve the radiative transfer equation and to calculate the Jacobians. The inversion is performed within an optimal estimation framework including prior information on the state variable magnitude and regularization constraints on their spectral and temporal variability. In each processed wavelength, the algorithm retrieves the parameters of the surface reflectance model, the aerosol total column optical thickness and single scattering properties. The CISAR algorithm functioning is illustrated with a series of simple experiments.

1 Introduction

Radiative coupling between atmospheric scattering and surface reflectance processes prevents the use of linear relationships for the retrieval of aerosol properties over land surfaces. The discrimination between the contribution of the signal reflected by the surface and that scattered by aerosols represents one of the major issues when retrieving aerosol properties using spaceborne passive optical observations over land surfaces. Conceptually, this problem can be modelled as solving a radiative system composed of at least two sets of layers, where the upper layers include aerosols and the bottom ones represent the soil/vegetation strata. The problem ~~is~~ can be further complicated by the intrinsic anisotropic radiative behaviour of natural surfaces due to the mutual shadowing of the scattering elements, which is also affected by the amount of incident radiation (Govaerts et al., 2010b, 2016). In most cases, an increase in aerosol concentration is responsible for an increase in the fraction of diffuse sky radiation which, in turn, smooths the effects of surface reflectance anisotropy. Though multi-spectral information is critical for the retrieval of aerosol properties, the spectral dimension alone does not allow full characterisation of the underlying surface reflectance which often offers a significant contribution to the total signal observed at the satellite level. In this regard, the additional information contained in multi-spectral and multi-angular observations have proven essential to characterize aerosol properties over land surfaces.

Pinty et al. (2000a) pioneered the development of a retrieval method dedicated to the joint retrieval of surface reflectance and aerosol properties based on the inversion of a physically-based radiative model. This method has been subsequently improved to permit the processing of any geostationary satellites accounting for their actual radiometric performance (Govaerts and Lattanzio, 2007). This new versatile version of Pinty's algorithm has permitted the generation of a global surface albedo product from archived data acquired by operational geostationary satellites around the globe (Govaerts et al., 2008). These data included observations acquired by an old generation of radiometers with only one broad solar channel on-board the European Meteosat First Generation satellite, the US Geosynchronous Operational Environmental Satellite (GOES) and the Japanese Geostationary Meteorological Satellite (GMS). It is now routinely applied in the framework of the Sustained and COordinated Processing of Environmental satellite data for Climate Monitoring (SCOPE-CM) initiative for the generation of essential climate variables (Lattanzio et al., 2013). An improved version of this algorithm has been proposed by Govaerts et al. (2010b) to take advantage of the multi-spectral capabilities of Meteosat Second Generation Spinning Enhanced Visible and Infrared Imager (MSG/SEVIRI) operated by EUMETSAT, and includes an Optimal Estimation (OE) inversion scheme using a minimization approach based on the Marquardt-Levenberg method (Marquardt, 1963).

The strengths and weaknesses of the algorithm proposed by Govaerts et al. (2010b) are discussed in Section (2). In their approach, the solutions of the Radiative Transfer Equation (RTE) are pre-calculated and stored in Look-Up Tables (LUTs) for a limited number of state variable values. Aerosol properties are limited to six different ~~classes~~ models dominated either by fine or coarse particles. Two major drawbacks result from the use of pre-defined aerosol ~~classes~~ models stored in pre-computed LUTs. Firstly, only a limited region of the solution space is sampled as a result of the reduced range of variability for state variables stored in the LUTs. For instance, in order to reduce the size of the LUTs, Pinty et al. (2000b) limit the maximum aerosol optical thickness to 1. Secondly, the use of pre-defined aerosol ~~classes~~ models constitutes a major drawback since the solution space is not continuously sampled. Dubovik et al. (2011) and Diner et al. (2012), among others, demonstrated the advantages of a retrieval approach based on continuous variations of the aerosol properties as opposed to a LUT-based approach relying on a set of pre-defined aerosol ~~classes~~models. Even considering a large number of aerosol ~~classes~~models, LUT-based approaches under-perform compare to methods with multi-variate continuity in the solution space (Kokhanovsky et al., 2010).

A new joint surface reflectance / aerosol properties retrieval approach is presented here that overcomes the limitations resulting from pre-computed RTE solutions stored in LUTs. ~~This new method takes advantage of the lessons learned from past attempts to retrieve simultaneously surface reflectance and aerosol properties.~~ The advantages of a continuous variation of the aerosol properties in the solution space against a LUT-based approach is discussed in Section (3). The proposed method expresses the single scattering albedo and phase function values as a linear mixture of basic aerosol ~~classes~~models. The forward radiative transfer model that includes the Jacobians, *i.e.* the partial derivative, computation is described in Section (4). With the exception of gaseous transmittance, this model no longer relies on LUTs, and the RTE is explicitly solved. The inversion method is described in Section (5). Finally, the ability to express aerosol single scattering properties as a linear combination is illustrated with simulated data representing various scenarios including small and large particles (6). Practical aspects of the application of the CISAR algorithm for the retrieval of both surface and aerosol properties from actual satellite data are addressed in Luffarelli and Govaerts (2018) (hereafter referred to as Part II).

2 Lessons learned from previous approaches

Pinty et al. (2000a) proposed an algorithm for the joint retrieval of surface reflectance and aerosol properties to demonstrate the possibility of generating Essential Climate Variables (ECV) from data acquired by operational weather geostationary satellites. Due to limited operational computational resources available at that time in the EUMETSAT ground segment, where the data were processed, the development of this algorithm was subject to strong constraints. The RTE solutions were pre-computed and stored in LUTs with a very coarse resolution, limiting the maximum Aerosol Optical Thickness (AOT) to 1, which represented a severe limitation over the Sahara region where AOT values can easily exceed such limit. Furthermore, the radiative coupling between aerosol scattering and gaseous absorption was not taken into account. This algorithm, referred to as Geostationary Surface Albedo (GSA) has been subsequently modified by Govaerts and Lattanzio (2007) to include an estimation of the retrieval uncertainty. This updated version has permitted the generation of a global aerosol product derived from observations acquired by operational weather geostationary satellites (Govaerts et al., 2008). Since then, it is routinely applied in the framework of the SCOPE-CM initiative to generate a Climate Data Record (CDR) of surface albedo (Lattanzio et al., 2013).

The GSA algorithm has been further improved for the processing of SEVIRI data on-board MSG for the retrieval of the total column AOT from observations acquired in ~~the VIS0.6, VIS0.8 and NIR1.6 spectral bands~~ three solar bands centred at 0.6 μm, 0.8 μm and 1.6 μm (Govaerts et al., 2010b; Wagner et al., 2010). The method developed by these authors relies on an OE approach where surface reflectance and daily aerosol load are simultaneously retrieved. The inversion is performed independently for each aerosol ~~class~~ model and the one with the ~~best fit~~ smallest cost function is selected. A physically-based radiative transfer model accounting for non-Lambertian surface reflectance and its radiative coupling with atmospheric scattering is inverted against daily accumulated SEVIRI observations. However, this Land Daily Aerosol (LDA) algorithm suffers from two major limitations: (*i*) the use of pre-defined aerosol ~~classes~~ models and, (*ii*) the algorithm delivers only one mean aerosol value per day when applied on MSG/SEVIRI data (Govaerts et al., 2010a). This latter issue has been addressed by Luffarelli et al. (2016) who retrieve an aerosol optical thickness value for each SEVIRI observation. The former issue prevents a continuous ~~variations~~ variation of the state variables characterizing the aerosol single scattering properties as required ~~by an OE approach (Rodgers, 2000).~~ to find the minimum of the cost function. A consistent implementation of such approach is not straightforward since aerosol ~~classes~~ models are defined as prior knowledge of the observed medium but ~~no uncertainties are~~ uncertainties cannot be easily assigned to this ~~information~~choice. Consequently, the estimated retrieval uncertainty is inconsistent as it does not account for the use of prior information and its associated uncertainties.

Diner et al. (2012) demonstrated the advantages of a retrieval method based on continuous variations of aerosol single scattering properties in the solution space as opposed to a LUT-based approach derived for a limited number of pre-defined aerosol ~~classes~~models. Dubovik et al. (2011) proposed an original method for the retrieval of aerosol micro-physical properties which also does not necessitate the use of predefined aerosol ~~classes~~models. This method retrieved more than 100 state variables requiring therefore a considerable number of observations, such as those provided by multi-angular and -polarisation radiometers like Polarisation et Anisotropie des Réflectances Au SOmmet de l'Atmosphère (PARASOL) (Serene and Corcoral, 2006) or the future Multi-viewing Multi-channel Multi-polarization Imaging (3MI) instrument on-board EUMETSAT's Polar System Second Generation (Manolis et al., 2013). Instruments delivering such a large number of observations are rather scarce as most of the current ~~or planned~~ passive optical sensors do not offer instantaneous multi-angular observation capabilities nor information on polarization. The primary objective of this paper is to address the limitations resulting from conventional approaches based on LUTs and/or a limited number of pre-defined aerosol ~~classes,~~ models by proposing a method that can be applied to observations acquired by single or multi-view instruments.

3 Continuous variation of aerosol properties in the solution space

Aerosol single scattering properties include the single scattering albedo ω_0 and the phase function Φ in RTE. Govaerts et al. (2010b) explained the benefits of representing pre-defined aerosol ~~classes~~ models in a two-dimensional solution space composed of these aerosol single scattering properties.

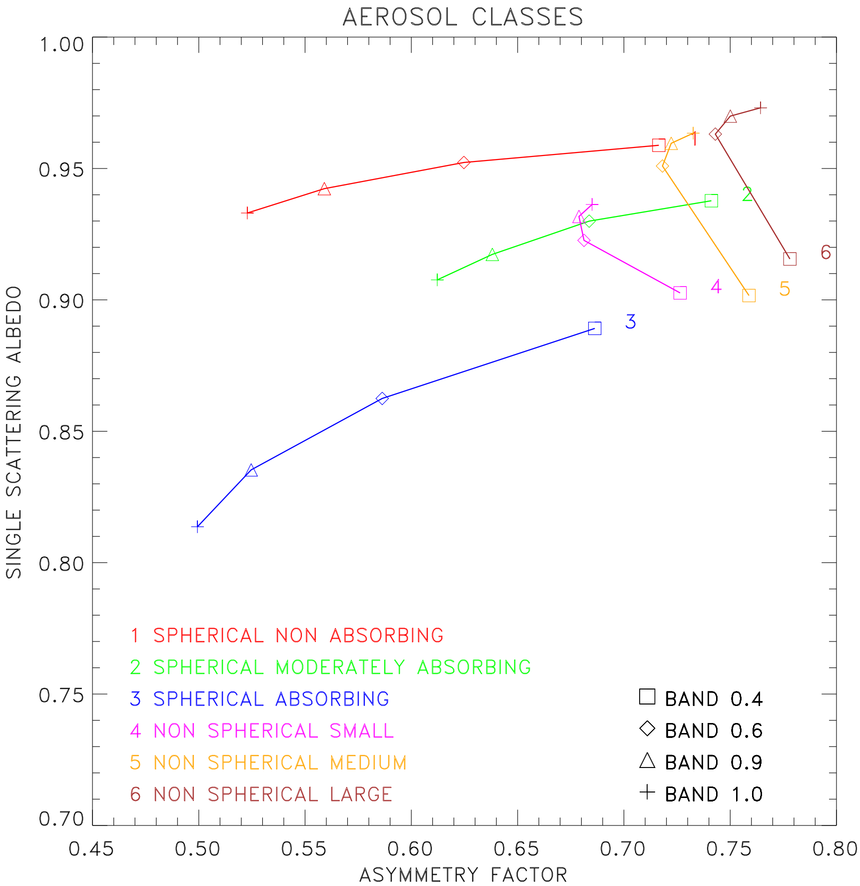

Fig. 1. Aerosol dual mode ~~classes~~ models after Govaerts et al. (2010b) in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space derived from the aggregation of aerosol single scattering properties retrieved from AERONET observations (Dubovik et al., 2006). Classes 1 to 3 are dominated by the fine mode and 4 to 6 by the coarse one.

For the sake of clarity, they limited the phase function in that 2D space to the first term of the Legendre coefficients, *i.e.*, the asymmetry parameter g. However, one should keep in mind that the reasoning applied in this Section should be applied to the entire phase function Φ. These aerosol single scattering properties are themselves determined by aerosol micro-physical properties, such as the particle size distribution, shape and their complex index of refraction. ~~Within a retrieval approach based on aerosol classes, the objective~~ The objective of retrievals that assume aerosol models is to provide ~~the best possible~~ a reasonable sampling of the ~~$[g,\omega_0]$ spacesuch as~~ $\{g,\omega_0\}$ space. Omitting areas of that space may produce biased retrievals, as discussed in Govaerts et al. (2010b). The inversion process proposed by ~~these authors~~ in this paper relies on a set of six ~~classes~~ models which have been defined from AErosol RObotic NETwork (AERONET) data aggregation (Dubovik et al., 2006). ~~These classes are supposed to provide the most likely sampling of the solution space but, since the scattering properties are not continuously varied, the inversion is typically~~ That choice of models was intended to provide a sampling of solution space representative of real-world conditions. The inversion is repeated for each aerosol class and the ~~one~~ result with the best fit is ~~selected (Wagner et al., 2010)~~reported, rather than vary the aerosol properties continuously, as would be preferable.

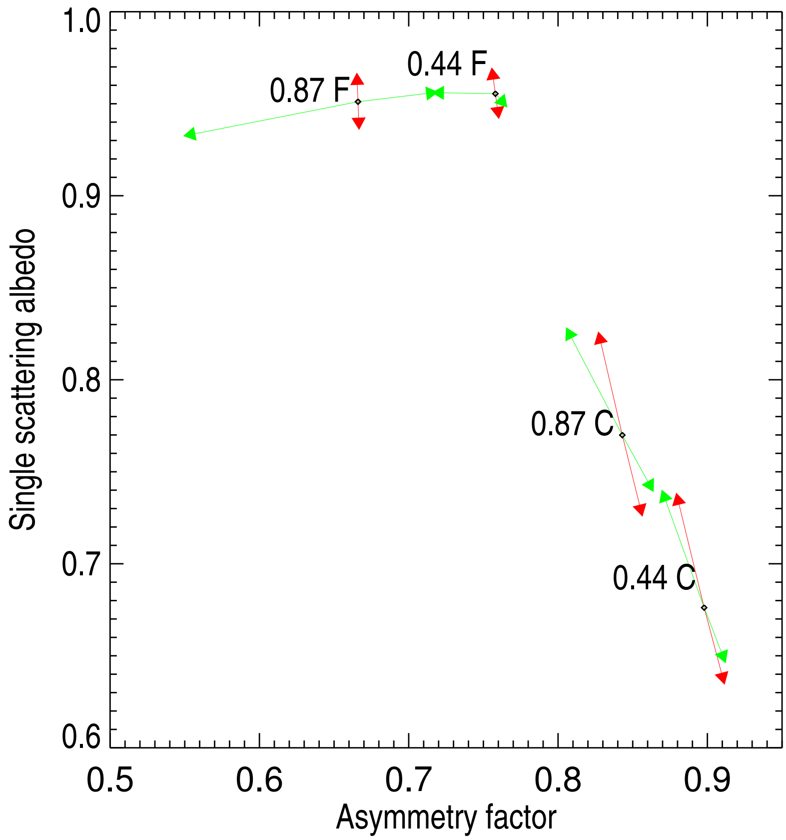

Fig. 2. Example of sensitivity of aerosol single scattering properties to particle median radius (green arrows) and imaginary part of the refractive index (red arrows) at 0.44 μm and 0.87 μm for fine mode F ($r_{mf} = 0.1\mu m$) and coarse mode C (~~$r_{mc} = 2.0\mu m$~~$r_{mc} = 2.0\mu$m). The length of the arrows reflects the magnitude of the change.

A visual inspection of Fig. (1) after Govaerts et al. (2010b) reveals that aerosol ~~classes~~ models occupy different regions in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space according to the dominant particle size distribution, *i.e.*, fine or coarse. Within that space, an aerosol ~~class~~ model is defined by the spectral behaviour of the $\{g(\lambda),\omega_0(\lambda)\}$ pairs where λ indicates the wavelength. The proposed fine mode ~~classes~~ models vary mostly as a function of ω_0 which is largely determined by the imaginary part of the refractive index n_i. Conversely, aerosol ~~classes~~ models dominated by coarse particles show little dependency on g and are therefore organised parallel to the ordinate axis. The main parameter discriminating these latter ~~classes~~ models is the median radius r_m, which essentially determines the asymmetry parameter value at a given wavelength.

To illustrate the dependence of g and ω_0 on the median radius r_m[1] and imaginary part of the refractive index n_i, fine and coarse mono-mode aerosol ~~classes~~ models were generated with $r_m = 0.15$ μm and 2.0 μm respectively. The other micro-physical values have been fixed to ~~$\sigma_r = 0.5\,\mu m$~~ $\sigma_r = 0.5\mu$m, $n_r = 1.42$ and $n_i = 0.008$ where σ_r is the radius standard deviation and n_r the real part of the refractive index. These values were selected to ease the explanation of the aerosol ~~classes~~ models organisation in Fig. (1). Black dots in Fig. (2) show the corresponding location of $\{g,\omega_0\}$ at 0.44 μm and 0.87 μm. The magnitude of the red arrows illustrate the sensitivity to a n_i change of ± 0.0025 and the green ones to a r_m change of $\pm 25\%$. For the fine mono-mode (F), changes in n_i essentially translate in displacement along the ω_0 axis while changes in r_m result in changes almost parallel to the g axis. There is also a clear relationship between the particle size and g for that mode. A change in the particle size results in a change in g while ω_0 remains ~~almost~~ relatively unchanged. The situation is quite different for the coarse mono-mode where changes in both n_i and r_m induce displacement parallel to the ω_0 axis with limited impact on g values.

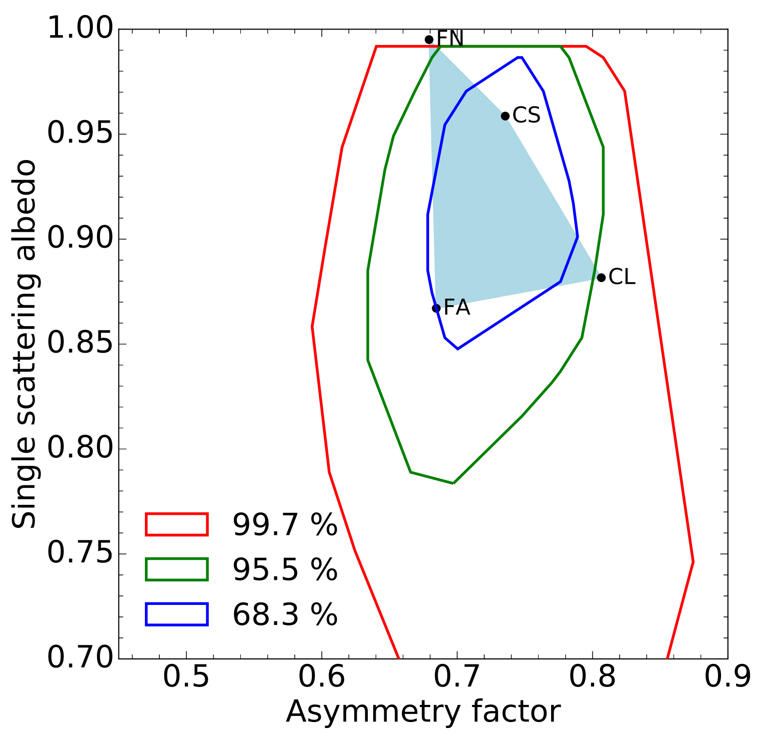

Fig. 3. Example of region (light blue area) in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ solution space at 0.44 μm defined by four aerosol vertices: single fine mode non-absorbing (FN), single fine mode absorbing (FA), coarse mode with small radius (CS) and coarse mode with large radius (CL). The isolines show the probability that the aerosol single scattering properties derived from AERONET observations with the method of Dubovik et al. (2006) fall within the delineated spaces.

[1] http://eodg.atm.ox.ac.uk/user/grainger/research/aerosols.pdf

The actual extent of solutions in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space for a given spectral band can be outlined by a series of vertices defined by aerosol single scattering properties (Fig. 3). Following Fig. (2), these vertices are defined by an absorbing and a non-absorbing fine mono-mode ~~classes~~ models with a small radius of about 0.1 μm, labelled respectively FA and FN, and by two coarse mono-modes with different radii, *i.e.*, large (1 μm) and small (0.3 μm), labelled respectively CL and CS. In Section (4), we will see how any pair of single scattering albedo and phase function values can be expressed as a linear combination of the vertex properties.

The choice of the position of these vertices is critical as they should encompass most likely aerosol single scattering properties that could be observed at a given time and location. Different approaches could be used to define the position of these vertices. The positions can be derived from the analysis of typical aerosol single scattering properties available in databases such as the Optical Properties of Aerosols and Clouds (OPAC) (Hess et al., 1998). Alternatively, it is also possible to follow a similar approach to the one proposed in Govaerts et al. (2010b) who analysed the single scattering albedo and phase function values derived from AERONET observations acquired in a specific region of interest for a given period (Dubovik et al., 2006). The red isoline in Fig. (3) delineates the area ~~of the $[g,\omega_0]$~~ $[g,\omega_0]$ of the solution space where 99.7% of the aerosol single scattering properties derived by Dubovik et al. (2006) from AERONET observations are located. The green and blue lines show respectively the 95% and 68% probability regions. These values have been derived using all available Level 2 AERONET observations since 1993. Finally, the model proposed by Schuster et al. (2005) can be used to determine the spectral variations of the single scattering properties outside the spectral bands measured by AERONET. ~~The present study~~ This work relies on simulated data and the aerosol vertices have been positioned to sample the solution space in a realistic way. When processing actual satellite data over a specific region or period, it is advised to calculate the isolines corresponding to that region of interest from AERONET observations and to adjust the position of the aerosol vertices accordingly as performed in Part II.

4 Forward Radiative Transfer Model

4.1 Overview

The forward model, named FASTRE, simulates the TOA Bidirectional Reflectance Factor (BRF) $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ as a function of the independent parameters $\mathbf{m}$ defining the observation conditions and a series of state variables $\mathbf{x}$ describing the state of the atmosphere and underlying surface. Model parameters $\mathbf{b}$ represent variables such as total column water vapour that influence the value of $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ but cannot be retrieved from the processed space-based observations due to the lack of information. The independent parameters $\mathbf{m}$ include the illumination and viewing geometries (Ω_0,Ω_v) and the wavelength dependence. The RTE is solved with the Matrix Operator Method (Fischer and Grassl, 1984) optimised by Liu and Ruprecht (1996) for a limited number of quadrature

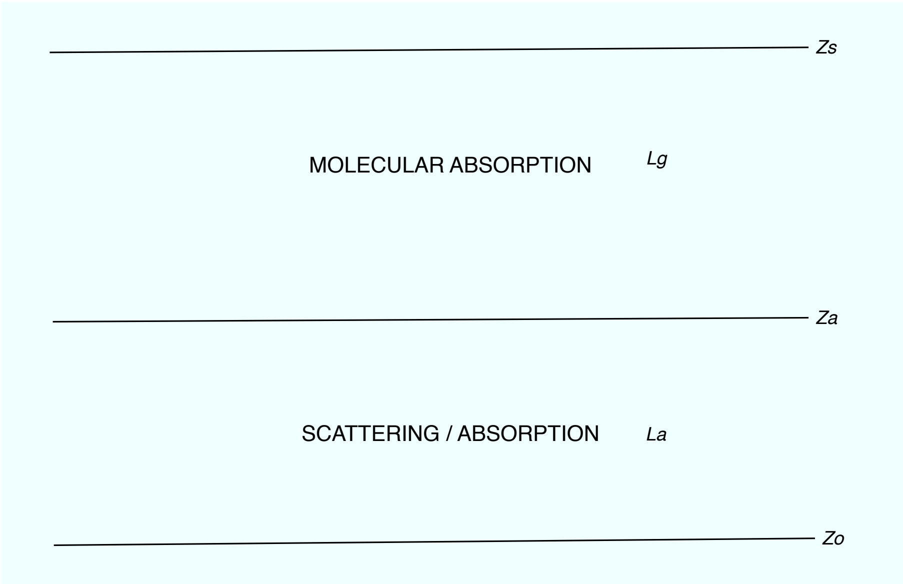

Fig. 4. Atmospheric vertical structure of the FASTRE model. The surface is at level Z_0 and radiatively coupled with the lower layer L_a extending from level Z_0 to Z_a. This layer includes scattering and absorption processes. The upper layer L_g runs from level Z_a to Z_s and only accounts for gas absorption processes.

points.

The model simulates observations acquired within spectral bands $\tilde{\lambda}$ characterized by their spectral response. Gaseous transmittances in these bands are precomputed and stored in LUTs. The model computes the contributions from single and multiple scattering separately, the latter being solved in Fourier space. In order to reduce the computation time, the forward model relies on the same atmospheric vertical structure as in Govaerts et al. (2010b), *i.e.*, a three-level system containing two layers (Fig. 4). The lowest level, Z_0, represents the surface. The lower layer L_a, ranging from levels Z_0 to Z_a, contains the aerosol particles. Molecular scattering and absorption are also taking place in that layer which is radiatively coupled with the surface for both the single and the multiple scattering. The upper layer L_g, ranging from Z_a to Z_s, is only subject to molecular absorption.

The surface reflectance $r_s(\mathbf{x_s},\mathbf{b};\mathbf{m})$ over land is represented by the so-called RPV (Rahman-Pinty-Verstraete) model characterised by four parameters $\mathbf{x_s} = \{\rho_0, k, \Theta, \rho_c\}$ that are all wavelength dependent (Rahman et al., 1993). The ρ_0 parameter, included in the [0,1] interval, controls the mean amplitude of the BRF and strongly varies with wavelengths. The k parameter is the modified Minnaert's contribution that determines the bowl or bell shape of the BRF and typically varies between 0 and 2. The asymmetry parameter Θ of the Henyey-Greenstein phase function ~~, Θ,~~ varies between -1 and 1. The ρ_c parameter controls the amplitude of the hot-spot due to the "porosity" of the medium. This parameter varies between -1 and 1. For the simulations over the ocean, the Cox-Munk model (Cox and Munk, 1954) is used as implemented in Vermote et al. (1997).

Aerosol single scattering properties in the layer L_a are represented by an external mixture of a series of predefined aerosol vertices as explained in Section (4.2). The L_g layer contains only absorbing gas not included in the scattering layer, such as high-altitude ozone, the part of the total column water vapour not included in layer L_a and few well-mixed gases.

The FASTRE model expresses the TOA BRF in a given spectral band $\tilde{\lambda}$ as a sum of the single $I_s^{\uparrow}$ and multiple $I_m^{\uparrow}$ scattering contributions as in

$$y_m(\mathbf{x},\mathbf{b};\mathbf{m}) = T_{L_g}(\mathbf{b};\mathbf{m})\,\frac{I_s^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m}) + I_m^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})}{E_0^{\downarrow}(\mathbf{m})\mu_0} \tag{1}$$

where

- $I_s^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})$ is the upward radiance field at level Z_a due to the single scattering;
- $I_m^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})$ is the upward radiance field at level Z_a due to the multiple scattering;
- $T_{L_g}(\mathbf{b};\mathbf{m})$ denotes the total transmission factor in the L_g layer;
- $E_0^{\downarrow}(\mathbf{m})$ denotes the solar irradiance at level Z_s corrected for the Sun-Earth distance variations.

The single scattering contribution writes

$$I_s^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m}) = \frac{E_0^{\downarrow}(\mathbf{m})\,\mu_0}{\pi}\exp\left(\frac{-\tau_{L_a}}{\mu_0}\right) r_s(\mathbf{x_s},\mathbf{b};\mathbf{m})\exp\left(\frac{-\tau_{L_a}}{\mu_v}\right) \tag{2}$$

where τ_{L_a} is the total optical thickness of layer L_a. μ_0 and μ_v are the cosine of the illumination and viewing zenith angles respectively.

The multiple scattering contribution $I_m^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})$ is solved in the Fourier space ~~in~~ for all illumination and viewing directions of the quadrature directions N_θ for $2N_\theta - 1$ azimuthal directions. The contribution $I_m^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})$ in the direction (Ω_0,Ω_v) is interpolated from the surrounding quadrature directions. Finally, the Jacobian $\mathbf{k}_{x_i} = \frac{\partial y_m(\mathbf{x_i},\mathbf{b};\mathbf{m})}{\partial x_i}$ of $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ for parameter x_i are calculated as finite differences.

4.2 Scattering layer L_a properties

The layer L_a contains a set of mono-mode aerosol ~~classes~~ models v characterized by their single scattering properties, *i.e.*, the single scattering albedo $\omega_{0,v}(\tilde{\lambda})$ and phase function $\Phi_v(\tilde{\lambda},\Omega_g)$ where Ω_g represents the scattering angle. The different vertices are combined into this layer according to their respective optical thickness $\tau_v(\tilde{\lambda})$ with the total aerosol optical thickness $\tau_a(\tilde{\lambda})$ of the layer being equal to

$$\tau_a(\tilde{\lambda}) = \sum_v \tau_v(\tilde{\lambda}) \tag{3}$$

The phase function $\Phi_v(\tilde{\lambda},\Omega_g)$ is characterized by a limited number N_κ of Legendre coefficients equal to $2N_\theta - 1$. The choice of this number results from a trade-off between accuracy and computational time. When N_κ is too small, the last Legendre moment is often not equal to zero and the delta-M approximation is applied (Wiscombe, 1977). In this case, the α_d coefficient of the delta-M approximation is equal to $\Phi_v(N_\kappa)$. The Legendre coefficients κ_j become

$$c_j = \frac{\kappa_j - \alpha_d}{1 - \alpha_d} \tag{4}$$

and the truncated phase function is denoted by Φ'_v. The corrected optical thickness $\tau'_v(\tilde{\lambda})$ and single scattering albedo $\omega'_{0,v}(\tilde{\lambda})$ of the corresponding aerosol ~~class~~ model become

$$\tau'_v(\tilde{\lambda}) = (1 - \omega_{0,v}\alpha_d)\tau_v(\tilde{\lambda}) \tag{5}$$

and

$$\omega'_{0,v}(\tilde{\lambda}) = \frac{1-\alpha_d}{1-\omega_{0,v}\alpha_d}\omega_{0,v}(\tilde{\lambda})\,. \tag{6}$$

The layer total optical thickness, τ_{L_a}, is the sum of the gaseous, τ_g, the aerosol, τ'_a and the Rayleigh, τ_r, optical depth

$$\tau_{L_a}(\tilde{\lambda}) = \tau_g(\tilde{\lambda}) + \tau'_a(\tilde{\lambda}) + \tau_r(\tilde{\lambda}) \tag{7}$$

with $\tau'_a(\tilde{\lambda}) = \sum_v \tau'_v(\tilde{\lambda})$. The single scattering albedo of the scattering layer is equal to

$$\omega'_0(\tilde{\lambda}) = \frac{\sum_c \omega'_{0,v}(\tilde{\lambda})\,\tau'_v(\tilde{\lambda})}{\tau'_a(\tilde{\lambda})} \tag{8}$$

and the layer average phase function

$$\Phi'(\tilde{\lambda},\Omega_g) = \frac{\sum_c \Phi'_v(\tilde{\lambda},\Omega_g)\,\tau'_v(\tilde{\lambda})}{\tau'_a(\tilde{\lambda})}\,. \tag{9}$$

4.3 Gaseous layer properties

It is assumed that only molecular absorption takes place in layer L_g. The height of level Z_a is used to partition the total column water vapour and ozone concentration in each layer assuming a US76 standard atmosphere vertical profile. This height is not retrieved and is therefore a model parameter of FASTRE which should be derived from some climatological values. T_{L_g} denotes the total transmission of that layer.

Table 1. Relative bias and root mean square error in percentage between FASTRE and the reference RTM in various spectral bands.

Spectral bands (μm)	0.44	0.55	0.67	0.87
Relative bias (%)	-1.1	-0.3	0.0	+0.3
Relative RMSE (%)	2.8	1.8	1.3	1.2

4.4 FASTRE model accuracy

The simple atmospheric vertical structure composed of two layers is the ~~most important~~ principal assumption of the FASTRE model. In order to evaluate the accuracy of FASTRE, a similar procedure as in Govaerts et al. (2010b) has been applied. The outcome of FASTRE has been evaluated against a more elaborated 1D Radiative Transfer Model (RTM) (Govaerts, 2006) for sun and viewing angles varying from 0 to 70°, for various types of aerosols, surface reflectance and total column water vapour values. This reference RTM represents the vertical structure of the atmosphere with 50 layers. The mean relative bias and relative Root Mean Square Error (RMSE) between the reference model and FASTRE have been estimated in the main spectral bands used for aerosol retrievals. The relative RMSE, R_r, is estimated as

$$R_r = \sqrt{\frac{1}{N}\sum_N \left(\frac{y_m(\mathbf{x},\mathbf{b};\mathbf{m}) - y_r(\mathbf{x},\mathbf{b};\mathbf{r})}{y_r(\mathbf{x},\mathbf{b};\mathbf{r})}\right)^2} \tag{10}$$

where $y_r(\mathbf{x},\mathbf{b};\mathbf{m})$ is the TOA BRF calculated with the reference model. In this paper, the FASTRE model solves the RTE using 16 quadrature points N_θ which provides a good compromise between speed and accuracy. Results are shown in Table (1). ~~As can be seen, the~~ The relative RMSE between FASTRE and the reference model is typically in the range of 1% – 3%. ~~An other~~ Another comparison of FASTRE has been performed against actual Project for On-Board Autonomy-Vegetation (PROBA-V) observations (Luffarelli et al., 2017). These comparisons show a RMSE in the range [0.024–0.038].

5 Inversion process

5.1 Overview

Surface reflectance characterisation requires multi-angular observations $\mathbf{y}_{\Omega\widetilde{\Lambda}}$, the acquisition of which can take between several minutes, as is the case for the Multi-angle Imaging SpectroRadiometer (MISR) instrument, and several days, as is the case for the Ocean and Land Colour Instrument (OLCI) on-board Sentinel-3 or the Moderate Resolution Imaging Spectroradiometer (MODIS). In the former case, data are often assumed to be acquired almost instantaneously, *i.e.*, with the atmospheric properties remaining unchanged during the acquisition time. Such a situation considerably reduces the calculation time required to solve the RTE, as the multiple scattering term $I_m^{\uparrow}(\mathbf{x},\mathbf{b};\mathbf{m})$ needs to be estimated only once per spectral band. In the latter case, atmospheric properties cannot be assumed to be invariant and the multiple scattering contribution needs to be solved for each observation. When geostationary observations are processed, the accumulation period is often reduced to one day, and the assumption that the atmosphere does not change can be converted into an equivalent radiometric uncertainty (Govaerts et al., 2010b). Strictly speaking, it should be assumed that atmospheric properties have changed when the accumulation time exceeds several minutes (Luffarelli et al., 2016).

The retrieved state variables in each spectral band $\widetilde{\lambda}$ are composed of the $\mathbf{x_s}$ parameters characterising the state of the surface and the set of aerosol optical thicknesses τ_v for the aerosol vertices that are mixed in layer L_a. Prior information consists of the expected values $\mathbf{x_b}$ of the state variables $\mathbf{x}$ characterising the surface and the atmosphere on one side, and regularization of the spectral and/or temporal variability of τ_v on the other side. Uncertainty matrices $\mathbf{S}_x$ are assigned to this prior information. Finally, uncertainties in the measurements $\mathbf{S}_y$ are assumed to be normally distributed with zero mean. The inversion process of the FASTRE model will be herein referred to as Combined Inversion of Surface and AeRosol (CISAR) algorithm.

5.2 Cost function

The fundamental principle of Optimal Estimation (OE) is to maximise the probability $P = P(\mathbf{x}|\mathbf{y}_{\Omega\widetilde{\Lambda}}, \mathbf{x_b}, \mathbf{b})$ with respect to the values of the state vector $\mathbf{x}$, conditional to the value of the measurements and any prior information. The conditional probability takes on the quadratic form (Rodgers, 2000):

$$\begin{aligned}
P(\mathbf{x}) \propto\, & \exp\left[-\left(y_m(\mathbf{x},\mathbf{b};\mathbf{m}) - \mathbf{y}_{\Omega\tilde{\Lambda}}\right)^T \mathbf{S}_y^{-1} \left(y_m(\mathbf{x},\mathbf{b};\mathbf{m}) - \mathbf{y}_{\Omega\tilde{\Lambda}}\right)\right] + \\
& \exp\left[-\left(\mathbf{x}-\mathbf{x}_b\right)^T \mathbf{S}_x^{-1}\left(\mathbf{x}-\mathbf{x}_b\right)\right] + \\
& \exp\left[-\mathbf{x}^T\, \mathbf{H}_a^T\, \mathbf{S}_a^{-1}\, \mathbf{H}_a\, \mathbf{x}\right] + \\
& \exp\left[-\mathbf{x}^T\, \mathbf{H}_l^T\, \mathbf{S}_l^{-1}\, \mathbf{H}_l\, \mathbf{x}\right]
\end{aligned} \tag{11}$$

where the first two terms represent weighted deviations from measurements and the prior state parameters, respectively, the third the AOT temporal smoothness constraints and the fourth the AOT spectral constraint, with respective uncertainty matrices $\mathbf{S}_a$ and $\mathbf{S}_l$. The algorithm proposed by Dubovik et al. (2011) implements similar temporal and spectral smoothness constraints. The two matrices $\mathbf{H}_a$ and $\mathbf{H}_l$, representing respectively the temporal and spectral constraints, can be written as block diagonal matrices

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}^{\rho_0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}^{k} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{H}^{\theta} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{H}^{\rho_c} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{H}^{\tau} \end{pmatrix} \tag{12}$$

where the four blocks $\mathbf{H}^{\rho_0}$, $\mathbf{H}^{k}$, $\mathbf{H}^{\theta}$ and $\mathbf{H}^{\rho_c}$ express the spectral constraints between the surface parameters. Their values are set to zero when these constraints are not active. The submatrix $\mathbf{H}_a^{\tau}$ can also be written using blocks $\mathbf{H}^{\tau}_{a;\tilde{\lambda},v}$ along the diagonal. For a given spectral band $\tilde{\lambda}$ and aerosol vertex v, the block $\mathbf{H}^{\tau}_{a;\tilde{\lambda},v}$ is defined as follows

$$\mathbf{H}^{\tau}_{a;\tilde{\lambda},v}\ \boldsymbol{\tau}_{\tilde{\lambda},v} = \begin{pmatrix} 1 & -1 & 0 & \dots & \dots \\ 0 & 1 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 1 & -1 \\ \dots & \dots & \dots & \dots & 0 \end{pmatrix} \begin{pmatrix} \tau_{\tilde{\lambda},v,1} \\ \tau_{\tilde{\lambda},v,2} \\ \vdots \\ \tau_{\tilde{\lambda},v,N_t-1} \\ \tau_{\tilde{\lambda},v,1,N_t} \end{pmatrix} \tag{13}$$

In the same way, the submatrix $\mathbf{H}^{\tau}_{l}$ can be written using blocks $\mathbf{H}^{\tau}_{l;v,t}$. For a given aerosol vertex v and time t, the block $\mathbf{H}^{\tau}_{l;v,t}$ is defined as follows

$$\mathbf{H}^{\tau}_{l;v,t}\ \boldsymbol{\tau}_{v,t} = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ -\frac{\epsilon_2}{\epsilon_1} & 1 & 0 & \dots & 0 \\ 0 & -\frac{\epsilon_3}{\epsilon_2} & 1 & \dots & 0 \\ \dots & \dots & \dots & \ddots & 0 \\ \dots & \dots & \dots & -\frac{\epsilon_{N_\lambda}}{\epsilon_{N_\lambda-1}} & 1 \end{pmatrix} \begin{pmatrix} \tau_{1,v,t} \\ \tau_{2,v,t} \\ \tau_{3,v,t} \\ \vdots \\ \tau_{N_{\tilde{\lambda}},v,t} \end{pmatrix} \tag{14}$$

where the ϵ_l represents the uncertainties associated with the AOT spectral constraints of the individual vertex v bounding the solution space. The spectral variations of τ_v between band $\tilde{\lambda}_l$ and $\tilde{\lambda}_{l+1}$ are assumed to vary as

$$\frac{\tau_{\tilde{\lambda}_l,v}}{\tau_{\tilde{\lambda}_{l+1},v}} = \frac{e_{\tilde{\lambda}_l}}{e_{\tilde{\lambda}_{l+1}}} \tag{15}$$

where $e_{\tilde{\lambda}_l}$ the extinction coefficient in band $\tilde{\lambda}_l$.

Maximising the probability function in Equation (11) is equivalent to minimising the negative logarithm

$$J(\mathbf{x}) = J_y(\mathbf{x}) + J_x(\mathbf{x}) + J_a(\mathbf{x}) + J_l(\mathbf{x}) \tag{16}$$

with

$$J_y(\mathbf{x}) = \left(y_m(\mathbf{x},\mathbf{b},\Omega) - \mathbf{y}_{\Omega\tilde{\Lambda}}\right) \mathbf{S}_y^{-1} \left(y_m(\mathbf{x},\mathbf{b},\Omega) - \mathbf{y}_{\Omega\tilde{\Lambda}}\right)^T \tag{17}$$

$$J_x(\mathbf{x}) = \left(\mathbf{x} - \mathbf{x}_b\right) \mathbf{S}_x^{-1} \left(\mathbf{x} - \mathbf{x}_b\right)^T \tag{18}$$

$$J_a(\mathbf{x}) = \mathbf{x}^T\, \mathbf{H}_a^T\, \mathbf{S}_a^{-1}\, \mathbf{H}_a\, \mathbf{x} \tag{19}$$

$$J_l(\mathbf{x}) = \mathbf{x}^T\, \mathbf{H}_l^T\, \mathbf{S}_l^{-1}\, \mathbf{H}_l\, \mathbf{x} \tag{20}$$

Notice that the cost function J is minimized with respect to the state variable $\mathbf{x}$, so that the derivative of J is independent of the model parameters $\mathbf{b}$. The need for angular sampling to document the surface anisotropy leads to an unbalanced dimension of n_x and n_y with $n_y > n_x$ where n_y and n_x represents the number of observations and state variables respectively. According to Dubovik et al. (2006), these additional observations should improve the retrieval as, from a statistical point of view, repeating similar observations implies that the variance should decrease. Accordingly, the magnitude of the elements of the covariance matrix should decrease as

$1/\sqrt{n_y}$. Thus, repeating similar observations results in some enhancements of retrieval accuracy which is proportional to the ratio n_y/n_x. Hence, the cost function which is actually minimized is $J_s(\mathbf{x}) = J_y(\mathbf{x}) + n_y/n_x\,(J_x(\mathbf{x}) + J_a(\mathbf{x}) + J_l(\mathbf{x}))$.

5.3 Retrieval uncertainty estimation

The retrieval uncertainty is based on the OE theory, assuming a linear behaviour of $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ in the vicinity of the solution $\hat{\mathbf{x}}$. Under this condition, the retrieval uncertainty $\sigma_{\hat{\mathbf{x}}}$ is determined by the shape of $J(\mathbf{x})$ at $\hat{\mathbf{x}}$

$$\sigma^2_{\hat{\mathbf{x}}} = \left(\frac{\partial^2 J_s(\mathbf{x})}{\partial \mathbf{x}^2}\right)^{-1} = \left(\mathbf{K}_x^T \mathbf{S}_y^{-1} \mathbf{K}_x + \mathbf{S}_x^{-1} + \mathbf{H}_a^T\,\mathbf{S}_a^{-1}\,\mathbf{H}_a + \mathbf{H}_l^T\,\mathbf{S}_l^{-1}\,\mathbf{H}_l\right)^{-1} \tag{21}$$

where $\mathbf{K}_x$ is Jacobian matrix of $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ calculated in $\hat{\mathbf{x}}$. Combining Equations (21) and (8), the uncertainty in the retrieval of ω_0 in band $\tilde{\lambda}$ writes

$$\sigma^2_{\hat{\omega}_0}(\tilde{\lambda}) = \sum_v \left(\frac{\omega_{0,v}(\tilde{\lambda}) - \omega_0(\tilde{\lambda})}{\tau_a(\tilde{\lambda})}\right)^2 \sigma^2_{\hat{\tau}_v}(\tilde{\lambda}) \tag{22}$$

A similar equation can be derived for the estimation of σ^2_g.

5.4 Acceleration methods

The minimization of Equation (16) relies on an iterative approach with $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ and the associated Jacobians $\mathbf{K}_x$ being estimated at each iteration. In order to reduce the calculation time dedicated to the estimation of $y_m(\mathbf{x},\mathbf{b};\mathbf{m})$ and $\mathbf{K}_x$, a series of methods have been implemented. All quantities that do not explicitly depend on the state variables, such as the observation conditions $\mathbf{m}$, model parameters $\mathbf{b}$, quadrature point weights, *etc*, are computed only once prior to the optimization.

When solving the RTE, the estimation of the multiple scattering term is by far the most time-consuming step. Hence, during the iterative optimisation process, when the change $\Delta\tau_a(\tilde{\lambda})$ ~~of $\tau_a(\tilde{\lambda})$~~ between iteration j and $j+1$ is small, the multiple scattering contribution at iteration $j+1$ is estimated with

$$I_m^{\uparrow}(\tau_a(j+1,\tilde{\lambda}),\mathbf{b};\mathbf{m}) = I_m^{\uparrow}(\tau_a(j,\tilde{\lambda}),\mathbf{b};\mathbf{m}) + \frac{\partial I_m^{\uparrow}(\tau_a(j,\tilde{\lambda}),\mathbf{b};\mathbf{m})}{\partial \tau_a}\,\Delta\tau_a(\tilde{\lambda})\,. \tag{23}$$

This approximation is not used ~~twice consecutively~~ in two successive iterations to avoid inaccurate results, and the single scattering contribution is always explicitly estimated.

6 Algorithm performance evaluation

6.1 Experimental setup

A simple experimental setup based on simulated data has been defined to illustrate the performance of the CISAR's algorithm as a function of the ~~delineated~~ chosen solution space. More specifically,

Table 2. List of aerosol properties used for the simulations. The parameters r_{mf} and r_{mc} are the median fine and coarse mode radii expressed in μm. Their respective standard deviations are $\sigma_{r_{mf}}$ and $\sigma_{r_{mc}}$. The parameters n_r and n_i are the real and imaginary part of the refractive index in the indicated bands. N_f and N_c are the fine and coarse mode particle concentration in number of particles per cm^3.

Centre band in μm			0.44	0.55	0.67	0.87		
Type	r_{mf}	r_{mc}	n_i	n_r	n_r	n_r	N_f	N_c
F0	0.08	-	~~1.3958~~ 1.396	~~1.3932~~ 1.393	~~1.3909~~ 1.391	~~1.3879~~ 1.388	-	-
F1	0.10	0.93	~~1.4189~~ 1.419	~~1.4269~~ 1.427	~~1.4357~~ 1.436	~~1.4417~~ 1.442	9.587	0.002
F2	0.08	0.77	~~1.4985~~ 1.498	~~1.5201~~ 1.520	~~1.5436~~ 1.544	~~1.5417~~ 1.542	8.975	0.024
	$\sigma_{r_{mf}}$	$\sigma_{r_{mc}}$	n_i	n_i	n_i	n_i		
F0	0.45	-	~~0.0123~~ 0.012	~~0.0123~~ 0.012	~~0.0122~~ 0.012	~~0.0121~~ 0.012	-	-
F1	0.43	0.62	~~0.0057~~ 0.006	~~0.0055~~ 0.005	~~0.0053~~ 0.005	~~0.0051~~ 0.005		
F2	0.50	0.62	~~0.0054~~ 0.005	~~0.0047~~ 0.005	~~0.0040~~ 0.004	~~0.0036~~ 0.004		

CISAR capability to continuously sample the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ solution space is examined in detail. For the sake of simplicity, a noise-free multi-angular observation vector $\mathbf{y}_{\Omega\tilde{\Lambda}}$, where Ω expresses the illumination and viewing geometries, is assumed to be acquired instantaneously in the principal plane and in the spectral bands listed in Table (1). A radiometric uncertainty of 3% is assumed to compose $\mathbf{S}_y$. In this ideal configuration, the Sun Zenith Angle (SZA) is set to 30°. ~~It is also assumed that the surface parameters are known a priori with zero bias and an~~ In these experiments, to concentrate on the retrieval of aerosol properties, the surface parameters prior values are set to the true values used in simulation (Table 5) with an ascribed uncertainty of 0.03~~for each RPV parameter, though these parameters are allowed to vary~~. The first guess values are randomly chosen within this uncertainty interval. Part II explains how prior information on the surface parameters can be derived. No prior information is assumed for the aerosol optical thickness, *i.e.*, the prior uncertainty is set to very large values. Only regularization on the spectral variations of τ_a is applied.

Table 3. Micro-physical parameter values for the four FA, FN, CS, CL vertices in the selected spectral bands. Radius are given in μm

Centre band in μm			0.44	0.55	0.67	0.87	0.44	0.55	0.67	0.87
Type	r_m	σ_{r_m}	n_r	n_r	n_r	n_r	n_i	n_i	n_i	n_i
FN	0.08	0.45	1.3958	1.3932	1.3909	1.3879	0.0006	0.0006	0.0006	0.0006
FA	0.08	0.45	1.3958	1.3932	1.3909	1.3879	0.0207	0.0207	0.0207	0.0205
CS	0.30	0.55	1.4889	1.4878	1.4845	1.4763	0.0029	0.0029	0.0029	0.0029
CL	1.00	0.55	1.4889	1.4878	1.4845	1.4763	0.0029	0.0029	0.0029	0.0029

The CISAR algorithm performance evaluation is based on a series of experiments corresponding to different selections of aerosol properties, both for the forward simulation of the observations and their inversion. Three different aerosol models are used in the forward simulations: F0 which only contains fine mode, F1 which contains a dual-mode particle size distribution dominated by small particles, and F2 composed of a dual-mode distribution dominated by the coarse particles. Table (2) contains the values of the size distribution and refractive indices of these aerosol ~~classes~~models. Values for the four FA, FN, CL, CS vertices enclosing the solution space as illustrated in Fig. (3) are given in Table (3). When the observations simulated with aerosol types F0, F1 or F2 are inverted, the list of vertices actually used depends on the type of experiments as indicated in Table (4). For all these scenarios, an AOT of 0.4 at 0.55μm is assumed.

Table 4. List of ~~experiment~~ experiments the name of which is provided in the first column. The active vertices in each ~~experiments~~ experiment are indicated with the $\times$ symbol. The last column indicates the name of the aerosol model used to simulate the observations.

Exp.	Active vertices				Forward type
	FA	FN	CS	CL	
F00	×	×			F0
F10	×	×			F1
F11	×	×	×		F1
F12	×	×		×	F1
F13	×	×	×	×	F1
F21	×	×	×		F2
F22	×	×		×	F2
F23	×	×	×	×	F2

Table 5. Values of the true and retrieved surface RPV parameters ~~used as prior information~~for experiment F00. Wavelengths are given in μm.

		True				Retrieved			
	Band	ρ_0	k	Θ	ρ_c	ρ_0	k	Θ	ρ_c
	0.44	0.025	0.666	-0.150	0.125	0.025±0.006	0.666±0.030	-0.150±0.030	0.125±0.030
~~Wavelengths~~	0.55	0.047	0.657	-0.114	0.023	0.047±0.004	0.657±0.029	-0.116±0.028	0.023±0.030
	0.67	0.056	0.710	-0.096	0.025	0.056±0.004	0.711±0.028	-0.096±0.026	0.025±0.030
	0.87	0.238	0.706	-0.019	0.030	0.238±0.011	0.705±0.025	-0.020±0.017	0.029±0.030
	height								

Values used for the RPV parameters in the four selected bands are indicated in Table (5). They correspond to typical BRF values that would be observed over a vegetated surface with a leaf area index value of 3 and a bright underlying soil.

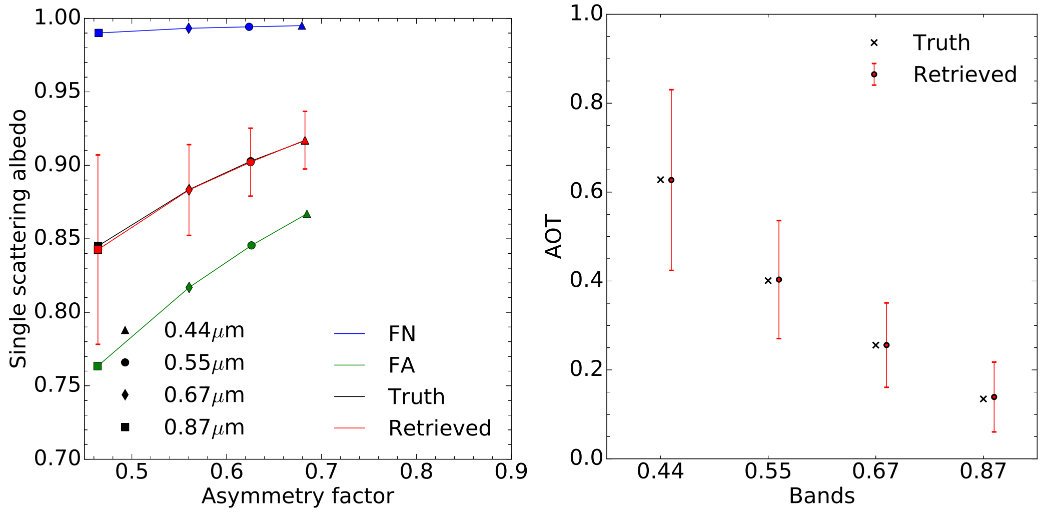

Fig. 5. Left panel: Results of experiment F00 in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space. The aerosol vertices used for the inversion are FN (blue) and FA (green). The forward aerosol properties are shown in black and the retrieved ones in red. Vertical and horizontal red bars indicate the uncertainty ~~, if any,~~ of the retrieved values. **Right panel**: Retrieved AOT (red circles). The retrieval uncertainty is shown with the vertical red lines. True values are indicated with black crosses. True and retrieved values are slightly staggered to ease the reading.

6.2 Results

6.2.1 Experiment F00

The purpose of the first experiment (F00) is to demonstrate that the CISAR algorithm can accurately retrieve aerosol properties in a simple situation, showing therefore that the inversion process works correctly. The F0 aerosol ~~class~~ model used to simulate the observations is only composed of fine particles with a median radius of 0.08μm, *i.e.*, the same value as for the FN and FA vertices used for the inversion. Hence, the retrieval is limited to the imaginary part of the index of refraction, the real part being set to 1.4. With a retrieval configuration restricted to the use of only two vertices, the solution space for each wavelength is limited to a straight line between the two vertices.

Results are shown in Fig. (5) for the atmosphere and Table (~~??~~5) for the surface. The asymmetry factor g and single scattering albedo ω_0 are almost exactly retrieved. There is practically no uncertainty in the retrieval of g because of the constraints imposed by the fact that the particle radius is the same as for the F0 aerosol ~~class~~model. The retrieved AOT is also in very good agreement with the true values as can be seen on the right panel. The retrieval error ϵ_τ is defined as the difference between the retrieved and the true AOT values. Results are summarised in Table (6). This first experiment demonstrates that it is possible to retrieve the properties of the aerosol ~~class~~ model F0 as a linear combination of the vertices FA and FN when only the absorption varies, the particle median radius being constant.

A comparison between ~~Tables~~ thr true and retrieved values in Table (5) ~~and (??)~~ shows that the surface parameters are very accurately retrieved. As stated in Section (6.1), prior information on the magnitude of the RPV parameter is assumed unbiased with an uncertainty of 0.03. The corresponding posterior uncertainties exhibit a significant decrease for the ρ_0 parameter at all wavelengths. A similar behaviour is not observed for the other parameters. As explained in Wagner et al. (2010), the k and Θ parameters, controlling the surface reflectance anisotropy, are strongly correlated with the amount of atmospheric scattering. Consequently, the retrieved uncertainties decrease with increasing wavelengths, *i.e.*, as a function of the actual AOT. Despite the observations taking place in the principal plane, the posterior uncertainty on the hot spot parameter remains equal to the prior one as a result of atmospheric scattering. This fact is attributed to the relatively high value of the true AOT, and the consequent amount of scattering attenuating the hot spot. Results for the surface parameter retrieval exhibits a very similar behaviour for the other experiments and will not be shown.

~~Values of the retrieved surface RPV parameters and associated uncertainties for experiment F00. Wavelengths are given in .~~

6.2.2 Experiment F10

Let us now examine the case where both r_m and n_i differ from those of the vertices used for the inversion. The aerosol type F1 is used for the forward simulation with $r_{mf} = 0.1$ μm for the predominant fine mode and $r_{mc} = 0.93\mu$m for the coarse mode. The same aerosol vertices as in experiments F00 are used for the inversion.

The results in Fig. (6) show that ω_0 is reasonably well retrieved unlike the g parameter, which is systematically underestimated. At any given wavelengths, it is not possible to retrieve g values outside the bounds defined by the FA and FN vertices. Consequently, the retrieved AOT values are underestimated by about 10% (Table 6). This example illustrates the retrieval failure when the actual solution lays outside the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space defined by the active vertices.

6.2.3 Experiments F11 - F13

In order to improve the retrieval of the F1 aerosol ~~class~~ model properties, the additional aerosol CS vertex with $r_m = 0.3$ μm has been added for the inversion process. Results of experiment F11 are displayed in Fig. (7). Retrieved g values are no longer underestimated. The single scattering albedo is slightly underestimated. It should be noted that the estimated uncertainty associated with g increases with wavelength and is particularly large at 0.87 μm, but rather underestimated at 0.44 μm. The improvement in the AOT retrieval accuracy is noticeable in the 0.44 μm and 0.55 μm bands where the magnitude of ϵ_r is reduced from 0.062 to 0.005 and from 0.042 to -0.021 respectively (Table 6). At larger wavelengths, the benefit of adding the CS vertex is less noticeable though the magnitude of ϵ_r remains below 0.05. Finally, the retrieval uncertainty slightly increases from 0.199 up to 0.239 for the 0.44 μm band because of the use of additional state variables τ_v associated with

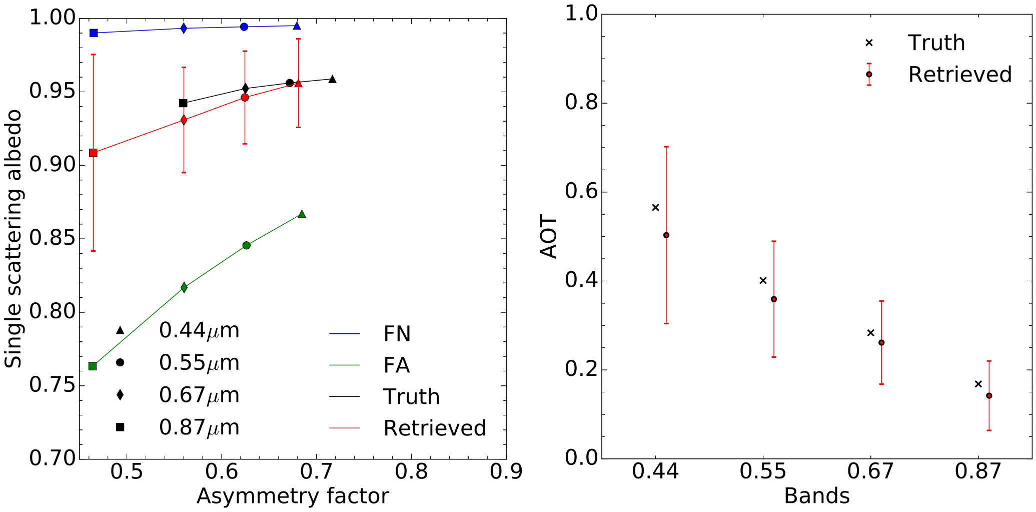

Fig. 6. Same as Fig. (5) but for experiment F10.

Table 6. Retrieved AOT error and uncertainties for the six experiments. The error ϵ_τ is calculated as the difference between the retrieved and the true values, δ_τ the relative error in percent and σ_τ the retrieval uncertainty estimated with Eq. (21). Wavelengths are given in μm.

BAND	0.44			0.55			0.67			0.87		
EXP	ϵ_τ	δ_τ	σ_τ	ϵ_τ	δ_τ	σ_τ	ϵ_τ	δ_τ	σ_τ	ϵ_τ	δ_τ	σ_τ
Units	–	(%)	–	–	(%)	–	–	(%)	–	–	(%)	–
F00	0.001	-0.1	0.203	-0.002	0.6	0.133	-0.000	0.0	0.095	-0.004	3.3	0.079
F10	0.062	-11.0	0.199	0.042	-10.5	0.130	0.022	-7.8	0.094	0.026	-15.6	0.078
F11	0.005	-0.9	0.239	-0.021	5.3	0.164	-0.037	13.2	0.125	-0.047	27.8	0.095
F12	0.041	-7.3	0.228	0.013	-3.3	0.152	-0.004	1.5	0.113	-0.015	8.6	0.089
F13	-0.001	0.1	0.295	-0.028	6.9	0.199	-0.041	14.5	0.145	-0.051	30.5	0.103
F21	0.018	-3.9	0.252	0.037	-9.2	0.172	0.042	-11.9	0.129	0.071	-22.9	0.096
F22	-0.018	3.9	0.236	-0.007	1.8	0.158	-0.004	1.1	0.116	0.008	-2.6	0.090
F23	-0.041	8.8	0.296	-0.031	7.8	0.200	-0.027	7.5	0.145	-0.018	6.0	0.103

the inclusion of an additional vertex. A similar behaviour is observed in the other bands.

For experiment F12, the CS vertex is substituted by vertex CL which has a median radius of 1.0μm. The use of this vertex instead of CS considerably improves the retrieval of g and of ω_0 at large wavelengths (Fig. 8). As can be seen in Fig. (2), the sensitivity of aerosol single scattering properties to particle median radius and imaginary part of the refractive index depends on the wavelength. Hence, a similar performance of the algorithm ~~in~~ at all wavelengths should not be expected. The errors ϵ_τ in this experiment F12 are further reduced compared to experiment F11 with the exception of the 0.44μm band. The CISAR algorithm ~~manages to correctly retrieve the total AOT~~retrieves total AODs consistent with the truth.

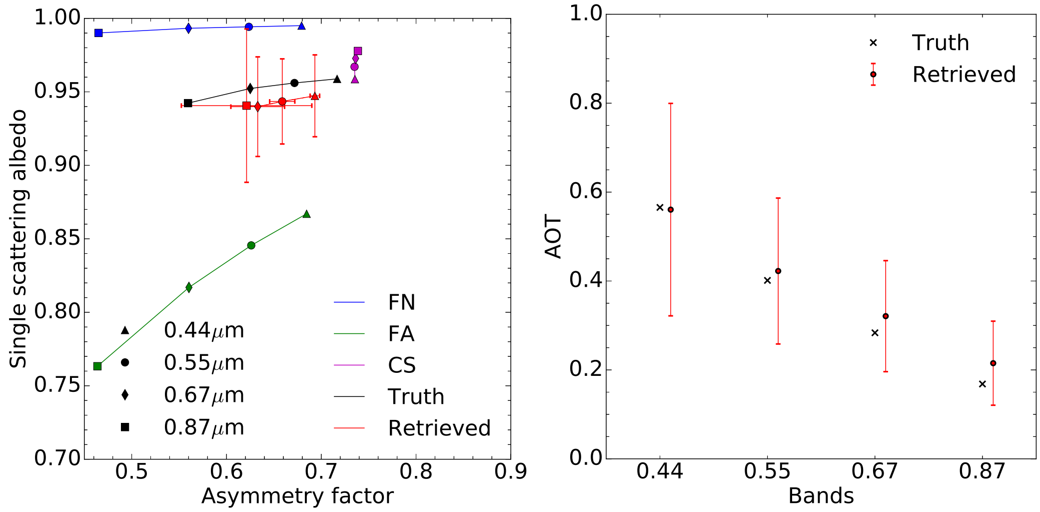

Fig. 7. Same as Fig. (5) but for experiment F11.

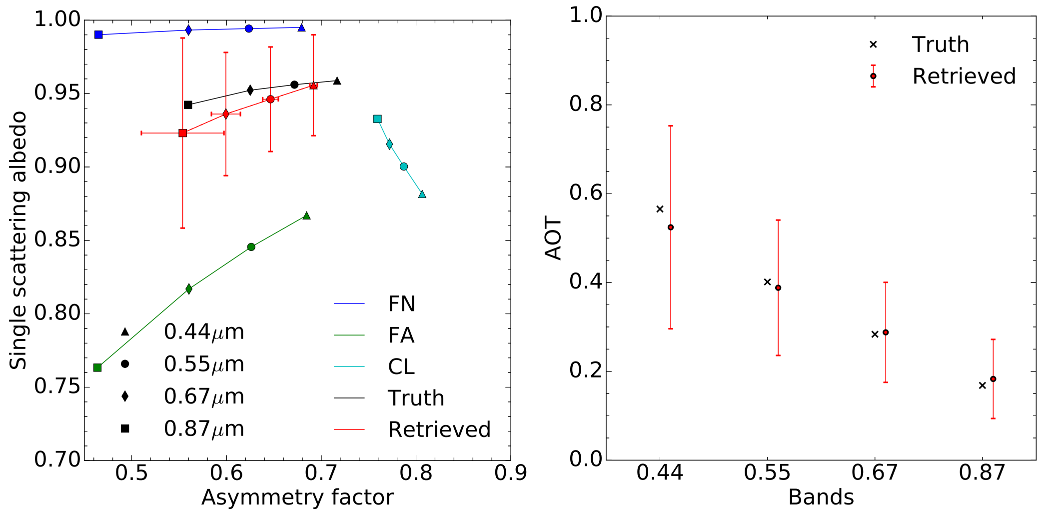

Fig. 8. Same as Fig. (5) but for experiment F12.

Finally, in experiment F13 the inversion was performed using all four vertices (Fig. 9). This additional "degree of freedom" translates into an increase of the estimated uncertainty $\sigma_{\hat{\tau}}$ as a result of the large number of possible way to combine these four vertices to retrieve the properties of the aerosol ~~class~~ model F1. In other words, ~~adding~~ using these two coarse mode vertices does not improve the characterization of F1. The actual benefit of adding this fourth vertex, *i.e.* expanding the solution space, is therefore not straightforward, and should be noted that increasing the number of vertices impacts the computational time. This series of experiments has shown that~~the~~ , of the four considered, the use of the FN, FA and CL vertices provides the best combination for the retrieval of ~~the properties of aerosol class~~ aerosol model F1. With this combination, the FN and FA vertices

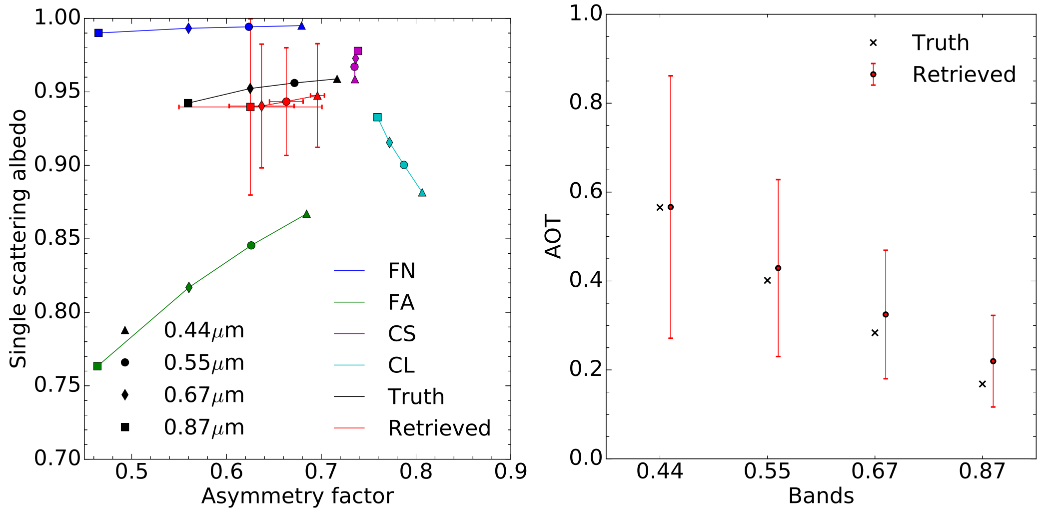

Fig. 9. Same as Fig. (5) but for experiment F13.

allow to control the amount of radiation absorbed by the aerosols and the CL vertex the effects of the particle size.

6.2.4 Experiments F21 - F23

The retrieval of aerosol ~~class~~ model F2, a dual mode particle size distribution dominated by coarse particles, is now examined. This ~~class~~ model is composed of a fine mode with radius $r_{mf} = 0.08$ μm and a coarse mode with radius $r_{mc} = 0.77$ μm. As for the retrieval of the F1 aerosol ~~class~~model, three combinations of vertices have been explored, *i.e.*, (FN, FA, CS) for experiment F21 (Fig. 10), (FN, FA, CL) for experiment F23 (Fig. 11) and (FN, FA, CS, CL) for experiment F22 (Fig. 11). Essentially the same conclusions hold as for the retrieval of aerosol ~~class~~ model F1. The retrieval of the ~~F2-class~~ F2-model properties expressed as a linear combination of the (FN, FA, CL) vertices provides the best solution with both g and ω_0 being well retrieved at all wavelengths.

7 Discussion and conclusion

This paper describes the CISAR algorithm designed for the joint retrieval of surface reflectance and aerosol properties. Previous attempts to perform such joint retrieval have been reviewed, discussing their advantages and weaknesses. ~~Retrieval~~ The limitations due to a combined used of discrete and continuous state variables in retrieval methods based on OE ~~applied only to a limited number of aerosol classes~~ as in Govaerts et al. (2010b) ~~represent a major drawback as it does not permit a continuous variation of the state variables in the solution space~~are discussed in Section (2). The new method presented in this paper specifically addresses ~~this issue~~these limitations, allowing continuous variations of the aerosol single scattering properties in the solution space without the aerosol micro-

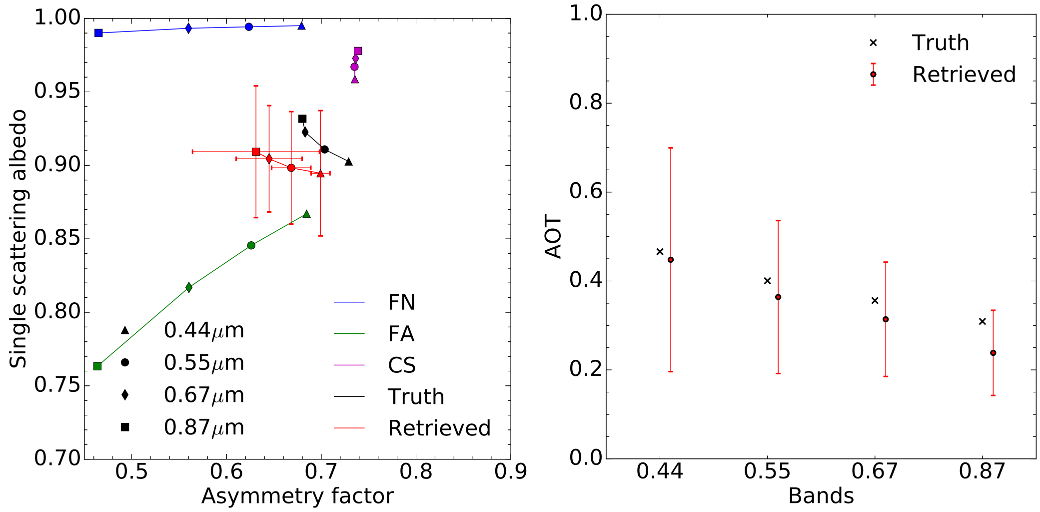

Fig. 10. Same as Fig. (5) but for experiment F21.

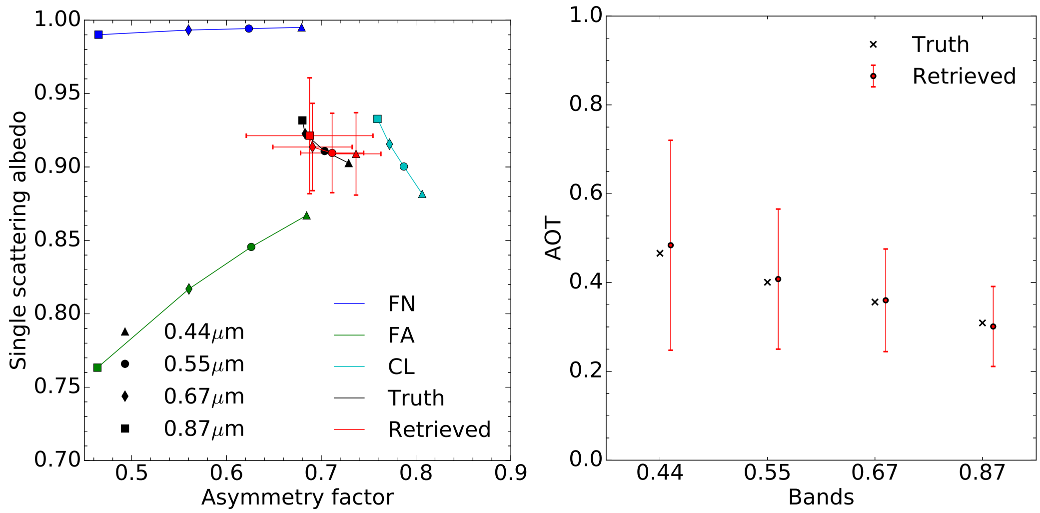

Fig. 11. Same as Fig. (5) but for experiment F22.

physical properties explicitly appearing as state variables.

A fast forward radiative transfer model has been designed, which solves the radiative transfer equation without relying on pre-computed look-up tables. This model considers two atmospheric layers. The upper layer only hosts molecular absorption. The lower layer accounts for both absorption and scattering processes due to aerosols and molecules and is radiatively coupled with the surface represented with the RPV BRF model. Single scattering aerosol properties in this layer are expressed as a linear combination of the properties of vertices enclosing part of the solution space.

A series of different experiments has been devised to analyse the behaviour of the CISAR algorithm and its capability to retrieve aerosol single scattering properties as well as the optical thickness.

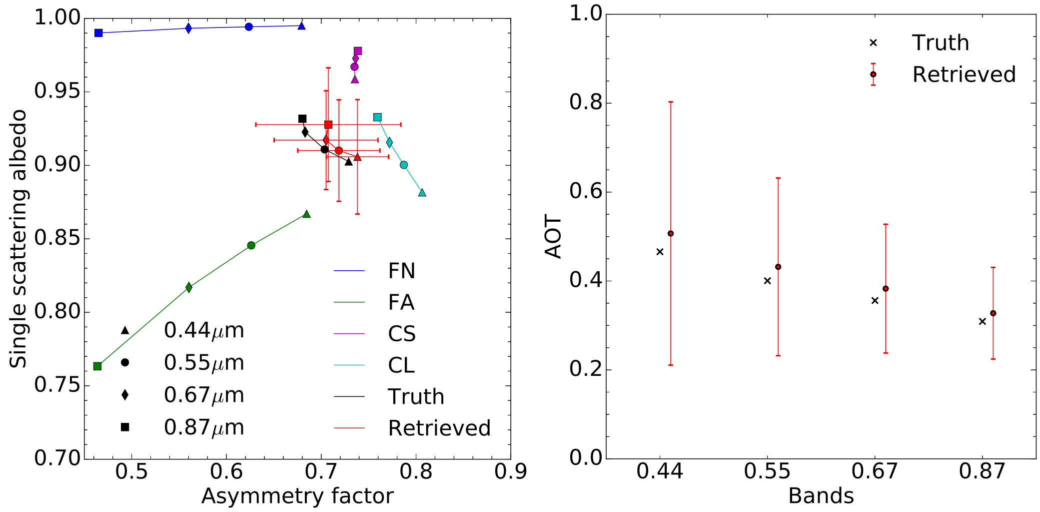

Fig. 12. Same as Fig. (5) but for experiment F23.

This discussion focuses on the retrieval of aerosol ~~classes~~ models dominated by the fine mode or a coarse mode. These two ~~classes~~ models have pretty different spectral behaviour in the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ space and yet the CISAR algorithm is capable of retrieving the corresponding single scattering properties in both cases with estimated uncertainties of about 15%.

These experiments illustrate the possibility to use Equations (8) and (9) for the continuous retrieval of the aerosol single scattering albedo and phase function. These equations assume a linear behaviour of ω_0 and g in the solution space. Such assumptions have proven to be valid for the case addressed in experiment F00. This assumption is not exactly true for the retrieval aerosol ~~classes~~ models of a fine and a coarse particle size modes. However, the retrieved aerosol single scattering properties are derived much more accurately than with a method based on a limited number of predefined aerosol ~~classes~~ models as in Govaerts et al. (2010b) where the single scattering properties of only predefined ~~classes~~ models are retrieved. It thus represents a major improvement with respect to these type of retrieval approaches without requiring the use of a large number of state variables as in the method proposed by Dubovik et al. (2011) where aerosol micro-physical properties are explicitly included in the set of retrieved state variables.

The choice of the vertices outlining the ~~$[g,\omega_0]$~~ $\{g,\omega_0\}$ solution space is critical. In these experiments, best retrieval is obtained using three vertices, *i.e.*, one vertex composed of small weakly absorbing particles (FN), one vertex composed of small absorbing particles (FA) and one vertex composed of large particles (CL). The use of a fourth vertex (CS) does not improve the retrieval and increases the estimated retrieval uncertainty.

This set of experiments represents ideal conditions, *i.e.*, noise-free observations in the principal plane with no bias on the surface prior. This choice is motivated by the need to keep the result interpretation simple to illustrate how the new retrieval concept developed in this paper works. These experiments show the possibility to retrieve aerosol single scattering properties within the solution space provided it is correctly bounded by the vertices. It is clear that adding noise in the observations will degrade the quality of the retrieval. Similar conclusions can hold in case the observations are taking place far from the principal plane where most of the angular variations occur. Part II addresses the CISAR performance when applied on actual satellite data.

8 Supplement

Includes the plots of case F22 adding a 3% Gaussian noise to the simulated TOA BRF for AOT = 0.05 (Fig. S1), AOT = 0.2 (Fig. S2), AOT = 0.4 (Fig. S3) and AOT = 0.8 (Fig. S4). Fig. S5 shows the merged results in the $\{g, \omega_0\}$ space of experiments F11, F12 and F13. Fig. S6 shows the merged results in the $\{g, \omega_0\}$ space of experiments F21, F22 and F23.

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