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Atmospheric Retrieval Algorithms for Long-Wave Infrared and Solar Radiance Scenarios

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ABSTRACT

Atmospheric retrieval is the extraction of atmospheric data from spectral radiance, as observed at a remote sensor. In particular, consider the retrieval of temperature and humidity profiles, and aerosol size distribution and the scattering refractive index from long-wave infrared and solar radiance spectra, respectively. The application of retrieval, in this report, primarily involves inversion of a radiative transfer equation (RTE). However, due to the ill-posed nature of the problem and the inherent errors involved, such inversions are non-trivial. This report presents a combined, generalised approach to retrieval via statistical inversion, which is derived in detail for the atmospheric parameters mentioned above.

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Executive Summary

One of the primary applications of electro-optic sensors for the Australian Defence Force is the accurate remote sensing of targets and background. Previous work of the Imaging Electro-Optics Systems group at Defence Science and Technology Organisation (IEOS, DSTO) has shown that target identification is sensitive to the influence and accurate modelling of the intervening atmosphere. Consequently, this report focuses on acquiring an accurate representation of the atmosphere and on accounting for atmospheric effects in electro-optic remote sensing scenarios. The challenge is to construct a valid description of the atmosphere from observed spectral radiance data.

The retrieval of atmospheric parameters, in this report, is achieved through inversion of a suitable approximation to the radiative transfer equation (RTE). Briefly; within the long-wave infrared spectral region, atmospheric emission is the dominant contributor to observed atmospheric radiance, characterised mainly by the vertical water vapour and temperature profiles of the atmosphere. In the solar spectral region, alternatively, the atmospheric radiance is primarily influenced by the scattering of solar radiation, characterised mainly by the aerosol and molecular properties of the atmosphere. For these two spectral regions then, appropriate approximations to the RTE, dominated by either atmospheric emission or scattering, can be obtained. The constructed radiative transfer formulae are then inverted in order to retrieve the temperature and humidity profiles or aerosol size distribution and refractive index, for long-wave infrared or solar spectral sensor data, respectively. Due to the ill-posed nature of the problem and the inherent errors involved, such inversions are non-trivial. The process involves the application of statistical regularisation to observed radiance data and *a priori* information.

This report focuses on constructing the mathematical and practical basis of a generic statistical inversion method for atmospheric retrieval. The purpose of developing a generic base is to demonstrate how the retrieval procedure can be technically applied and adapted to a variety of scenarios. In this report, the process is tailored to the scenarios of long-wave infrared and solar spectral waveband sensing. The final result is the construction of appropriate "retrieval equations", obtained for the retrieval of temperature and humidity profiles, as well as aerosol size distribution and refractive index of the atmosphere. Extrapolation of these results is investigated with the application to ground-based target identification, which is found to ultimately rely on the information available and the particular scenario presented. Finally, the report concludes that further research at DSTO would enable improved atmospheric models for Australian conditions and more accurate atmospheric compensation in target detection algorithms. To this end, a follow-up report will apply these formulae to specific Defence simulated and experimental scenarios.

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Michelle Hackett completed a Bachelor of Science, majoring in mathematics and physics, followed by Honours in Applied Mathematics at the University Queensland in 2001. She joined the Defence Science and Technology Organisation (DSTO) as a graduate in 2002 and has been working in the Imaging Electro-Optics Systems (IEOS) group of the Intelligence, Surveillance and Reconnaissance Division (ISRD) until the present. During her time in the IEOS group, Ms Hackett has been researching the retrieval of atmospheric properties from remotely sensed hyperspectral data. She has presented this work at a number of internal and collaborative meetings. During this time Ms Hackett has also contributed to the analysis of data in the Atmospheric Aerosol Research task, run by Dr Stephen Carr. June 2005 has seen Ms Hackett complete her Graduate Certificate in Sciences (Defence Signal Information Processing) with the University of Adelaide, where she is also currently pursuing a Masters of Arts (International Studies) .

Contents

1. Introduction

Atmospheric retrieval involves the extraction of information about the atmosphere and its constituents from remotely sensed radiance data.

Transfer of radiation through the atmosphere to a sensor is influenced by various atmospheric processes. The gases, aerosols and physical conditions of the atmosphere determine the extent to which this radiation will be absorbed, emitted and scattered. The radiance data collected by a remote sensor, therefore, contains information about the various processes and constituents of the atmosphere. It is ultimately through manipulation of this data that atmospheric characteristics can be retrieved.

Various scenarios and processes of extraction have been studied in the field of atmospheric retrieval. This report draws upon the plethora of research documentation in the field to present two applications that have particular relevance to Defence; electro-optic solar (*ie.* visible and short-wave infrared) and long-wave infrared sensing. One of the primary applications of electro-optic sensors in Defence is to provide accurate remote sensing of targets and background. Previous work of the Imaging Electro-Optics Systems group at Defence Science and Technology Organisation (IEOS, DSTO) has shown that target identification is sensitive to the influence and accurate modelling of the intervening atmosphere [2]. Application of atmospheric retrieval is expounded in this report in a generic form, for these two sensing scenarios.

1.1 Purpose

The purpose of this report is to inform the reader of the processes by which to technically perform atmospheric retrieval, via statistical inversion. This includes the mathematical construction of radiation transfer through the atmosphere and the statistical analysis necessary to retrieve atmospheric characteristics from observed radiance data. In particular, the report will investigate two scenarios; the retrieval of atmospheric temperature and humidity profiles, and the retrieval of aerosol size distribution and refractive index. This is made possible with the data obtained through passive sensing of long-wave infrared and solar wavebands, respectively.

The retrieval processes for the two different applications are presented concurrently, in order to emphasise that atmospheric retrieval of various phenomena can be conducted by following a generic formula. Utilisation of several sensors, of differing wavebands, could then allow us to probe the various aspects of the atmosphere that contribute to its configuration. Ultimately this could give us a clearer understanding of the atmosphere through which we are sensing. One applications of this, which is particularly relevant in Defence, is towards more accurate knowledge of the atmosphere in remote target detection.

The purpose of this report is not to validate a new technique for atmospheric retrieval, but rather to introduce an unfamiliar reader to the theory and mathematics underlying common atmospheric retrieval procedures. The point of this is to help readers apply the mathematics to their own specific circumstances. Application of the formulae to simulated or experimental data can be seen in the referenced papers mentioned throughout the report. The retrieval formulae of this report are well-tested, applied and documented in the literature, but it is the mathematical development of these equations that is not well documented in a generic unified way. The importance of this is two-fold; one, a report that expounds the mathematical derivations enables others to also duplicate or follow the work in this field; and two, understanding the underlying assumptions of the resultant retrieval formulae enables more accurate adaptation of the techniques to particular circumstances and scenarios. Whilst including specific examples would be beyond the scope of this report, it is planned that a less theoretical report will follow-up this paper in the future, which will apply these retrieval formulae to specific DSTO examples.

1.2 Outline

This report has be organised such that the foundational mathematics can be accessed by those that need to adapt the forms to their own needs (Chapter 2 and appendices), but also such that the specific applications can be examined without having to delve into the underlying mathematics of the statistical retrieval (Chapter 3 and 4). A summary of the basic mathematics of the generic retrieval equation is presented in Chapter 2.

The following chapters (Chapters 3 and 4) apply this formula to the retrieval of temperature and humidity profiles from observed long-wave infrared radiances, and the aerosol size distribution and refractive index from observed solar radiances. The scenarios consider the radiation observed from ground-based sensors directed with zenith angle towards the sky. The sensors will detect radiation affected by various processes, including radiation emitted, scattered and absorbed by the atmosphere. The atmospheric processes are mathematically modelled according to the application, and then used to retrieve the required information via the retrieval formula described in Chapter 2. More detailed explanation and derivation of the various factors involved in the retrieval equations are presented in the appendices (Appendices A and B).

The end of Chapter 3, "Application for Long-Wave Infrared Sensors: Retrieval of Temperature and Humidity Profiles", briefly explores the added application of remote target detection. Within Defence, this is one of the primary objectives of atmospheric retrieval. As previously stated, knowledge of the atmosphere and its effect on the radiance, observed by a remote electro-optic sensor, is extremely beneficial in accurate target detection. This report will highlight the adjustments necessary for inclusion of target radiance in the long-wave infrared scenario and the added complications that this can produce.

Finally, the report will conclude with a summary of the procedures, an assessment of the validity of the applications, and suggestions for future progress.

2. Mathematical Basis of Atmospheric Retrieval

2.1 Radiative Transfer Equation (RTE)

The problem, as described so far, is to retrieve values for atmospheric characteristics from experimentally taken radiance measurements. This observed radiance information is linked to the unknown characteristics via a Radiative Transfer Equation (RTE).

The RTE describes the change in spectral radiance over a distance (ds) along a path through the atmosphere.

Electromagnetic radiation transfer could be envisaged as an initial emission from a source (target, the Earth or the sun), which is transmitted through the atmosphere to a sensor. Various processes, involving atmospheric gaseous and particulate components, affect the radiance along a path from an initial radiator to a sensor. These processes include scattering of radiation out of the path, absorption of radiation along the path, multiple scattering of indirect diffuse radiation into the path, single scattering of direct solar radiation into the path, and emission of infrared radiation into the path. Thus the RTE, which describes these processes, is expressed as,

$$dL(\lambda) = dL_{\text{emission}}(\lambda) + dL_{\text{scat in}}(\lambda) + dL_{\text{multiscat}}(\lambda) - dL_{\text{scat out}}(\lambda) - dL_{\text{absorp}}(\lambda), \quad \textbf{\textit{eqn(1)}}$$

where $dL(\lambda)$ is the spectral change in radiance.

Depending on the applications of the project, a RTE can be represented by variations on the above equation. As different processes take dominance within different spectral regions and circumstances, the above RTE can be simplified by removing less consequential terms.

In order to appropriately construct this simplified radiative transfer equation, the role of the unknown characteristics to be retrieved must be considered, as will be demonstrated in the application chapters to follow. This chapter will explore the mathematical basis of the retrieval problem without going into application-specific detail. Firstly, we will integrate and manipulate the RTE into a generic, linearised form, as a function of the sensor radiance. Then, using the generic radiance function and other "information equations", we will investigate the fundamentals of the statistical inversion, as required to retrieve atmospheric characteristics.

2.2 Discretisation and Linearisation of the RTE

The radiative transfer equation can describe the transfer of electromagnetic radiation through the atmosphere with an analytic function. It is from this function, in its various forms, that we need to extract information or characteristics of the atmosphere.

In its current form, the RTE (eqn(1)) is a function of all atmospheric processes. However, as will be seen in the following chapters, with specific application this RTE can be simplified to only include the dominant processes. This is done with the aim to produce an equation for the radiance at the sensor, as a function of the required atmospheric characteristics. For the specific applications to follow (Chapters 3 and 4), the unknown atmospheric characteristics are temperature, humidity, aerosol size distribution and refractive index. We will represent these unknowns with the variable x.

Integration of the RTE, with respect to the path length (ds), will give a ***radiance equation*** for the sensor data as a function of the unknown atmospheric characteristics, x,

$$L_{\text{sensor}}(\lambda, s) = \int_{ds} dL(\lambda) = L_{\text{RTE}}(\lambda, s, x)$$

where $L_{\text{sensor}}(\lambda, s)$ is the observed sensor data at altitude $z(s)$, and $L_{\text{RTE}}(\lambda, s, x)$ is the RTE integrated over the path length to the sensor, as a function of the unknown variable x.

In these applications, as also in other scenarios, the integration of the RTE is not analytically possible. To solve this problem, we will firstly discretise the unknown variable x into vector form, as follows.

2.2.1 Discretisation

Currently we have assumed that x is a continuous function. Consider instead, that the unknown variable is now an unknown ***vector***, $\mathbf{x}$.

For our applications, the unknown temperature and humidity profiles of the atmosphere are continuous functions of the altitude, $T(z)$ and $\rho(z)$. Let us now instead consider the atmosphere as 'virtually' constructed of discrete consecutive layers, each of which emits and absorbs electromagnetic radiation. We then have layer altitudes z_i for which we can determine approximate temperature and humidity values, and hence a temperature and humidity vector, *ie.* $\mathbf{x} = [\mathbf{T}^{\text{T}}, \boldsymbol{\rho}^{\text{T}}]^{\text{T}}$, or explicitly, $\mathbf{x} = [T(z_1), T(z_2), ..., \rho(z_1), \rho(z_2), ...]^{\text{T}}$.

Similarly, the aerosol size distribution is a continuous function of radius, $n(r)$. The effects of particulate-scattering processes on the radiation in the atmosphere are fundamentally determined by the size of the individual aerosols and their scattering cross-section. Let us now consider individual radii bins r_i with which to retrieve a discretised aerosol size distribution vector. Similarly, the refractive index, $m(\lambda)$, can be discretised into specific wavelengths, corresponding to the radiance measurements, *ie.* $\mathbf{x} = [\mathbf{n}^{\text{T}}, \mathbf{m}^{\text{T}}]^{\text{T}}$, or explicitly, $\mathbf{x} = [n(r_1), n(r_2), ..., m(\lambda_1), m(\lambda_2), ...]^{\text{T}}$.

Also, for the expedience of matrix formation, the observed radiance can be presented as a vector of wavelengths, $\mathbf{L}_{\text{sensor}} = [L(\lambda_1), L(\lambda_2), ...]^{\text{T}}$.

With appropriate discretisation of the variables, and other application-specific assumptions, the RTE can be integrated along the path to the sensor, and now presented as the radiance equation,

$$\mathbf{L}_{\text{sensor}} = \mathbf{L}_{\text{RTE}}(\mathbf{x}).$$

2.2.2 Linearisation

As will be demonstrated in the applications to follow, the relationship between the observed radiance, $\mathbf{L}_{\text{sensor}}$, and the unknown atmospheric characteristics, $\mathbf{x}$, is often not well defined or simple. That is, the integrated RTE is not in a form that is practicably invertible. One solution is to linearise the equation with a "first guess" of the atmospheric unknown variable.

Let us approximate the unknown solution about an initial estimate, vector $\mathbf{x0}$, using a multivariate Taylor's expansion,

$$L_{\text{sensor}}(\lambda_j) = L_{\text{RTE}}(\lambda_j, \mathbf{x}) \approx L_{\text{RTE}}(\lambda_j, \mathbf{x0}) + \sum_i \left(J(\lambda_j, \mathbf{x0}_i)\left(\mathbf{x}_i - \mathbf{x0}_i\right)\right) + \text{H.O.T.} \qquad \textbf{\textit{eqn(2)}}$$

where $J(\lambda_j, \mathbf{x0}_i) = \left.\dfrac{\partial L_{\text{RTE}}(\lambda_j, \mathbf{x})}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}}$. ***eqn(3)***

Let us assume for these linearised systems that the higher order terms (H.O.T.) are neglected without compromise. This will be discussed in greater detail later, for the individual applications.

Hence we have a discretised linear equation (eqn(2)) that requires the observed total radiance of the atmosphere data $L_{\text{sensor}}(\lambda)$, the radiance of an atmosphere with virtual "first guess" characteristics $L_{\text{RTE}}(\lambda, \mathbf{x0})$, and a calculation of how the atmosphere would change with respect to this virtual unknown profile $\partial L_{\text{RTE}}(\lambda, \mathbf{x0})/\partial \mathbf{x}|_{\mathbf{x0}}$. These parameters can be calculated with the assistance of various atmospheric modelling software packages and *a priori* information, as will be discussed for the specific applications.

After discretisation and linearisation, the general form of the radiance equation as expressed in equation (2), can be most succinctly expressed in a simple, generic matrix form,

$$\mathbf{L}_{\text{sensor}} - \mathbf{L}_{\text{RTE}}(\mathbf{x0}) = \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0})$$

eqn(4)

where $\hat{\mathbf{J}}$ is the Jacobian matrix of the derivatives as described in eqn(3), and $\mathbf{L}_{\text{sensor}}$ and $\mathbf{L}_{\text{RTE}}(\mathbf{x0})$ are now vectors of specific wavelengths.

With a generic equation (eqn(4)) defined by a simple matrix function of the unknown atmospheric vector and its Jacobian matrix, it now seems more feasible to retrieve a solution. Currently, however, the inversion problem is ill-posed; for hyperspectral data we have an over-determined system, with more information than unknowns (and thus no unique solution), and for multispectral data we have an under-determined system, with an inadequate amount of information for a solution.

It is also evident that there exists both measurement and estimation errors. These complicate the inversion procedure further. In order to find the optimal solution with all the information available, whilst accounting for these errors, some form of statistical regularisation is necessary, tempered with knowledge of the physical reality of the scenario. It is beneficial to firstly declare all information in a generic form and the associated errors, and then extrapolate to the particular retrieval scenarios.

2.3 Information Equations for Retrieval of Unknown Vectors

The problem, as originally described, is to retrieve values for atmospheric unknowns from remote sensor radiance measurements. This observed radiance data is now linked to the unknown atmospheric vector via a linearised radiance equation. Due to the ill-posed nature of the radiance equation and the inherent errors associated with it, we require more information than that provided by the sensor. Statistical techniques need to be used to find an optimal solution that takes into account all information available: Consider these as 'real' and 'virtual' forms of information.

2.3.1 Real Information

Real information or data is that which is collected or measured from observed phenomena. Thus far, the sensor radiances $\mathbf{L}_{\text{sensor}}$ for different wavelengths and (later) scattering angles have been considered. With any physical measurement, the equipment used will always have some degree of uncertainty and error, $\mathbf{E}_{\text{instrument}}$. Added to this, the integrated radiative transfer equation (eqn(4)) used to link the observed real data to the unknown vector has inherent formulation errors, due to approximations *etc.*, $\mathbf{E}_{\text{formula}}$. Let us attempt to account for these errors in our retrieval. Let,

$$\mathbf{L}(\mathbf{x}) = \mathbf{L}_{\text{sensor}} \pm \mathbf{E}_{\text{instrument}} \quad \text{and} \quad \mathbf{L}(\mathbf{x}) = \mathbf{L}_{\text{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{E}_{\text{formula}},$$

where $\mathbf{L}(\mathbf{x})$ is the true value of the radiance; $\mathbf{L}_{\text{sensor}}$ is the observed data; $\mathbf{E}_{\text{instrument}}$ is the measurement (*eg.* sensor instrument) error; and $\mathbf{E}_{\text{formula}}$ is the formula (*eg.* RTE approximation and linearisation) error. So that,

$$\mathbf{L}_{\text{sensor}} = \mathbf{L}_{\text{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{El}, \text{ where } \mathbf{El} = \mathbf{E}_{\text{formula}} + \mathbf{E}_{\text{instrument}}.$$

The retrieval procedure, as considered so far, has been directed towards inverting a radiative transfer equation to obtain the desired atmospheric variables. That is, the primary information utilised has been the observed total radiance, $\mathbf{L}_{\text{sensor}}$, and the radiance equation (integrated RTE) that attempts to link the true value of the total radiance, $\mathbf{L}(\mathbf{x})$, to the unknown vector $\mathbf{x}$. Previously, $\mathbf{L}_{\text{sensor}}$ and $\mathbf{L}(\mathbf{x})$ were interchangeable, but with addition of error terms, we must redefine our equations as above. The true value of $\mathbf{L}(\mathbf{x})$ is unknown due to inherent errors, thus we are left with the question of how to retrieve $\mathbf{x}$, with the observed radiance information $\mathbf{L}_{\text{sensor}}$, within the error constraints.

Let us define the observed 'real' information as $\mathbf{L}^*$. The unknown variable, $\mathbf{x}$, is presently bound in the integrated RTE equation. Thus, as will be demonstrated later, it is beneficial to view the current problem as how to best calculate the integrated RTE from the observed radiance data, in order to extract $\mathbf{x}$, *ie*.

$$\mathbf{L}^* = \mathbf{L}_{\text{sensor}} = \mathbf{L}_{\text{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{El}\ .$$

The validity of the observed radiance information equation is, at present, still compromised by the assumptions and estimations made in the Taylor's linearisation. The formula error term in the above equation can be used to account for the higher order terms that are neglected in this linearization. However, we have also introduced a new source of data, $\mathbf{x0}$, without explanation of the origins and inherent errors associated with it. The "first guess" data $\mathbf{x0}$ is, in its own right, a form of information, but since it is derived from means other than direct observation, let us classify it as 'virtual' information.

2.3.2 Virtual Information

Virtual information can be obtained from statistics of the atmospheric region, extrapolation of previous results, or known constraints on the form of the retrieved data, *etc.*. Thus far we have introduced only one form of virtual information; the "first guess" profile, which is an estimation of the retrieved solution $\mathbf{x}$,

$$\mathbf{x}^* = \mathbf{x0} = \mathbf{x} \pm \mathbf{Ex}\ .$$

where $\mathbf{x}^*$ is the approximated solution, often represented as a first guess $\mathbf{x0}$; $\mathbf{Ex}$ is the expected error in our approximation; and $\mathbf{x}$ is the real profile required.

Linearisation of the integrated RTE was achieved by using a Taylor's approximation about a chosen parameter $\mathbf{x0}$. By defining $\mathbf{x0}$ as the first guess of $\mathbf{x}$, and then interpreting this first guess as the real value of $\mathbf{x}$ with sufficiently small error, we ensure that the linearisation of the RTE is supportable. That is, with $\mathbf{x0}$ sufficiently close to $\mathbf{x}$, the linearised RTE should provide a reliable function about real value $\mathbf{x}$.

In the case of the aerosol retrieval, it is also necessary that the retrieved solution be well-behaved; that is, smooth and continuous. Let us then introduce another virtual information equation that will smooth the solution. As is presented in Appendix B.3, the appropriate smoothing matrix $\mathbf{B}$ is chosen such that,

$$\mathbf{0}^* = \mathbf{0} = \hat{\mathbf{B}}\,\mathbf{x} \pm \mathbf{Eb}\ .$$

2.3.3 Optimisation of the Information Equations

All real and virtual information about the system can be represented by a generic function,

$$\mathbf{f}^* = \mathbf{f}(\mathbf{x}) \pm \mathbf{Ef}\ .$$

eqn(5)

In order to manipulate the various information equations, it is recommended that the functions $\mathbf{f}(\mathbf{x})$ be discretised and linearised, as already shown for the observed radiance information equation using Taylor's approximation (eqn(4)).

Assuming that $\mathbf{x0}$ is a close approximation to $\mathbf{x}$ (with error $\mathbf{Ex}$), in generic terms; $\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{x0}) + \hat{\mathbf{J}}_{\mathrm{f}}(\mathbf{x} - \mathbf{x0}) + \mathrm{o}\left((\mathbf{x}\text{-}\mathbf{x0})^2\right)$.

Therefore our "real" and "virtual" ***information equations*** are;

$$\mathbf{L}_{\mathrm{sensor}} = \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{El}$$

$$\mathbf{x0} = \mathbf{x0} + \hat{\mathbf{J}}_{\mathrm{x}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{Ex} \qquad \text{where } \hat{\mathbf{J}}_{\mathrm{x}} = \partial\mathbf{x}/\partial\mathbf{x} = \hat{\mathbf{I}} \text{ and}$$

$$\mathbf{0} = \hat{\mathbf{B}}\,\mathbf{x0} + \hat{\mathbf{J}}_{\mathrm{B}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{Eb} \qquad \text{where } \hat{\mathbf{J}}_{\mathrm{B}} = \partial\hat{\mathbf{B}}/\partial\mathbf{x} = \hat{\mathbf{B}}\,.$$

These equations, at first glance, may appear to convolute rather than aid in the retrieval of the unknown atmospheric variables $\mathbf{x}$. However, conversion of all information into the above forms is a useful way to appreciate the amount and reliability of the information that we have about $\mathbf{x}$. From this platform, we are able to decide on a method of retrieval, or more particularly, on a method of statistical inversion.

2.4 Statistical Regularisation and Inversion

We are presented now with several linearised functions from which to gain information about the unknown atmospheric vector, $\mathbf{x}$. How we choose to use such information equations is dependent on the statistical technique best suited to the application.

2.4.1 Implementing the Inversion

One method of statistical inversion is to simultaneously optimise all of the information equations with respect to $\mathbf{x}$. Each information equation is considered optimum when the error is minimised, such that $\mathbf{f}^* \to \mathbf{f}(\mathbf{x})$. In terms of probability theory, we wish to find the $\mathbf{x}$ that maximises the probability of finding $\{\mathbf{f}_0(\mathbf{x}), \ldots, \mathbf{f}_k(\mathbf{x})\}$ given $\{\mathbf{f}_0^*, \ldots, \mathbf{f}_k^*\}$. This technique is known as Maximum Likelihood [3]. The mathematics of the statistical regularisation technique employed here is detailed in Appendix A.

Since, essentially we wish to minimise the error variance, Maximum Likelihood is one method that facilitates this. However, various other statistical regularisation techniques are equally applicable, and conclude with the same final "retrieval equation" forms (eqns (16) and (34)) [4] [5]. The choice of method depends on the scenario and information available [6] [7].

As described in detail in Appendix A, Maximum Likelihood can be applied as follows: By combining all information equations $\mathbf{f}_k(\mathbf{x})$, such that the errors are minimised, we are able to produce a formula for the optimum solution of the atmospheric variable required, $\mathbf{x}$ (see Appendix A.2);

$$\sum_{k=1}^{K}\left(\frac{d}{d\mathbf{x}}\{\mathbf{f}_k(\mathbf{x})-\mathbf{f}_k{}^*\}\right)\left(\hat{\mathbf{C}}_k{}^{-1}+(\hat{\mathbf{C}}_k{}^{-1})^T\right)\left(\mathbf{f}_k(\mathbf{x})-\mathbf{f}_k{}^*\right)=\mathbf{0}\,. \qquad \textbf{\textit{eqn(6)}}$$

where $\hat{\mathbf{C}}_k$ are the covariance matrices of the information equations.

When a specific application is applied, this equation can be easily manipulated into a retrieval equation. That is, the unknown vector $\mathbf{x}$ can be expressed as a function of the other terms and variables,

$$\mathbf{x}=\mathrm{fn}\left\{\mathbf{L}_{\mathrm{sensor}},\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}),\hat{\mathbf{J}},\mathbf{x0},\hat{\mathbf{C}}_{\mathrm{k}},\hat{\mathbf{B}}\right\}.$$

eqn(7)

The retrieval of the unknown vector $\mathbf{x}$ then becomes a search for reliable values of the terms in equation (7); the observed radiance $\mathbf{L}_{\mathrm{sensor}}$, the first guess profile $\mathbf{x0}$, the corresponding radiance $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ and its Jacobian $\hat{\mathbf{J}}$, and the covariance matrices $\hat{\mathbf{C}}_k$. This, in itself, is a complex and error prone procedure with assumptions, statistical data and atmospheric modelling packages as the main tools.

From this phase onward it is best to investigate atmospheric retrieval from the application-orientated point of view. In the following chapters we will apply the above mathematical retrieval basis to the cases of temperature, humidity, aerosol size distribution and refractive index retrieval. This will cover the particularities and irregularities of the parameters needed and hopefully give a clearer, better understanding of the abstract mathematics presented above.

3. Application for "Long-Wave Infrared" Sensors: Retrieval of Temperature and Humidity Profiles

3.1 Introduction

This application considers the radiation observed by a ground-based sensor, s0, directed with zenith angle θ towards the sky. The remote sensor will detect radiation from several sources, including that emitted from the atmosphere, the sun and any obstruction. All sources of radiation are attenuated as they pass through the remaining atmosphere, through processes of absorption and scattering. "The processes that affect radiation along the beam are scattering radiation out of the beam, absorption of radiation along the beam, multiple scattering of indirect, diffuse radiation into the beam, single scattering of direct solar radiation into the beam, and emission of infrared radiation into the beam." [8].

The constituents and physical condition of the atmosphere determine the significance and magnitude of the radiation processes within specific spectral regions. In the visible and short-wave infrared range, radiation in the atmosphere is predominantly effected by atmospheric absorption and the scattering of solar radiation into or out of the path of observation. In the long-wave infrared region, the processes of atmospheric absorption and emission, rather than scattering, are dominant. The ability of the atmospheric constituents to absorb and emit radiation is dependent on the temperature of the atmosphere and the specific wavebands over which we are sensing. For example, within the 8-12μm region, water vapour (or the water continuum) is the atmospheric constituent that dominantly effects the radiation. Thus, with the aim to retrieve both the temperature and humidity profiles of the atmosphere, one method is to consider the 8-12μm long-wave infrared radiance data from a remote sensor.

In the following sections we will construct simplified radiative transfer equations specifically for the long-wave infrared region. With this, we will briefly revisit the statistical analysis of the previous chapter and apply it directly to this scenario. Finally, we will analyse the application to remote identification of ground-based targets.

3.2 Mathematical Background

The first application of atmospheric retrieval to be considered involves solving for unknown temperature and humidity profiles. We will attempt to determine the quantity of water vapour and the effective temperature at any altitude in the atmosphere.

The primary atmospheric effects that are influenced by temperature and humidity are the absorption and emission of radiation by the atmospheric gases. The mass density of water in the air directly affects the amount of electromagnetic radiation that is absorbed by the atmosphere. Temperature, on the other hand, is a macroscopic measure of the random motion of gases and particles that compose the atmosphere.

In order to retrieve information about the humidity and temperature profiles, it is beneficial to investigate the radiance measured in a spectral region that is dominated by the processes of emission and absorption of radiation by atmospheric gases. In particular, this is served by sensing in the long-wave infrared region, 8-12μm. In this scenario, whilst the effects of aerosol scattering of radiation out of the path must be accounted for in the transmittance, the radiation observed from scattered solar radiation is negligible. (Scattering of solar radiation into the path contributes orders of magnitude *less* radiance than does atmospheric emission, in the 8-12μm band, according to MODTRAN execution [9]). Thus, it is possible to neglect the contribution of scattered radiation when constructing a radiative transfer equation.

The atmospheric constituents at any altitude will absorb and scatter out a percentage of the radiation introduced to it; will allow the remaining percentage of radiation to be transmitted onward; and also, will emit a degree of thermal radiation. The final radiance that is seen from a remote observer, looking either upwards or downwards, is the accumulated effect of the transmittance and emittance of the atmosphere on an initial radiance (*eg*. Earth, target, sun).

3.2.1 Radiative Transfer Equation

The radiative transfer equation describes the change in spectral radiance over the distance ds along a path (eqn(1)). For the long-wave infrared application, the RTE is,

$$dL(\lambda) = dL_{\text{emission}}(\lambda) - dL_{\text{scat out}}(\lambda) - dL_{\text{absorp}}(\lambda)$$
$$\textit{ie. } dL(\lambda) = dL_{\text{emission}}(\lambda) - dL_{\text{ext}}(\lambda)$$

eqn(8)

where $dL_{\text{ext}}(\lambda) = L(\lambda)\sigma_{\text{ext}}(\lambda)ds$ is the radiance absorbed and scattered out of the path by the atmosphere (atmospheric extinction), and $dL_{\text{emission}}(\lambda) = B(\lambda)\sigma_{\text{absp}}(\lambda)ds$ is the radiance emitted into the path by the atmosphere.

$\sigma_{\text{ext}}(\lambda)$ is the extinction coefficient (measures the loss of electromagnetic radiation due to absorption and scattering, per unit distance); and $B(\lambda)$ is the blackbody radiance of the atmosphere.

Let us define the angle θ as the observation zenith angle, $dz = \cos(\theta)ds$, where z is the altitude; and let us define the incremental optical depth as $d\tau_{\text{ext}} = -\cos(\theta)\sigma_{\text{ext}}ds$.

For down-welling radiation, optical depth is defined as,

$$\tau_{\text{ext}}(s) = \cos(\theta)\int_{\infty}^{s} \sigma_{\text{ext}}(\lambda, s')ds'.$$

Thus, the RTE (eqn(8)) becomes,

$$dL(\lambda) = \frac{1}{\cos(\theta)} L(\lambda)d\tau_{\text{ext}} + \frac{-1}{\cos(\theta)} B(\lambda)d\tau_{\text{ext}}.$$

In order to describe the observed radiance data as a function of the atmospheric processes, let us integrate the RTE above. For a ground-based sensor, integrating over the entire path length from space to $s0$ gives the radiance equation**,**

$$L_{\text{sensor}}(\lambda) = L_{\text{RTE}}(\lambda, s0) = L_{\text{initial}}(\lambda, \infty)\, e^{\frac{-\tau_{\text{tot}}(\lambda)}{\cos(\theta)}} + \frac{-1}{\cos(\theta)} \int_{\tau_{\text{tot}}(\lambda)}^{0} B(\lambda)\, e^{\frac{-\tau'}{\cos(\theta)}}\, d\tau' \qquad \textbf{\textit{eqn(9)}}$$

which is simply $L_{\text{sensor}} = L_{\text{initial}}\mathit{trans}_{\text{atmosphere}} + L_{\text{atmosphere}}$. ***eqn(10)***

The transmittance, $\mathit{trans}(\lambda)$, is defined as the fraction of radiation allowed to pass through a portion of the atmosphere, without being absorbed or scattered out. For the downwelling-radiation case (*eg*. ground sensor to space),

$$trans(\lambda,s) = \frac{L(\lambda,s)}{L_{\text{initial}}(\lambda,\infty)} = \frac{L_{\text{initial}}(\lambda,\infty)\, e^{-\frac{\tau(\lambda,s)}{\cos(\theta)}}}{L_{\text{initial}}(\lambda,\infty)} = \exp\left\{-\int_{\infty}^{s} \sigma_{\text{ext}}(\lambda,s')ds'\right\}. \quad \textbf{\textit{eqn(11)}}$$

If we were to position the sensor's line of sight (path) directly at the sun, then the initial radiation, $L_{\text{initial}}(\lambda)$, would be the initial solar radiation. Let us assume this is not the case in our scenario, so that there is no initial radiation and the sensor records only atmospheric effects. Thus,

$$L_{\text{RTE}}(\lambda,s0) = L_{\text{atm}}(\lambda) = \frac{-1}{\cos(\theta)}\int_{\tau_{\text{tot}}(\lambda)}^{0} B(\lambda)\, e^{\frac{-\tau'}{\cos(\theta)}} d\tau' = \int_{trans_{\text{tot}}(\lambda)}^{1} B(\lambda)\, dtrans\,. \quad \textbf{\textit{eqn (12)}}$$

The integrated RTE, radiance equation (eqn(12)), is now simplified as a function of blackbody atmospheric radiance and transmittance.

The analytical form of Planck's blackbody equation $B(T(s),\lambda)$, is well known and defined as a function of temperature and wavelength alone, and thus is a function of the altitude in so much as the temperature varies through the atmosphere.

The transmittance, $trans(\lambda,s)$, is not a well-behaved or differentiable function. The extinction coefficient $\sigma_{\text{ext}}(\lambda,s)$, from which it is derived, is dependent on the composition of the atmosphere at a particular height, and its corresponding extinction properties. The extinction coefficient and transmittance are directly dependent on the water composition or absolute humidity of the atmosphere at any altitude. The temperature is indirectly related to the transmittance, as a mutual consequence of the altitudinal composition. In an unfamiliar atmosphere the exact composition and properties of all elements in the atmosphere is unknown. The long-wave infrared waveband used for this retrieval is dominantly influenced by water vapour content and temperature, which enables us to use model approximations of the other constituents without too great an error or complications. Thus transmittance can be described by the temperature and humidity profiles of the atmosphere. However, since the extinction coefficients are ultimately only known through empirical observation (data tables), we do not have transmittance as a well-behaved, continuous function of temperature and humidity.

In summary, the radiance equation above is not presently in an invertible form. Transmittance is an ill-posed function of temperature and humidity, as well as various other factors that are unknown for the atmosphere of interest. We can approximate the other characteristics to an acceptable degree, but require further approximations before inversion retrieval can be performed.

3.2.2 Assuming a Layered Atmosphere

Consider the unknown atmosphere as structured with consecutive, homogeneous altitudinal layers. Each layer contributes to the extinction and emittance of radiation in the path to the sensor. It is through introduction of atmospheric layers (and linearisation) that we will solve the problem of ill-posed transmittance functions, and thus the retrieval of temperature and humidity for specific altitudes.

$$L_{\mathrm{RTE}}(\lambda, s0) = \frac{-1}{\cos(\theta)} \int_{\tau_{\mathrm{tot}}(\lambda)}^{0} B(\lambda, T(\tau'))\, e^{\frac{-\tau'}{\cos(\theta)}} d\tau'$$

Extraction of the unknown temperature and humidity profiles from the integral equation above is analytically unachievable. We do not have analytic equations for the transmittance or optical depth as functions of the unknown profiles. Empirical data tables, however, exist for the extinction coefficients under specific conditions. Therefore, if we consider the atmosphere to be homogeneous over chosen altitudinal intervals, we can establish values of optical depth for specific values of temperature, humidity and altitude, $\tau(T_i, \rho_i, \lambda, s)$. We consider optical depth rather than transmittance here, since it is proportional to altitude, and thus more accurately discretised with respect to altitude.

Therefore, let us firstly define the unknown temperature and humidity functions as atmospheric profiles in vector $\mathbf{x}$,

$$\mathbf{x} = \left[\mathbf{T}^{\mathrm{T}}, \boldsymbol{\rho}^{\mathrm{T}}\right]^{\mathrm{T}}$$

where $\mathbf{T} = [T(z_1), T(z_2), \ldots]^{\mathrm{T}}$ and $\boldsymbol{\rho} = [\rho(z_1), \rho(z_2), \ldots]^{\mathrm{T}}$,

and let us assume that the optical depth can be described by the temperature and water content of the atmosphere alone, $\tau(\lambda, z_i) \equiv \tau(\lambda, z_i, \mathbf{T}, \boldsymbol{\rho})$.

So that we can now describe the radiance equation as a discrete summation over atmospheric layers, as follows,

$$L_{\mathrm{RTE}}(\lambda, s0) \approx \sum_{i=1} \frac{-1}{\cos(\theta)} B(\lambda, \mathbf{T}_i) e^{\frac{-\tau(\mathbf{T}_i, \boldsymbol{\rho}_i)}{\cos(\theta)}} \Delta\tau(\mathbf{T}_i, \boldsymbol{\rho}_i),$$

eqn(13)

or simply,

$$L_{\mathrm{RTE}}(\lambda, s0) = \sum_{i=1} \Delta L_{\mathrm{emission}}(\lambda, z_i, \mathbf{T}, \boldsymbol{\rho})\, trans(\lambda, z_i, \mathbf{T}, \boldsymbol{\rho}).$$

eqn (14)

The radiance equation (eqn(14)) now presents the sensor observed radiance as constructed from the sum of the emitted radiation from each layer in the atmosphere (which are in turn transmitted through the rest of the atmosphere to the sensor).

Each atmospheric layer is composed of varying percentages of gases and particles, including water vapour. It is the thermal properties and condition of these constituents that determine the temperature at any altitude. The discretised radiance equation (eqn(14)) assumes homogeneity within the constructed layers of the atmosphere. For our calculations, therefore, there is an assumption that the temperature (and thus Planck's radiance) and the constituent concentrations are constant within each layer. This discretisation, then, is only valid for sufficiently small layers. Consideration as to the size of the layer must include the atmospheric conditions and the positioning. For example, layers closer to the ground will need to be narrower than those at higher altitudes, due to the relatively steep change in temperature with altitude near the Earth's surface.

3.2.3 "First guess" Temperature and Humidity Profiles

The blackbody radiance emitted by each atmospheric layer is a well-posed function of $T(z_i)$ and $\rho(z_i)$, however, the transmittance $trans(\lambda, z_i)$ and optical depth $\tau(\lambda, z_i)$ are not. An analytic statistical inversion of the current radiance equation (eqn(14)), then, is not possible.

One solution is to linearise the equation with a "first guess" of the atmospheric conditions. In this way, the transmittance for the "first guess" atmosphere can be empirically sought, and our equation becomes an explicit, invertible function of the unknown temperature and humidity vector.

Let us approximate the radiance equation about an initial profile, $\mathbf{x0} = [\mathbf{T0}^{\mathrm{T}}, \boldsymbol{\rho}\mathbf{0}^{\mathrm{T}}]^{\mathrm{T}}$, using a multivariate Taylor's expansion;

$$L_{\text{sensor}}(\lambda_j) \approx L_{\text{RTE}}(\lambda_j, \mathbf{x0}) + \sum_{n=1}^{N}\left(\left.\frac{\partial L_{\text{RTE}}(\lambda_j)}{\partial \mathbf{T}_n}\right|_{\mathbf{x0}} (\mathbf{T}_n - \mathbf{T0}_n) \right) + \sum_{p=1}^{P}\left(\left.\frac{\partial L_{\text{RTE}}(\lambda_j)}{\partial \boldsymbol{\rho}_p}\right|_{\mathbf{x0}} (\boldsymbol{\rho}_p - \boldsymbol{\rho}\mathbf{0}_p) \right) + \text{H.O.T.}$$

where $L_{\text{sensor}}(\lambda)$ is the observed data, and $L_{\text{RTE}}(\lambda, \mathbf{x0})$ is the radiance equation (eqn(14)) as a function of "first guess" temperature and humidity $\mathbf{x0}$.

In matrix form, the above linearised equation becomes,

$$\mathbf{L}_{\text{sensor}} - \mathbf{L}_{\text{RTE}}(\mathbf{x0}) \approx \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0})$$

where $\hat{\mathbf{J}}$ is the Jacobian of the radiance equation (eqn(14)),

$$\hat{\mathbf{J}}_{j,i} = \left.\frac{\partial L_{\text{RTE}}(\lambda_j)}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \qquad \textbf{\textit{eqn(15)}}$$

and $i = n + p$ is the number of the atmospheric layer being described, and j is the number of the radiance wavelength.

Hence we have a discretised linear equation that requires the observed total radiance, $\mathbf{L}_{\text{sensor}}$, and the radiance values of the atmosphere at varying altitudes for selected "first guess" atmospheric conditions of temperature and humidity. Now that we have an expression in the generic form of equation (4), as required in Chapter 2, we can investigate the inclusion of error and the other information equations and from thence, the statistical inversion.

3.2.4 Temperature and Humidity Profile Retrieval Equation

For the case in which we are required to retrieve temperature and humidity profiles, smoothing (Appendix B.3) is not necessary. Thus we only include two information equations in our minimisation; the linearised radiance equation above, and the "first guess" approximation of the profiles, $\mathbf{x0}$. By combining the information equations so that the errors are minimised, we are able to produce a formula for the optimum solution to the atmospheric parameter required, $\mathbf{x}$. Appendix A.2.1 has details of the minimisation technique used and the specific application to temperature and humidity profile retrieval.

By substituting $\mathbf{f}_0(\mathbf{x}) = \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ and $\mathbf{f}_1(\mathbf{x}) = \mathbf{x}$ into the minimisation equation in Chapter 2 (eqn(6)), as seen in Appendix A.2.1, we can rearrange and manipulate our minimisation equation into the form below.

This is now the referral equation by which we can calculate retrieved values for temperature and humidity,

$$\boxed{\mathbf{x} = \mathbf{x0} + \left(\hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \hat{\mathbf{J}} + \hat{\mathbf{C}}_{\mathrm{Ex}}^{-1}\right)^{-1}\ \hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \left(\mathbf{L}_{\mathrm{sensor}} - \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})\right)}$$

eqn(16)

where $\mathbf{x}$ is the unknown temperature and humidity profile; $\mathbf{L}_{\mathrm{sensor}}$ is the measured radiance from the sensor; $\mathbf{x0}$ is the approximate estimate; $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ is the radiance of this estimate; $\hat{\mathbf{J}}$ is the Jacobian (eqn(15)); and the $\hat{\mathbf{C}}$ are the covariance matrices of the errors, as described in Appendix B.2.

This completes the mathematical background of the atmospheric retrieval in the long-wave infrared region. We have developed a specific retrieval equation that can be used to solve for the temperature and humidity profiles of an unknown atmosphere (eqn (16)). From this stage onward, the specific application and scenario must be considered, and the use of comprehensive modelling packages becomes prominent. The following section will summarise the findings above and give a brief overview of the practicalities involved in its application.

3.3 Temperature and Humidity Retrieval: Summary and Practicalities

In summary, we consider the scenario in which we are ground sensing the radiance, at long-wave infrared wavelengths, which has been emitted and transmitted by the atmosphere. We are interested in retrieving values for the temperature and humidity of the atmosphere from this observed radiance data.

Due to a lack of a well-defined transmittance function, as previously explained, the spectral data from a remote sensor must be supplemented by a reasonable "first guess" of the temperature and humidity, from which we can extrapolate the true solution. An understanding of the errors involved in the measurement and the retrieval procedures is also necessary for accurate atmospheric retrieval.

Through statistical regularisation of the information available, the following equation can be created, via which we can retrieve the temperature and humidity of the atmosphere at consecutive altitudes.

$$\boxed{\mathbf{x} = \mathbf{x0} + \left(\hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \hat{\mathbf{J}} + \hat{\mathbf{C}}_{\mathrm{Ex}}^{-1}\right)^{-1}\ \hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \left(\mathbf{L}_{\mathrm{sensor}} - \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})\right)}$$

where,

$\mathbf{x}$ is the vector of unknown temperature and humidity variables to be retrieved,
$\mathbf{x} = [T(z_1), T(z_2), \ldots, T(z_N), \rho(z_1), \rho(z_2), \ldots, \rho(z_P)]^{\mathrm{T}}$;

$\mathbf{L}_{\mathrm{sensor}}$ is the vector of measured radiance values from the sensor,
$\mathbf{L}_{\mathrm{sensor}} = [L_{\mathrm{sensor}}(\lambda_1), L_{\mathrm{sensor}}(\lambda_2), \ldots, L_{\mathrm{sensor}}(\lambda_M)]^{\mathrm{T}}$;

$\mathbf{x0}$ is the vector of first guess approximations of the unknown $\mathbf{x}$,
$\mathbf{x0} = [T0(z_1), T0(z_2), \ldots, T0(z_N), \rho 0(z_1), \rho 0(z_2), \ldots, \rho 0(z_P)]^{\mathrm{T}}$;

$\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ is the vector of radiance created by simulating an atmosphere with $\mathbf{x0}$ profile, using eqn(14),
$\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) = [L_{\mathrm{RTE}}(\lambda_1, \mathbf{x0}), L_{\mathrm{RTE}}(\lambda_2, \mathbf{x0}), \ldots, L_{\mathrm{RTE}}(\lambda_M, \mathbf{x0})]^{\mathrm{T}}$;

$\hat{\mathbf{J}}$ is the Jacobian matrix of the radiance equation, eqn(15). The derivatives are calculated with respect to the unknown variables and then calculated for $\mathbf{x0}$,

$$\hat{\mathbf{J}}_{j,n} = \left.\frac{\partial L_{\mathrm{RTE}}(\lambda_j)}{\partial \mathbf{T}_n}\right|_{\mathbf{x0}} \quad \text{and} \quad \hat{\mathbf{J}}_{j,p+N} = \left.\frac{\partial L_{\mathrm{RTE}}(\lambda_j)}{\partial \boldsymbol{\rho}_p}\right|_{\mathbf{x0}} ;$$

for $j = 1 \ldots M$ wavelengths, $n = 1 \ldots N$ temperature altitudinal layers, and $p = 1 \ldots P$ pressure altitudinal layers;

and $\hat{\mathbf{C}}$ are the covariance matrices that account for inherent errors in the process,
$\hat{\mathbf{C}}_{\mathrm{El}} = \hat{\mathbf{I}}\,[C_{\mathrm{El}}(\lambda_1), \ldots, C_{\mathrm{El}}(\lambda_M)]^{\mathrm{T}}$ and
$\hat{\mathbf{C}}_{\mathrm{Ex}} = \hat{\mathbf{I}}\,[C_{\mathrm{Ex}}(T(z_1)), \ldots, C_{\mathrm{Ex}}(T(z_N)), C_{\mathrm{Ex}}(\rho(z_1)), \ldots, C_{\mathrm{Ex}}(\rho(z_P))]^{\mathrm{T}}$.

We initially assume that the covariance matrices are diagonal (that is, errors are independent). However, iteration during the retrieval process can allow for variation, as will be explained in section 3.3.1.2.

Establishing the "optimal" inversion equation (eqn(16)) is the first step in the retrieval procedure. Following this, the individual components must be correctly calculated and the incorporated errors must be estimated to an acceptable degree. This involves the composition of non-trivial matrices and many strictures imposed on the processes involved, as will be discussed below. (More detailed descriptions of the Jacobian and Covariance matrices are presented in Appendices B.1 and B.2.)

3.3.1 Practicalities

3.3.1.1 Atmospheric Models

For the atmosphere under observation, the exact gas and aerosol composition is unknown. Atmospheric modelling packages, like MODTRAN, offer several models that represent various 'typical' atmospheres. These model atmospheres are composed of specific combinations and quantities of water, carbon dioxide, ozone, pollution, *etc.* and refer to average climatological temperature profiles. The optical properties of the atmospheric constituents have been empirically tested for each model in MODTRAN and the extinction coefficients are data-based within the program.

The "first guess" temperature and humidity profiles, $\mathbf{x0}$, can be calculated through atmospheric simulation packages, such as MODTRAN and FASCODE [10], or taken from meteorological data available for the region. Depending on the sensing scenario, an appropriate model can be chosen to represent the atmosphere. The temperature and humidity profiles of this model atmosphere can then be used as the "first guess" profile $\mathbf{x0}$. The linearisation of the radiance equation that occurs in the retrieval calculations requires this first guess to be adequately close to the true value of $\mathbf{x}$. This can lead to difficulties if the location that is being observed is foreign and unmodelled. One method of calculation of initial guess profiles from ground based sensors, as developed by Theriault *et al*. [11] [12], involves manipulation of radiance data collected at highly absorbent frequencies *eg.* for CO_2. Alternatively, statistical or climatological profiles can be used as an appropriate "first guess" [13].

From the initial approximation of the unknown, $\mathbf{x0}$, the values for the virtual radiance $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ and the Jacobian matrix $\hat{\mathbf{J}}$ must be calculated. Unlike the observed radiance, the radiance that corresponds to the first guess profile cannot be measured directly. A suitable RTE (eqn(14)) must be used to calculate $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ from the `virtual' atmospheric profile $\mathbf{x0}$. Options for the user to input their own temperature and gas profiles are available in MODTRAN or FASCODE, and it is through this that values for the virtual radiance, $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$, can be created. The inclusion of aerosol extinction and the effect of other particulate and gaseous constituents in the accurate formation of the RTE and retrieval work are often heavily based on *a priori* model atmospheres such as those in MODTRAN.

Similarly, the Jacobian of the radiance equation, $\hat{\mathbf{J}}$, requires a simulation package (or data-base) to model the coefficients of an unknown atmosphere. As previously explained, we cannot form an analytic function of the transmittance with respect to temperature and humidity. Thus direct calculation of the derivatives of the radiance equation is impossible. The Jacobian matrix, therefore, is constructed by approximating the derivatives by assessing the effect of small linear changes in the temperature to the observed radiance. The radiance is calculated for the "first guess" profile and the subdominant constituents are approximated by the appropriate atmospheric model, in order to create estimates of the transmittance as required in the formula. More detailed explanation of this process is provided in Appendix B.1.

3.3.1.2 Newtonian Iteration of the Solution

The form of our retrieval equation (eqn(16)) is such that an iterative process can be applied to acquire more accurate results. We can substitute the resultant $\mathbf{x}$ back into the equation as the new $\mathbf{x0}$ value and recalculate. This practice, however, may lead to misleading results if the Jacobian $\hat{\mathbf{J}}$ and first guess radiance $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ are not also updated with the new $\mathbf{x0}$. The majority of the convergence towards the real solution occurs within the first iteration. The covariance matrix $\hat{\mathbf{C}}_{\mathrm{Ex}}$, also, can be iteratively calculated with statistical regularisation. In this way, a better adjustment for error, which accounts for possible correlations, can be acquired. For further information on this approach to the covariance matrices see Rodgers [14].

3.3.1.3 Sources of Error

The accuracy of $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ relies on the suitability of the modelling software program used and the accuracy of the "first guess". The errors inherent in the calculation of $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ therefore come from two sources; "first guess" error variance of the temperature and humidity profiles, and error in the model representation approximations of all other atmospheric contributions. The first of these errors is accounted for in the "first guess" error covariance matrix of the retrieval equation, $\hat{\mathbf{C}}_{\mathrm{Ex}}$. This allows the solution to vary within defined limits. The error in the atmospheric model RTE is hopefully diminished by the appropriate choice of spectral range. The dominant radiative processes in the long-wave infrared range should be summarised by the temperature and humidity profile of the atmosphere. The scenario and specific circumstances of the application will define whether this is accurate enough for the project.

The Jacobian matrix, $\hat{\mathbf{J}}$, is limited by the errors above, and also by the practical approximation that is required for its calculation. The analytic derivatives of the RTE cannot be calculated due to the discrete nature of the transmittance. Thus the "small linear change" of the radiance equation with respect to $\mathbf{x}$, as explained in Appendix B.1, will unavoidably produce error. This is one source of error that must be considered when constructing the radiance error covariance matrix of the retrieval equation, $\hat{\mathbf{C}}_{\mathrm{El}}$. This matrix attempts to account for the errors in the first RTE information equation, which includes the error involved in the linearisation of the RTE and in any of the terms. The radiance error covariance matrix also must account for the error in observational measurement. This should be the known variance error of the sensor.

3.4 Atmospheric Retrieval for Target Detection

One motivation for the retrieval of atmospheric characteristics is the need for better representation of atmospheric influence in remote, passive target detection. We will now investigate the scenario of a remote hyperspectral sensor collecting radiance data, in the long-wave infrared region, from a target on the ground. The result of this is to hopefully determine the characteristics and identify this target, through consequent calculation of its emissivity and temperature.

Previous study by the IEOS group at DSTO Edinburgh (South Australia), has indicated that the accurate detection of remote targets, in this scenario, requires adequate representation of the atmospheric characteristics [13]. It was found that even 1% improvement of the temperature profiles and 5% improvement of the humidity profile gained substantially better results for retrieval of temperature and emissivity of a target. It is with this motivation that achieving more accurate temperature and humidity profiles of the atmosphere between the target and sensor is considered beneficial.

The scenario presented here differs from the previous section in that we are now interested in the upwelling radiation observed by a remote sensor. The radiative transfer equation must accommodate the inclusion of an initial radiance and adjust for this new orientation.

3.4.1 Modelling Upwelling Radiative Transfer

The application described in this chapter, "Application to Retrieval of Temperature and Humidity Profiles", is constructed with the aim towards characterising the atmosphere without reference to an initial emitter. The scenario was described as a ground-based sensor directed into the sky. Let us now re-adjust our perspective so that we have a sky-based sensor directed at the Earth's surface. The first problem that must be dealt with, then, is to investigate the remotely observed radiance over ground surface that is known. The method for doing this is dependent on the specific scenario of the experiment.

In section 3.2.1 we presented the observed sensor radiance as a function of the initial radiation, atmospheric radiation and atmospheric transmittance, $L_{\text{sensor}} = L_{\text{initial}} trans_{\text{atmosphere}} + L_{\text{atmosphere}}$.

Let us present this now in the appropriate orientation- for upwelling radiation as observed by a remote sky-based sensor at height $z(S)$;

$$L_{\text{sensor}}(\lambda, S) = L_{\text{earth}}(\lambda, s0)\, trans_{\text{atm}}^{\uparrow}(\lambda) + L_{\text{atm}}^{\uparrow}(\lambda).$$

where $L_{\text{atm}}^{\uparrow}(\lambda)$ and $trans_{\text{atm}}^{\uparrow}(\lambda)$ are up-welling atmospheric radiation and transmittance. The path of the radiation is now between the sensor S and the ground $s0$, rather than space. Total transmittance is now defined as, $trans^{\uparrow}(\lambda, S) = \exp\left\{-\int_{s0}^{S} \sigma_{\text{ext}}(\lambda, s')ds'\right\}$.

3.4.1.1 Ground Surface Radiance

In the previous sections the initial radiation term was not applicable. We now consider the case in which the initial radiation of the Earth is observed and thus included in our radiance equation. The initial Earth radiance is a result of the emitted thermal radiation of the Earth (and target) and the reflected solar and atmospheric radiation from the Earth's surface,

$$L_{\text{earth}}(\lambda) = L_{\text{emitted}}(\lambda) + L_{\text{reflected}}(\lambda)$$
$$L_{\text{earth}}(\lambda, s0) = \varepsilon_{\text{earth}}(\lambda) B(\lambda, T_{\text{earth}}) + \rho_{\text{earth}}(\lambda)\left(L^{\downarrow}_{\text{solar}}(\lambda, s0) + L^{\downarrow}_{\text{atm}}(\lambda, s0)\right). \qquad \textbf{\textit{eqn(17)}}$$

The emissivity, $\varepsilon(\lambda)$, is a measure of how effectively a material can emit radiation; defined as the ratio of emitted radiation from the source (Earth) to the emitted radiation from a blackbody of the same temperature. It is specific to the material investigated and a function of wavelength. Blackbody radiation $B(\lambda, T)$ is solely a function of wavelength and temperature. The reflectivity, $\rho(\lambda)$, of a solid opaque object in thermal equilibrium with its surroundings is $\left(1-\varepsilon(\lambda)\right)$. $L^{\downarrow}_{\text{solar/atm}}(\lambda, s0)$ is the downwelling radiance, contributed by the sun or the atmosphere, as measured at the Earth's surface, $s0$.

In order to retrieve information about the atmosphere from the upwelling radiation measured at the sensor, we firstly need to know the emissivity and temperature of the ground surface. This leaves us with a circular problem; the purpose of target detection analysis is to retrieve (ground) target emissivity and temperature, which are themselves necessary for the retrieval equation.

Atmospheric retrieval is a useful tool in target detection for acquiring a better approximation of the atmosphere than a "first guess" simulated model. Let us assume, in the following section, that there is a region of ground surface sufficiently close to the target, which has a recognisable emissivity signature. By considering the atmospheric characteristics retrieved nearby the target, this will hopefully give a better approximation of the atmosphere in the line of sight to the target.

3.4.2 Retrieval of "Surrounding" Atmospheric Characteristics

Let us attempt to retrieve the atmospheric characteristics by analysing the radiance observed in the area surrounding the target, for which the surface material is familiar. The simplest case of this would be if the ground surface were approximately a blackbody ($\varepsilon = 1$) or greybody, for example, the ocean, which has almost constant emissivity [14]. Other scenarios include familiar ground surfaces for which the emissivity is known, for example concrete or desert. In order for the assumption of *a priori* information about the emissivity, it may be necessary for all the suitable data from the surrounding area to be collated and used as an average radiance measure of the average surrounding atmosphere and surface properties.

The average temperature of the surrounding ground surface, $T(s0)$, is then included as an element of the unknown vector, $\mathbf{x}$, with extra elements being added to the first guess vector, $\mathbf{x0}$, and Jacobian, $\hat{\mathbf{J}}$. This is not done with the final aim to find an accurate temperature for the average surface $T(s0)$, but to ensure the use of an accurate ground temperature in the retrieval of the average *atmospheric* properties of the surrounding area. This scenario requires Earth radiance terms, with known emissivity, to be included in the relevant RTEs that are needed to calculate $\mathbf{L}_{\text{RTE}}(\mathbf{x0})$ and $\hat{\mathbf{J}}$. With this information, the retrieval equation below, unchanged from the previous section, can be used to retrieve the temperature and humidity profiles for the atmosphere surrounding the target;

$$\mathbf{x} = \mathbf{x0} + \left(\hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \hat{\mathbf{J}} + \hat{\mathbf{C}}_{\mathrm{Ex}}^{-1}\right)^{-1}\ \hat{\mathbf{J}}^{\mathrm{T}}\ \hat{\mathbf{C}}_{\mathrm{El}}^{-1}\ \left(\mathbf{L}_{\text{sensor}} - \mathbf{L}_{\text{RTE}}(\mathbf{x0})\right)$$

where now

$$L_{\text{RTE}}(\lambda, S, \mathbf{x}) = \left(\varepsilon_{\text{earth}}(\lambda) B(\lambda, T_{\text{earth}}) + (1-\varepsilon_{\text{earth}}(\lambda))\left(L_{\text{solar}}^{\downarrow}(\lambda, s0) + L_{\text{atm}}^{\downarrow}(\lambda, s0)\right)\right) trans_{\text{atm}}^{\uparrow}(\lambda) + L_{\text{atm}}^{\uparrow}(\lambda, S)$$

eqn(18)

for $L_{\text{atm}}^{\uparrow/\downarrow}(\lambda) = \sum_{j=s0} \Delta L_{\text{emission}}^{\uparrow/\downarrow}(\lambda, z_j, \mathbf{T}, \boldsymbol{\rho}) trans^{\uparrow/\downarrow}(\lambda, z_j, \mathbf{T}, \boldsymbol{\rho})$

and $L_{\text{solar}}^{\downarrow}(\lambda, s0) = F_{\text{solar}}(\lambda)\ trans^{\downarrow}(\lambda, \mathbf{T}, \boldsymbol{\rho})$, (see section 4.2.2.1).

The atmospheric properties of temperature and humidity retrieved here can then be used to determine approximate transmittance and atmospheric radiance values for the line of sight of the sensor to target. These can then be used to calculate the emissivity and temperature of the ground target.

This method will invariably add more uncertainty to the retrieval of the atmospheric temperature and humidity. The ground surface radiance is the dominant contributor in the long-wave infrared range that we are examining. The inclusion of correspondingly large Jacobian terms, due to this, will cause less sensitive retrieval of atmospheric profiles. Thus this approach cannot retrieve the atmospheric characteristics with as much accuracy as the case where the surrounding ground temperature is known.

3.4.3 Alternative Technique

Accurate modelling of the atmosphere is essential for good estimation and retrieval of ground characteristics, and thus target identification. As such, any improvement on the assumed or "first guess" atmosphere model is worth investigating. The accuracy of retrieval via statistical inversion is dependent on the information available and the scenario involved, as is presented above.

In regards to target detection for unknown or foreign Earth surfaces, the inversion method can facilitate the retrieval of atmospheric characteristics for only limited scenarios. An alternative approach is to use a numerical optimisation method. This involves repeatedly forward-modelling the scenario with different atmospheres until the "best" model solution is found. An example of this technique is given in [17] and [18]. This approach is best suited to the classification of targets, rather than accurate retrieval of atmospheric characteristics. Thus the choice of retrieval method is dependent on the final aim of the project.

4. Application for "Solar" Sensors: Retrieval of Aerosol Size Distribution and Refractive Index

4.1 Introduction

In the long-wave infrared region, the temperature and water content of the atmosphere can be retrieved due to the dominant influence of absorption and emission on the radiation in an observation path. In the solar spectral region, however, the effects of atmospheric thermal emission are surpassed by the influence of scattering of solar radiation into and out of the path, by the atmospheric constituents. Aerosol size and refractive index influence the degree of scattering of solar radiation by an atmospheric particle. Thus through manipulation of the observed atmospheric radiance in the visible and short-wave infrared spectral regions, we can potentially gain information about the atmospheric aerosol size distribution and refractive index in the sensor line of sight.

The atmospheric constituents at any altitude will scatter the radiation incident on it; will allow the remaining percentage of radiation to be transmitted onward; and also, will emit a negligible degree of thermal radiation in this spectral region. The final radiance that is seen from a remote observer, looking either upwards or downwards, is the accumulated effect of the transmittance and scattering of the atmosphere on the initial radiance (*eg.* from a target). The complications with including the reflection off the Earth's surface and accounting for this in any retrieval, suggests that downward looking retrieval via inversion techniques is unlikely to give accurate or stable results [19]. Particularly in the solar region, the influence of the Earth's surface dominates and renders the retrieval of aerosol characteristics almost impossible.

Let us then assume that we are observing the atmosphere along a path that is looking upwards, with a ground-based sensor and the primary radiance source from the sun. In this case we have two scenarios to consider, involving Sun and Sky radiances.

4.2 Mathematical Background

4.2.1 Aerosol Size Distribution and Refractive Index

The aerosol size distribution is a measure of the number of particles (~ 0.001 - 100 μm), in a unit volume of atmosphere, which are of a certain radii size or fit within a specific radii bin.

The function $n(r) = \dfrac{dN(r)}{d\log r}$ is the aerosol size distribution that we wish to solve for. The function $N(r)$ is the number concentration (#/cm^3), which is the number of particles in a radius size bin per unit volume of air. The total number concentration of particles, then, is the sum over all size bins, $N_{\mathrm{T}} = \sum_r N(r)$. There are four continuous size distributions that are commonly used to describe an aerosol sample; the lognormal, the power law, Marshall-Palmer, and the modified gamma distributions [20]. We will deal mainly with the first of these and will thus henceforth refer only to the lognormal size distribution of aerosols. The appropriate use of other functions should be considered with reference to the project application.

The lognormal aerosol size distribution function is,

$$n(r) = \sum_i \frac{dN(r)}{d\log r} = \sum_i \frac{N_{\mathrm{T}}{}^i}{\sqrt{2\pi}(\log\sigma_r{}^i)} \exp\left\{ \frac{-\left(\log r - \log \bar{r}^i\right)^2}{2(\log\sigma_r{}^i)^2} \right\} \qquad \textbf{\textit{eqn(19)}}$$

where $\bar{r}^i$ are the mean aerosol radii for the population data, $\log\bar{r}^i$ are the means of lognormal distributions, and $\log\sigma_r{}^i$ are the standard deviations of the distributions.

The complex refractive index, m, of the atmosphere is a measure of the ability of the atmospheric particles to absorb and scatter radiation, $m = \eta + i\chi$. It is a function of the wavelength, $m = m(\lambda)$, and thus not independent of the observed sensor radiance $L_{\mathrm{sensor}}(\lambda)$. The index can be retrieved simultaneously with the aerosol size distribution at a fixed wavelength [21] [22], or, with more difficulty, as a function of wavelength [23] [24].

As with the retrieval of temperature and humidity, the retrieval of both aerosol size distribution and refractive index is achieved via reference to an appropriate radiative transfer equation (RTE).

4.2.2 Radiative Transfer Equation

The scenario to be considered for this application involves a ground-based electro-optic sensor that observes radiation in the solar region (0.4 – 1.5μm) along a path at angle θ, with sun zenith θ_{s} and scattering angles Ω. With this orientation and spectral region, we can construct a RTE that neglects Earth radiation and atmospheric thermal emission.

The change in spectral radiance over the distance ds along a path, gives the RTE

$$dL(\lambda,\Omega) = dL_{\mathrm{scat\ in}}(\lambda,\Omega) + dL_{\mathrm{multi\ scat}}(\lambda) - dL_{\mathrm{absp}}(\lambda) - dL_{\mathrm{scat\ out}}(\lambda)$$

where Ω is the scattering angle, corresponding to the chosen path and sun orientations.

Let us consider two scenarios, one in which the sensor is directed at the sun and one in which it is not. In the first case, the sensor will collect radiation that is coming directly from the sun. The atmospheric particles will absorb and scatter a proportion of this radiation out of the path, with the remaining being transmitted directly to the sensor. A percentage of the solar radiation that is not directly in the line of sight of the sensor will also be scattered into the path through multiple scattering processes. In the second case, when the sensor is not directed at the sun, the radiance collected will primarily come from solar radiation that is scattered by atmospheric particles into the sensor line of sight or `path'. There is no direct sun radiation component.

These two scenarios use the above RTE, with varying emphasis on the terms involved, to gain information about the atmosphere. We will see how this can be combined to retrieve aerosol size distribution and refractive index. Let us call these two cases direct sun radiation and sky radiation respectively.

4.2.2.1 Direct Sun Radiance RTE

For this scenario we have the path zenith angle of the sensor, θ, equal to that of the sun zenith angle, θ_s. In this case, the scattering of surrounding radiance into the path is negligible compared to the direct solar radiation that will be transmitted (with extinction) directly to the observer. The appropriate approximation to the RTE includes the effects of absorption and scattering extinction of the initial solar radiation, at various wavelengths.

The change in spectral radiance over the distance ds along a beam is, $dL(\lambda) = -dL_{\text{scat out}}(\lambda) - dL_{\text{absp}}(\lambda) + \text{o}(dL_{\text{multi scat}}(\lambda))$; that is, $dL(\lambda) = -L(\lambda)\sigma_{\text{scat out}}(\lambda) - L(\lambda)\sigma_{\text{absp}}(\lambda) + \text{o}(dL_{\text{multi scat}}(\lambda))$.

The extinction of radiation from the sensor's path in the atmosphere is determined by absorption and scattering of radiation by gases and aerosols. The total extinction coefficient and optical depth can be expressed as $\sigma_{\text{ext}}(\lambda) = \sigma_{\text{scat out}}(\lambda) + \sigma_{\text{absp}}(\lambda)$ and $\tau_{\text{ext}}(\lambda) = \tau_{\text{scat out}}(\lambda) + \tau_{\text{absp}}(\lambda)$, respectively.

Therefore, the RTE for direct sun scenario becomes,

$$dL(\lambda) \approx -L(\lambda)\sigma_{\text{extinction}}(\lambda)ds .$$

With integration from space to the ground, the direct sun RTE defines the radiance observed from a ground based sensor at $s0$,

$$L_{\text{sensor}}^{\text{SUN}}(\lambda) = L_{\text{RTE}}^{\text{SUN}}(\lambda, s0) = F_{0,\text{solar}}(\lambda)e^{-\int_{\infty}^{s0}\sigma_{\text{ext}}(\lambda,s)ds} = F_{0,\text{solar}}(\lambda)e^{\frac{-\tau_{\text{ext}}^{\text{tot}}(\lambda)}{\cos(\theta)}}$$

Expressed simply,

$$L_{\text{sensor}}^{\text{SUN}} = F_{0,\text{solar}} trans_{\text{atmosphere}} .$$

As the initial solar irradiance $F_{0,\text{ solar}}$ is known for specific frequencies [25], the direct sun radiance is often stated by the total atmospheric optical depth, $\tau_{\text{RTE}}^{\text{SUN}}(\lambda, s0) = \tau_{\text{ext}}^{\text{tot}}(\lambda)$, instead of $L_{\text{RTE}}^{\text{SUN}}(\lambda, s0)$. That is;

$$\tau_{\text{sensor}}^{\text{SUN}}(\lambda) = \tau_{\text{RTE}}^{\text{SUN}}(\lambda, s0) = -\cos(\theta)\log_{e}\left(\frac{L_{\text{sensor}}^{\text{SUN}}(\lambda)}{F_{0,\text{solar}}(\lambda)}\right). \qquad \textbf{\textit{eqn(20)}}$$

With this optical depth data, the direct sun radiance equation can be formed;

$$\tau_{\text{sensor}}^{\text{SUN}}(\lambda) = \tau_{\text{RTE}}^{\text{SUN}}(\lambda, s0) = \tau_{\text{ext}}^{\text{aerosol}}(\lambda, s0) + \tau_{\text{ext}}^{\text{gas}}(\lambda, s0) .$$

eqn(21)

The optical depth $\tau(\lambda)$ is a measure of the "penetrability" of an atmosphere to a sensor. It is an exponential function of the transmittance, which can be used to measure the ability of the atmosphere to transmit radiation that is emitted from a remote source. The various processes of absorption and scattering by gases and aerosols are the main influences that affect the optical depth of an atmosphere. Amongst others, it can be shown that the optical depth is a function of the unknown variables- the aerosol size distribution and refractive index.

Before further defining the relationship between optical depth and aerosol size distribution and refractive index, let us investigate the RTE of sky radiance, to draw a comprehensive picture.

4.2.2.2 Sky Radiance RTE

Consider the second scenario, in which the path observation angle, θ, is not the same as the sun zenith angle, θ_s. The upward looking observer, then, is not directly in the path of any incident radiation source, and the only significantly contributing factor is the sun radiation that is scattered into the path and then transmitted (with extinction) through the remaining atmosphere, to the sensor. The sky radiance RTE is,

$$dL(\lambda, \Omega) = -dL_{\text{ext}}(\lambda) + dL_{\text{scat in}}(\lambda, \Omega) + \text{o}(dL_{\text{multi scat}}(\lambda)) . \qquad \textbf{\textit{eqn(22)}}$$

The single scatter contribution, $dL_{\text{scat in}}$, is the percentage of the solar radiance from the sun that is transmitted to a point on the observation path, $s*$, and then scattered into the direction of the sensor;

$$dL_{\text{scat in}}(\lambda, \Omega) = L_{\text{solar}}(\lambda) trans(\text{Sun to s*}) \times (\text{\% scattered into path}) ds .$$

That is,

$$dL_{\text{scat in}}(\lambda, \Omega) = F_{0,\text{solar}}(\lambda) e^{\frac{-\tau_{\text{ext}}(\lambda, s)}{\cos(\theta_s)}} \frac{1}{4\pi} \left[\sigma_{\text{scat}}^{\text{gas}}(\lambda) P^{\text{gas}}(\lambda, \Omega) + \sigma_{\text{scat}}^{\text{aero}}(\lambda) P^{\text{aero}}(\lambda, \Omega) \right] ds$$

where $P^{\text{gas / aero}}$ are the scattering Phase Functions for gas or aerosol constituents, as will be defined in the following section.

The extinction term, dL_{ext}, in the RTE (eqn(22)), accounts for the absorption and scattering of radiation out of the remaining path to the observer, $s*$ to $s0$. The RTE is then integrated over every scattering point along the path, $s* = s$, to account for all contributions to the final observed radiance.

Substituting the extinction and single scattering terms into equation (22), where $\varpi(\lambda)=\dfrac{\sigma_{\text{scat}}^{\text{total}}(\lambda)}{\sigma_{\text{ext}}^{\text{total}}(\lambda)}$ is the single scattering albedo, the transformation of the RTE with respect to $d\tau$ gives;

$$dL(\lambda,\Omega)=L(\lambda,\Omega)\frac{d\tau(s)}{\cos(\theta)}+-F_0(\lambda)\,e^{\frac{-\tau_{\text{ext}}}{\cos(\theta_S)}}\frac{1}{4\pi}\varpi(\lambda)\left[\sum_{\text{X=gas, aero}}\frac{\sigma_{\text{scat}}^{\text{X}}}{\sigma_{\text{scat}}^{\text{gas + aero}}}P^{\text{X}}(\lambda,\Omega)\right]\frac{d\tau(s)}{\cos(\theta)}\,.$$

eqn(23)

The RTE, in this form, is not an integrable function of optical depth or path length. In order to integrate the RTE and describe the observed radiance as a function of the unknown aerosol characteristics, then, we must apply several assumptions, as detailed in the following sections.

4.2.3 Assuming a Homogeneous Atmosphere

Consider an atmosphere that appears, from a ground sensor, to be optically equivalent to our scenario but is in fact composed only of a single homogeneous atmospheric layer, of arbitrary height. So that, whilst the final optical depths are equivalent for this and our real scenario, the coefficients of this new scenario are now independent of the altitude. By replacing our atmosphere with one such as this, we are able to integrate the sky RTE analytically.

The optical depth of the atmosphere is defined as the integral of the coefficient σ(s) over the path length; $\tau_{\text{absp/ ext/ scat}}(s)=\int_s^\infty -\cos(\theta)\sigma_{\text{absp/ ext/ scat}}(s')ds'$.

If we instead consider an equivalent atmosphere that is homogeneous within an imagined total path length, s to $\bar{S}$, then the corresponding "uniform" coefficients, $\bar{\sigma}$, are constant over that path. The optical depth can then be alternatively expressed as, $\tau_{\text{absp/ ext/ scat}}(s)=-\cos(\theta)\,\bar{\sigma}_{\text{absp/ ext/ scat}}(\bar{S}-s)$.

For a ground based sensor, let us define the arbitrary path length $\bar{S}$, such that $\tau_{\text{absp/ ext/ scat}}(s0)=\bar{\sigma}_{\text{absp/ ext/ scat}}$.

For the sky radiative transfer equation, this means that the single scattering albedo, $\bar{\varpi}$, the scattering mixing ratios (per unit volume) $\bar{\sigma}_{\text{scat}}^{\text{X}}/\bar{\sigma}_{\text{scat}}^{\text{gas +aero}}$ and the aerosol phase function P^{aero} are constant over, and thus independent of, the optical depth of the atmosphere.

With this assumption, we can integrate the sky RTE from the top of the atmospheric path to the ground sensor along the line of sight, with respect to optical depth. Such that equation (23) becomes,

$$L_{\text{sensor}}^{\text{SKY}}(\lambda,\Omega) = L_{\text{RTE}}^{\text{SKY}}(\lambda,\Omega,s0) = F_0 \frac{\cos(\theta_S)}{\cos(\theta_S)-\cos(\theta)} \left(e^{\frac{-\tau_{\text{ext}}^{\text{tot}}(\lambda)}{\cos(\theta_S)}} - e^{\frac{-\tau_{\text{ext}}^{\text{tot}}(\lambda)}{\cos(\theta)}} \right) \frac{1}{4\pi} \bar{\varpi}(\lambda) P^{\Theta}(\lambda,\Omega)$$

eqn(24)

where $$P^{\Theta}(\lambda,\Omega) = \frac{\tau_{\text{scat}}^{\text{gas}}(\lambda)}{\tau_{\text{scat}}^{\text{total}}(\lambda)} P^{\text{gas}}(\lambda) + \frac{\tau_{\text{scat}}^{\text{aerosol}}(\lambda)}{\tau_{\text{scat}}^{\text{total}}(\lambda)} P^{\text{aerosol}}(\lambda,\Omega) \quad .$$ ***eqn(25)***

This form of the sky radiance equation is presented in terms of optical depth, rather than coefficients, since we can express the single scattering albedo and the scattering mixing ratios as follows,

$$\bar{\varpi}(\lambda) = \frac{\bar{\sigma}_{\text{scat}}^{\text{total}}(\lambda)}{\bar{\sigma}_{\text{ext}}^{\text{total}}(\lambda)} = \frac{\tau_{\text{scat}}^{\text{total}}(\lambda)}{\tau_{\text{ext}}^{\text{total}}(\lambda)} \quad \text{and} \quad \frac{\bar{\sigma}_{\text{scat}}^{\text{gas/ aerosol}}(\lambda)}{\bar{\sigma}_{\text{scat}}^{\text{total}}(\lambda)} = \frac{\tau_{\text{scat}}^{\text{gas/ aerosol}}(\lambda)}{\tau_{\text{scat}}^{\text{total}}(\lambda)} \quad .$$ ***eqn(26)***

The assumption of homogeneity is in part justified by the fact that the spectral regions over which we are sensing are dominated by scattering rather than thermal effects. The ability of particles to scatter solar radiation is a function of the number and size of the particles. The majority of particles, especially larger aerosols, are located within the lower altitudes of the atmosphere (the boundary layer). With the orientation of our sensor as ground based, looking upwards, the radiance scattered into the line of sight will predominantly be the result of the particles in the lower altitudes of the atmosphere. The atmosphere itself is obviously not vertically homogeneous, however, the ground-based radiance can be formulated as if it is, using "uniform" coefficients.

Thus we now have the integrated sun and sky RTEs described as functions of the radiance observed at the sensor (eqns (21), (24)). Before we can construct the relationship between the observed radiance and the unknowns, we need to define the various factors involved.

4.2.4 Assuming Discretised Aerosol Radii Bins

Presently, we have sun and sky radiance equations that describe the observed sensor data $L_{\text{sensor}}(\lambda)$ as a function of phase functions P^{X}, optical depth $\tau_{\text{ext}}(\lambda)$ and/or extinction coefficients $\sigma_{\text{ext}}(\lambda)$. If we wish to retrieve values for the aerosol size distribution and refractive index from the radiance equations, we firstly need to express these variables in terms of their constituents. In doing so we will see, in the following subsections, that these variables themselves are not well-posed and can only be described in terms of discrete radius values.

In order to obtain well-posed radiance functions for inversion, we need to create discrete vectors to describe the aerosol size distribution and refractive index. Instead of a continuous distribution of atmospheric particles, let us construct logarithmically spaced radii "bins", in order to transform the aerosol size distribution into a vector format. The refractive index is a complex function of wavelength and thus is represented by both its real (Re) and imaginary (Im) parts, in its vector form.

Let us define the unknown aerosol size distribution and refractive index as vector $\mathbf{x}$,

$$\mathbf{x} = \left[\mathbf{n}^{\mathrm{T}}, \mathbf{m}^{\mathrm{T}}\right]^{\mathrm{T}}$$

where $\mathbf{n} = [n(r_1), n(r_2), ..., n(r_N)]^{\mathrm{T}}$ and

$\mathbf{m} = [\mathrm{Re}(m(\lambda_1)), ..., \mathrm{Re}(m(\lambda_M)), \mathrm{Im}(m(\lambda_1)), ..., \mathrm{Im}(m(\lambda_M))]^{\mathrm{T}}$.

4.2.4.1 Radius-binned Aerosol Coefficients and Optical Depths

The extinction and scattering coefficients, $\sigma_{\mathrm{ext/scat}}$, measure the loss of radiation at any point along the atmospheric path due to the presence of gases and aerosols. For aerosols, they are defined as the product of the respective cross-sections and the aerosol size distribution. This size distribution will vary through the atmosphere, which is often represented by a series of 'sum of lognormal' functions. Our assumption of vertical homogeneity requires us to treat this as a vertical column of arbitrary height with a single aerosol size distribution function, $n(r)$.

$$\tau^{\mathrm{aero}}_{\mathrm{ext/scat}}(\lambda, s0) = \bar{\sigma}^{\mathrm{aero}}_{\mathrm{ext/scat}}(\lambda) = \int \beta_{\mathrm{ext/scat}}(\lambda) dN(r) = \int \beta_{\mathrm{ext/scat}}(\lambda) \frac{dN(r)}{d\log r} d(\log r)$$

ie.
$$\tau^{\mathrm{aero}}_{\mathrm{ext/scat}}(\lambda, s0) = \int \beta_{\mathrm{ext/scat}}\, n(r)\, d(\log r) \qquad \textbf{\textit{eqn(27)}}$$

where r is the aerosol radius, $\beta_{\mathrm{ext/scat}}$ is the extinction/scattering cross-section for a single particle, and the function $n(r)$ is the aerosol size distribution that we wish to solve for.

The cross-section $\beta_{\mathrm{ext/scat}}$ is defined as the product of the geometric cross-section of a single particle with the extinction/scattering efficiency, Q_{ext}. The efficiency Q_{ext} is a complex function of the wavelength, particle radius and refractive index, *m*. The formula for Q_{ext} is obtained from Mie theory of particle scattering [26], [27]. However, it can only be calculated for specific values of radii. That is, the efficiency Q_{ext} is not an integrable function of radius. As such, the aerosol cross-section $\beta_{\mathrm{ext/scat}}$ is not integrable and the aerosol coefficient cannot be expressed analytically as a function of radius and aerosol size distribution. It is necessary, therefore, to discretise the aerosol coefficients with respect to radius. Such that,

$$\tau^{\mathrm{aero}}_{\mathrm{ext/scat}}(\lambda, \mathbf{n}, \mathbf{m}) \approx \sum_{i\ =\text{radius bin } 1} \beta_{\mathrm{ext/scat}}(\lambda, r_i, m).n(r_i)\Delta(\log r_i)\,. \qquad \textbf{\textit{eqn(28)}}$$

The total extinction optical depth, $\tau^{\mathrm{total}}_{\mathrm{ext}}(\lambda)$, is available as observed spectral data through manipulation of the direct sun RTE, eqn(20). With knowledge and approximations of the molecular component of the total optical depth, we can use this data to present the direct sun total optical depth as a function of aerosol size distribution and refractive index. Such that the direct sun radiance equation becomes,

$$\boxed{\tau_{\text{RTE}}^{\text{SUN}}(\lambda, s0, \mathbf{n}, \mathbf{m}_\lambda) = \tau_{\text{ext}}^{\text{gas}}(\lambda, s0) + \sum_{i\text{ =radius bin 1}} \beta_{\text{ext}}(\lambda, r_i, m(\lambda)).n(r_i)\Delta(\log r_i)}$$

eqn(29)

4.2.4.2 Radius-binned Aerosol Phase Function

The way in which a particle interacts with electromagnetic radiation depends on the relative size of the particle radius to the radiation wavelength. For gas species, the wavelength is much larger than the particle radius $\lambda >> r$ and the interaction falls into the Rayleigh regime [28]. This regime defines the Phase function of such constituents to be a function of scattering angle alone, $P_{\text{gas}} = \text{fn}(\Omega)$.

For aerosol species however, the wavelength of solar radiation can be the same magnitude as the particle radius $\lambda \sim r$ and the interaction is described by the Mie regime. In the Mie regime, the Phase function of an optically homogeneous atmosphere is defined as,

$$P_{\text{aero}}(\lambda, \Omega) = \frac{\lambda^2}{2\pi} \frac{1}{\bar{\sigma}_{\text{scat}}^{\text{aero}}(\lambda, \mathbf{n}, \mathbf{m})} \int Amp(\lambda, \Omega, r, m(\lambda))\, n(r)\, d\log r$$

where $Amp(\lambda, \Omega, r, m)$ is a complex function of the wavelength, particle radius and refractive index. The formula for $Amp(\lambda, \Omega, r, m)$ can be derived from the Mie theory of particle scattering [29], [30]. Similar to the formation of the efficiency factor, however, the Amp function can only be calculated for specific values of the radius. That is, it is not an analytically integrable function, and thus not in a form suitable for analytic inversion.

Again, by referring to radii "bins", we can discretise the phase function as follows;

$$P_{\text{aero}}(\lambda, \Omega, \mathbf{n}, \mathbf{m}) = \frac{\lambda^2}{2\pi} \frac{1}{\tau_{\text{scat}}^{\text{aero}}(\lambda, \mathbf{n}, \mathbf{m})} \sum_{i\text{ = radii bin 1}} Amp(\lambda, \Omega, r_i, m(\lambda))\, n(r_i)\, \Delta\log r_i\ .$$

eqn(30)

With the aerosol phase function and the aerosol optical depth as functions of **n** and **m**, we can now express the sky radiance equation as,

$$\boxed{L_{\text{RTE}}^{\text{SKY}}(\lambda, \Omega, s0, \mathbf{m}, \mathbf{n}) = \frac{F_0(\lambda)\cos(\theta_s)}{\cos(\theta_s) - \cos(\theta)} \left(e^{\frac{-\tau_{\text{ext}}^{\text{tot}}(\lambda, s0, \mathbf{m}, \mathbf{n})}{\cos(\theta_s)}} - e^{\frac{-\tau_{\text{ext}}^{\text{tot}}(\lambda, s0, \mathbf{m}, \mathbf{n})}{\cos(\theta)}} \right) \frac{1}{4\pi} \varpi(\lambda, \mathbf{m}, \mathbf{n}) P^{\Theta}(\lambda, \Omega, \mathbf{m}, \mathbf{n})}$$

where $P^{\Theta}(\lambda,\Omega,\mathbf{m},\mathbf{n}) = \dfrac{\tau_{\text{scat}}^{\text{gas}}(\lambda)}{\tau_{\text{scat}}^{\text{total}}(\lambda,\mathbf{m},\mathbf{n})} P^{\text{gas}}(\lambda) + \dfrac{\tau_{\text{scat}}^{\text{aerosol}}(\lambda,\mathbf{m},\mathbf{n})}{\tau_{\text{scat}}^{\text{total}}(\lambda,\mathbf{m},\mathbf{n})} P^{\text{aerosol}}(\lambda,\Omega,\mathbf{m},\mathbf{n})$.

eqn(31)

We now have equations for the aerosol coefficients and phase functions as discretised functions of wavelength, radius, scattering angle and the unknown variables- aerosol size distribution and refractive index (eqn(29), eqn(31)). With knowledge of the molecular components, as given below, we have constructed the observed sun and sky radiances as functions of the unknown atmospheric characteristics. It is these functions that will be the primary information equations in the statistical regression and retrieval.

4.2.5 Assuming Molecular Characteristics

For practical application, the observed radiance frequencies are chosen in solar bands that are known not to include molecular absorption. Gaseous absorption within the solar spectral region is known to be minimal, thus this is easily accomplished; $\bar{\sigma}_{\text{absorption}}^{\text{gas}}(\lambda) \approx 0$. Alternatively, various authors have accommodated for the presence of ozone O_3 and nitrogen dioxide NO_2 in the atmosphere [31], [32].

The molecular scattering, as described by the Rayleigh regime, is not dependent on the size of the gas species, as they are more than an order of magnitude smaller than the solar wavelengths that they scatter. An approximation of the molecular optical depth can be given via knowledge of the ground-level pressure for specific wavelengths in the solar region [33]. According to Hansen and Travis (1974), this relationship is,

$$\tau_{\text{scat out}}^{\text{gas}}(\lambda) = 0.008569\lambda^{-4}(1 + 0.0113\lambda^{-2} + 0.00013\lambda^{-4})\frac{P}{P_0}$$

where λ is the wavelength in μm, P is the atmospheric pressure in mb, $P_0 = 1013.25\ \text{mb}$ is the standard pressure.

4.2.6 "First guess" Aerosol Size Distribution and Refractive Index

Similarly to the application for temperature and humidity retrieval, inversions of the integrated RTEs presented in equations (29) and (31) are not possible. Even though in this scenario we do have well-defined functions of the unknowns, the complex summation nature of their structure makes them impossible to manipulate. Thus, again, it is recommended that we linearise the RTEs around an estimate of the unknowns and construct the appropriate information equations.

Let us approximate the observed radiance about an 'initial guess' profile, $\mathbf{x0}$, using a multivariate Taylor's expansion.

$$L_{\text{sensor}}(\lambda,\Omega) = L_{\text{RTE}}(\lambda,\Omega,\mathbf{x}) \approx L_{\text{RTE}}(\lambda,\Omega,\mathbf{x0}) + \sum_{n=1}^{N}\left(\left.\frac{\partial L_{\text{RTE}}(\lambda,\Omega)}{\partial \mathbf{n}_n}\right|_{\mathbf{x0}}(\mathbf{n}_n - \mathbf{n0}_n)\right)$$
$$+ \sum_{k=1}^{M}\left(\left.\frac{\partial L_{\text{RTE}}(\lambda,\Omega)}{\partial \mathbf{m}_k}\right|_{\mathbf{x0}}(\mathbf{m}_k - \mathbf{m0}_k)\right) + \text{H.O.T.}$$

In matrix form, the linearised equations are,

$$\mathbf{L}^{\text{SKY}}_{\text{sensor}} - \mathbf{L}^{\text{SKY}}_{\text{RTE}}(\mathbf{x0}) \approx \hat{\mathbf{J}}^{\text{SKY}}(\mathbf{x}-\mathbf{x0}) \quad \text{and} \quad \boldsymbol{\tau}^{\text{SUN}}_{\text{sensor}} - \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}}(\mathbf{x0}) \approx \hat{\mathbf{J}}^{\text{SUN}}(\mathbf{x}-\mathbf{x0})$$

eqn(32)

where $\hat{\mathbf{J}}^{\text{SUN/SKY}}$ are the Jacobians of the radiance equations (eqn(29) and eqn(31)),

$$\hat{\mathbf{J}}^{\text{SUN}}_{j,i} = \left.\frac{\partial \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \quad \text{and} \quad \hat{\mathbf{J}}^{\text{SKY}}_{j,i} = \left.\frac{\partial \mathbf{L}^{\text{SKY}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \qquad \textbf{\textit{eqn(33)}}$$

and where $j = 1\ldots(M+P)$ is the number of wavelengths and scattering angles, and $i = 1\ldots(N+2M)$ is the number of radii bins plus wavelength elements.

Hence we have two discretised linear equations (eqns(32)) that require the observed radiance and the radiance values of the atmosphere for selected "first guess" atmosphere conditions of $\mathbf{n}$ and $\mathbf{m}$. Now that the radiative transfer equations are expressed in the generic form of equation (4) as required in section 2.2.2, we can investigate the inclusion of the other information equations and from thence, the statistical inversion.

4.2.7 Retrieval Equation for Aerosol Size Distribution and Refractive Index

For the case in which we are required to retrieve aerosol size distribution and refractive index, there are four information equations to consider: Radiance and optical depth as the real data; and "first guess" and smoothing as the virtual information.

By combining the information equations so that the errors are minimised, we are able to produce a formula for the optimum solution to the atmospheric parameter required, $\mathbf{x}$. Appendix A.2.2 has information of the minimisation technique used and the specific application to aerosol size distribution and refractive index retrieval.

This is now the referral equation by which we can calculate retrieved values for aerosol size distribution and refractive index;

$$\boxed{\begin{gathered}\mathbf{x} = \mathbf{x0} + \left(\left(\hat{\mathbf{J}}_{\text{SUN}}{}^{\text{T}}\,\hat{\mathbf{C}}_{\text{Elsun}}{}^{-1}\hat{\mathbf{J}}_{\text{SUN}}\right) + \left(\hat{\mathbf{J}}_{\text{SKY}}{}^{\text{T}}\,\hat{\mathbf{C}}_{\text{Elsky}}{}^{-1}\hat{\mathbf{J}}_{\text{SKY}}\right) + \left(\hat{\mathbf{C}}_{\text{Ex}}{}^{-1}\right) + \left(\hat{\mathbf{B}}^{\text{T}}\hat{\mathbf{C}}_{\text{Ex}}{}^{-1}\hat{\mathbf{B}}\right)\right)^{-1} \times \\ \left(\left(\hat{\mathbf{J}}_{\text{SUN}}{}^{\text{T}}\,\hat{\mathbf{C}}_{\text{Elsun}}{}^{-1}\left(\boldsymbol{\tau}^{\text{SUN}}_{\text{sensor}} - \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}}(\mathbf{x0})\right)\right) + \left(\hat{\mathbf{J}}_{\text{SKY}}{}^{\text{T}}\,\hat{\mathbf{C}}_{\text{Elsky}}{}^{-1}\left(\mathbf{L}^{\text{SKY}}_{\text{sensor}} - \mathbf{L}^{\text{SKY}}_{\text{RTE}}(\mathbf{x0})\right)\right) - \left(\hat{\mathbf{B}}^{\text{T}}\hat{\mathbf{C}}_{\text{Eb}}{}^{-1}\hat{\mathbf{B}}\,\mathbf{x0}\right)\right)\end{gathered}}$$

eqn(34)

where $\mathbf{x}$ is the unknown aerosol size distribution and refractive index; $\mathbf{L}_{\text{sensor}}$, $\boldsymbol{\tau}_{\text{sensor}}$ are the measured radiances from the sensor; $\mathbf{x0}$ is the approximate estimate; $\mathbf{L}_{\text{RTE}}(\mathbf{x0})$, $\boldsymbol{\tau}_{\text{RTE}}(\mathbf{x0})$ are the radiances of this estimate; $\hat{\mathbf{J}}$ are the Jacobians of the radiance equations (29) and (31); and $\hat{\mathbf{C}}$ are the covariance matrices of the errors, as described in Appendix B.2.

4.3 Aerosol Size Distribution and Refractive Index Retrieval: Summary and Practicalities

In summary; we consider the scenario in which we are ground-sensing solar radiance at various wavelengths and scattering angles, that has been influenced by the intervening atmosphere. We are interested in retrieving values for the aerosol size distribution at specific radii values and the refractive index at specific wavelengths.

As has been previously explained, the spectral data from a remote sensor is not sufficient for this problem. We must supplement the data with *a priori* or statistical information; for example, a "first guess" of the distribution and index, from which we can extrapolate the true solution. We also require an understanding of the errors involved in the measurement and the retrieval procedures, as presented in the preceding sections.

Through statistical regularisation of the information available, the following equation can be obtained, via which we can retrieve the aerosol size distribution and refractive index for a vector of radii and wavelengths.

$$\boxed{\begin{aligned}\mathbf{x} = \mathbf{x0} + \left(\left(\hat{\mathbf{J}}_{\text{SUN}}{}^{\text{T}}\hat{\mathbf{C}}_{\text{Elsun}}{}^{-1}\hat{\mathbf{J}}_{\text{SUN}}\right) + \left(\hat{\mathbf{J}}_{\text{SKY}}{}^{\text{T}}\hat{\mathbf{C}}_{\text{Elsky}}{}^{-1}\hat{\mathbf{J}}_{\text{SKY}}\right) + \left(\hat{\mathbf{C}}_{\text{Ex}}{}^{-1}\right) + \left(\hat{\mathbf{B}}^{\text{T}}\hat{\mathbf{C}}_{\text{Ex}}{}^{-1}\hat{\mathbf{B}}\right)\right)^{-1} \times \\ \left(\left(\hat{\mathbf{J}}_{\text{SUN}}{}^{\text{T}}\hat{\mathbf{C}}_{\text{Elsun}}{}^{-1}\left(\boldsymbol{\tau}^{\text{SUN}}_{\text{sensor}} - \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}}(\mathbf{x0})\right)\right) + \left(\hat{\mathbf{J}}_{\text{SKY}}{}^{\text{T}}\hat{\mathbf{C}}_{\text{Elsky}}{}^{-1}\left(\mathbf{L}^{\text{SKY}}_{\text{sensor}} - \mathbf{L}^{\text{SKY}}_{\text{RTE}}(\mathbf{x0})\right)\right) - \left(\hat{\mathbf{B}}^{\text{T}}\hat{\mathbf{C}}_{\text{Eb}}{}^{-1}\hat{\mathbf{B}}\,\mathbf{x0}\right)\right)\end{aligned}}$$

where,

$\mathbf{x}$ is the vector of unknown aerosol size distribution and refractive index variables to be retrieved,
$\mathbf{x} = [n(r_1),\ldots,n(r_N),\mathrm{Re}\left(m(\lambda_1)\right),\ldots,\mathrm{Re}\left(m(\lambda_M)\right),\mathrm{Im}\left(m(\lambda_1)\right),\ldots,\mathrm{Im}\left(m(\lambda_M)\right)]^{\text{T}}$;

$\mathbf{L}_{\text{sensor}}$ is the vector of measured sky radiance values from the sensor,
$\mathbf{L}_{\text{sensor}} = [L_{\text{sensor}}(\lambda_1,\Omega_1), L_{\text{sensor}}(\lambda_2,\Omega_1),\ldots,L_{\text{sensor}}(\lambda_M,\Omega_1), L_{\text{sensor}}(\lambda_1,\Omega_2),\ldots,L_{\text{sensor}}(\lambda_M,\Omega_P)]^{\text{T}}$
$\boldsymbol{\tau}_{\text{sensor}}$ is the vector of measured direct sun optical depth values from the sensor,
$\boldsymbol{\tau}_{\text{sensor}} = [\tau_{\text{sensor}}(\lambda_1), \tau_{\text{sensor}}(\lambda_2),\ldots,\tau_{\text{sensor}}(\lambda_M)]^{\text{T}}$;

$\mathbf{x0}$ is the vector of first guess approximations of the unknown $\mathbf{x}$,
$\mathbf{x0} = [n0(r_1),\ldots,n0(r_N),\mathrm{Re}\left(m0(\lambda_1)\right),\ldots,\mathrm{Re}\left(m0(\lambda_M)\right),\mathrm{Im}\left(m0(\lambda_1)\right),\ldots,\mathrm{Im}\left(m0(\lambda_M)\right)]^{\text{T}}$;

$\mathbf{L}_{\text{RTE}}(\mathbf{x0})$ is the vector of sky radiance created by simulating an atmosphere with $\mathbf{x0}$ profile, using eqn(31),

$\mathbf{L}_{\text{RTE}}(\mathbf{x0}) = [L_{\text{RTE}}(\lambda_1, \Omega_1, \mathbf{x0}), \ldots, L_{\text{RTE}}(\lambda_M, \Omega_1, \mathbf{x0}), L_{\text{RTE}}(\lambda_1, \Omega_2, \mathbf{x0}), \ldots, L_{\text{RTE}}(\lambda_M, \Omega_P, \mathbf{x0})]^{\text{T}}$

$\boldsymbol{\tau}_{\text{RTE}}(\mathbf{x0})$ is the vector of direct sun optical depth created by simulating an atmosphere with $\mathbf{x0}$ profile, using eqn(29),

$\boldsymbol{\tau}_{\text{RTE}}(\mathbf{x0}) = [\tau_{\text{RTE}}(\lambda_1, \mathbf{x0}), \ldots, \tau_{\text{RTE}}(\lambda_M, \mathbf{x0})]^{\text{T}}$;

$\hat{\mathbf{J}}$ are the Jacobian matrices of the radiance equations (eqn(29) and eqn(31)). The derivatives are calculated with respect to the unknown variables and then calculated for $\mathbf{x0}$,

$$\hat{\mathbf{J}}^{\text{SUN}}_{j,i} = \left.\frac{\partial \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \quad \text{and} \quad \hat{\mathbf{J}}^{\text{SKY}}_{j,i} = \left.\frac{\partial \mathbf{L}^{\text{SKY}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}}$$

with $j = 1 \ldots M * P$ frequency by scattering angle elements and $i = 1 \ldots N + 2 * M$ radii bins and frequency elements;

and $\hat{\mathbf{C}}$ are the covariance matrices that account for inherent errors in the process,

$\hat{\mathbf{C}}_{\text{El}} = \hat{\mathbf{I}}\,[C_{\text{El}}(\lambda_1, \Omega_1), \ldots, C_{\text{El}}(\lambda_M, \Omega_P)]^{\text{T}}$ and

$\hat{\mathbf{C}}_{\text{Ex}} = \hat{\mathbf{I}}\,[C_{\text{Ex}}(\mathbf{n}_1), \ldots, C_{\text{Ex}}(\mathbf{n}_N), C_{\text{Ex}}(\mathbf{m}_1), \ldots, C_{\text{Ex}}(\mathbf{m}_{2M})]^{\text{T}}$.

We initially assume that the covariance matrices are diagonal. However, iteration during the retrieval process can allow for variation, as previously explained in section 3.3.1.2.

4.3.1 Practicalities

4.3.1.1 Atmospheric Models

Unlike the application of temperature and humidity retrieval, the variables in the radiative transfer equations that depend on the unknown aerosol characteristics are not empirically derived. That is, we have calculable equations for the aerosol coefficients and phase function. Though these equations are not continuous or simple, with the discretisation of the RTE (with respect to radii) we have a series of equations with aerosol size distribution specifically defined. The consequence of this is that it is possible to find the analytic derivative of the radiance equation with respect to aerosol size distribution **n.** This is also true, but less easily accomplished, for the refractive index **m.** Thus the Jacobian matrices required in the retrieval equation above can be obtained (Appendices B.1.2 and B.1.3).

The possible problems with this approach include the accuracy of the RTE used to represent the atmospheric processes. The radiative transfer equations given in the sections above outline a general approach to the solar waveband sensing scenario, with approximations made in order to create the retrieval equation. However, more accurate representations of the RTE can be attained by using atmospheric modelling software. The choice to use the analytic derivatives to create the Jacobian matrices, or to use the "small change" Δ approach given in temperature and humidity application, is dependent on the specific circumstances. For example; how accurately the molecular contributions can be measured.

Similarly, the first guess radiance $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ can be calculated via forward modelling in atmospheric software. Unlike the application to temperature and humidity retrieval, however, MODTRAN does not facilitate the input of new aerosol size distribution and refractive index specifically.

4.3.1.2 Sources of Error and Alternatives

The retrieval equation itself, in this application, will need to be dealt with carefully in the calculations. The matrices, especially the Jacobians, if unchecked, can tend towards extremely large-valued elements. The inversion of the term required in equation (34) then, which includes the Jacobians, can often lead to singularities. Careful inclusion of an appropriate covariance matrix $\hat{\mathbf{C}}_{\mathrm{Ex}}$ can reduce this possibility. Various techniques for mathematically managing the collected data and retrieval algorithms are presented in Dubovik and King [34]. These include referring to the radii in terms of logarithmic variables, and expressing the aerosol size distribution as a volume distribution. Supplementing this, statistical techniques for confining the inversion term, in the formation of the relevant matrices, can be applied [35].

The retrieval of the refractive index, $\mathbf{m}$, is somewhat more complicated than that of size distribution. This is due to the fact that $m(\lambda)$ is a complex function of the coefficients and phase function, and is dependent on the wavelength and thus not independent of the observed radiance spectra. Consequently, many applications of this retrieval will treat the refractive index as a constant, as this approach allows more easily calculated Jacobians and does not require techniques to make the solution distinguishable from noise. The paper by Romanov *et al.* [36] gives a novel approach to the retrieval problem. It attempts to retrieve refractive index as a function of frequency and uses solar aureole observations (*i.e.* forward scattered light around the sun disk, which is primarily due to the scattering by aerosols) to simplify the RTE. The use of solar aureole is not unique, but the retrieval of observation angle to make the RTE more accurate, is.

In regards to these options, the chosen form in the retrieval of aerosol size distribution and refractive index is dependent on the scenario, information available and results required. The retrieval of aerosol characteristics, from "solar" sensors, can ultimately be used to aid the accurate modelling of the atmosphere in a region, or to aid the processes of ground-based target detection.

5. Conclusion

Passive electro-optic remote sensing can enable the retrieval of the temperature profile, the humidity profile, aerosol size distribution and the refractive index of the atmosphere. This report has attempted to present a generic design for atmospheric retrieval, via statistical inversion, for the specific application to sensors operating in the long-wave infrared and solar spectral wavebands.

The inversion algorithm is applied to radiative transfer equations, which have been constructed using suitable mathematical approximations, assumptions and *a priori* information. The specific models of radiative transfer are given for both of these scenarios as a basic guide, but do not encompass the complexity of the processes that are occurring. With this mathematical foundation, however, statistical analysis of the retrieval equations is accessible.

The inversion of the radiance equations is not a well-defined problem and thus must be solved via statistical techniques and regularisation. Introduction of a "first guess" of the unknown atmospheric characteristics redefines the problem as an attempt to gain a better solution to established atmospheric models or statistical *a priori* data. The accuracy of the results, then, is dependent on the error analysis and appropriate modelling of the atmosphere being considered.

The culmination of radiance data collected for both long-wave infrared and solar sensors could ultimately be used in correlation, to divulge information of the gaseous, particulate and physical condition of the atmosphere. This information, available in the temperature profile, humidity profile, aerosol size distribution and refractive index, gives a more comprehensive exposition of the atmosphere. The applications of this for the Australian Defence Organisation involve improved atmospheric models for Australian conditions, and more accurate atmospheric compensation in target detection algorithms. To pursue these ends, the continuation of research by DSTO in atmospheric retrieval is recommended.

This report was written with the aim to provide a framework for atmospheric retrieval via inversion, for a variety of scenarios. This framework can be extrapolated to include phenomena such as clouds in the long-wave infrared scenario, and applications such as identification of sky-borne targets. The specific project and required outcomes, and the availability of *a priori* information, will determine the mode and execution of the atmospheric retrieval. Understanding of the assumptions and processes behind the algorithms used to achieve this is vital for accurate variable representation, and ultimately, for reliable solutions to the atmospheric characteristics we wish to retrieve.

The purpose of this report was the elucidation of the underlying mathematics and assumptions in the development of a unified, generic description of atmospheric retrieval. A following report will utilise these tools in application to simulated and experimental data from DSTO scenarios, with consideration for the specific conditions present.

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Appendix A: Statistical Regularisation

A.1. Maximum Likelihood Method

In Chapter 2, section 2.3.3, the information equations are given in the generic form,

$$\mathbf{f}_k(\mathbf{x}) = \mathbf{f}_k * + \mathbf{E}_k,$$

where $k = \{0,1,2,\ldots K\}$, $\mathbf{f}_k(\mathbf{x})$ is the true value of the function with the true $\mathbf{x}$ value, $\mathbf{f}_k *$ is the data that is available or observed, and $\mathbf{E}_k$ is the uncertainty or error.

The aim of using the Maximum Likelihood method is to combine all data, both real and virtual in our scenarios, to gain the best estimate of the unknown vectors. That is, we wish to maximise the conditional probability of finding $\mathbf{f}(\mathbf{x})$ given $\mathbf{f}*$; $\mathrm{P}\{\mathbf{f}_1(\mathbf{x}),\mathbf{f}_2(\mathbf{x}),\ldots,\mathbf{f}_K(\mathbf{x}) \mid \mathbf{f}_1*,\mathbf{f}_2*,\ldots,\mathbf{f}_K*\}$.

There are a few assumptions that need to be made in order to do this: Firstly, that all information equations are independent of each other; and secondly, that the errors are random, uncorrelated and normalised. If sufficient data is recorded, then the errors, if unbiased, will come from a Normal distribution [37]. Using these assumptions enables us to construct the conditional probability above as a Gaussian probability density function;

$$\mathrm{P}\{\mathbf{f}_k(\mathbf{x}) \mid \mathbf{f}_k*\} \sim \exp\left\{\frac{-1}{2}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)^{\mathrm{T}} \hat{\mathbf{C}}_k^{-1}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)\right\}$$

where $\hat{\mathbf{C}}_k$ are the covariance matrices of the information functions.

And since, $\mathrm{P}\{\mathbf{f}_1(\mathbf{x}),\mathbf{f}_2(\mathbf{x}),\ldots,\mathbf{f}_K(\mathbf{x}) \mid \mathbf{f}_1*,\mathbf{f}_2*,\ldots,\mathbf{f}_K*\} = \prod_k \mathrm{P}\{\mathbf{f}_k(\mathbf{x}) \mid \mathbf{f}_k*\}$, this implies

$$\mathrm{P}\{\mathbf{f}_1(\mathbf{x}),\mathbf{f}_2(\mathbf{x}),\ldots,\mathbf{f}_K(\mathbf{x}) \mid \mathbf{f}_1*,\mathbf{f}_2*,\ldots,\mathbf{f}_K*\} \sim \exp\left\{\frac{-1}{2}\sum_k\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)^{\mathrm{T}} \hat{\mathbf{C}}_k^{-1}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)\right\}.$$

In order to maximise the conditional probability, we need to maximise the exponential equation above. This is accomplished by minimising the absolute of the index of the exponential equation; that is, the weighted error variance.

A.2. Retrieval Equations

Essentially, we need to minimise the weighted error variance of the information equations. In the simplest terms, the local solution can be found as follows:

Minimising $\sum_{k=0}^{K}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)^{\mathrm{T}}\hat{\mathbf{C}}_k^{-1}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)$ with respect to $\mathbf{x}$, implies

$$\frac{d}{d\mathbf{x}}\left\{\sum_{k=0}^{K}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)^{\mathrm{T}}\hat{\mathbf{C}}_k^{-1}\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right)\right\} = 0 \quad \text{and}$$

$$\sum_{k=0}^{K}\left(\frac{d}{d\mathbf{x}}\{\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\}\right)\left(\hat{\mathbf{C}}_k^{-1} + (\hat{\mathbf{C}}_k^{-1})^{T}\right)\left(\mathbf{f}_k(\mathbf{x}) - \mathbf{f}_k*\right) = 0\,. \qquad \textit{eqn(35)}$$

In order to extract the unknown vector $\mathbf{x}$ from the above equation, the particular form of the information equations, for the application involved, are required.

A.2.1 Application 1: Temperature and Humidity Retrieval Equations

Firstly, let us examine Application 1; the retrieval of temperature and humidity profiles, $\mathbf{x} = [\mathbf{T}^{\mathrm{T}}, \boldsymbol{\rho}^{\mathrm{T}}]^{\mathrm{T}}$.

Since, in equation (15), we converted the temperature and humidity radiance equation into the general form as described in Chapter 2 (eqn (4)), we can consequently include error terms and present the resulting linearised equation as our first information equation, $\mathbf{L}_{\mathrm{sensor}} = \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}\left(\mathbf{x} - \mathbf{x0}\right) \pm \mathbf{El}$; so that,

$$\mathbf{f}_0{}^* = \mathbf{L}_{\mathrm{sensor}} \quad \text{and} \quad \mathbf{f}_0(\mathbf{x}) = \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}\left(\mathbf{x} - \mathbf{x0}\right),$$

where $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ and $\hat{\mathbf{J}}$ are calculated from the temperature and humidity radiance equation (eqn(14)).

The second information equation involves the error in the "first guess", $\mathbf{x0} = [\mathbf{T0}^{\mathrm{T}}, \boldsymbol{\rho}\mathbf{0}^{\mathrm{T}}]^{\mathrm{T}}$ as stated in the Chapter 2.3.2, $\mathbf{x0} = \mathbf{x} \pm \mathbf{Ex}$; so that,

$$\mathbf{f}_1{}^* = \mathbf{x0} \quad \text{and} \quad \mathbf{f}_1(\mathbf{x}) = \mathbf{x}.$$

For the retrieval of temperature and humidity profiles, smoothing is not necessary. Thus we only need to include these two information equations in the minimisation. By combining all information equations $\mathbf{f}_k(\mathbf{x})$ such that the errors are minimised, we are able to produce a formula for the optimum solution to the atmospheric parameter required $\mathbf{x}$ in equation (35) above. Let us now input these information equations into equation (35) and manipulate to retrieve $\mathbf{x}$.

Firstly, $\dfrac{d}{d\mathbf{x}}\left\{\mathbf{f}_0(\mathbf{x}) - \mathbf{f}_0{}^*\right\} = \dfrac{d}{d\mathbf{x}}\left\{\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) - \mathbf{L}_{\mathrm{sensor}}\right\} = \hat{\mathbf{J}}$, and

$\dfrac{d}{d\mathbf{x}}\left\{\mathbf{f}_1(\mathbf{x}) - \mathbf{f}_1{}^*\right\} = \dfrac{d}{d\mathbf{x}}\left\{\mathbf{x} - \mathbf{x0}\right\} = \hat{\mathbf{I}}$.

So that, equation (35) becomes;

$$\hat{\mathbf{J}}^{\mathrm{T}}\left(\hat{\mathbf{C}}_{\mathrm{El}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{El}}{}^{-1})^{\mathrm{T}}\right)\left(\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}\left(\mathbf{x} - \mathbf{x0}\right) - \mathbf{L}_{\mathrm{sensor}}\right) + \hat{\mathbf{I}}\left(\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1})^{\mathrm{T}}\right)\left(\mathbf{x} - \mathbf{x0}\right) = \mathbf{0}.$$

Let us assume here that the errors are uncorrelated, such that the covariance matrices are diagonal matrices, and thus $\hat{\mathbf{C}}^{-1} = (\hat{\mathbf{C}}^{-1})^{\mathrm{T}}$.

Rearranged, we obtain the required retrieval equation;

$$\boxed{\mathbf{x} = \mathbf{x0} + \left(\hat{\mathbf{J}}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{El}}^{-1}\,\hat{\mathbf{J}} + \hat{\mathbf{C}}_{\mathrm{Ex}}^{-1}\right)^{-1}\,\hat{\mathbf{J}}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{El}}^{-1}\,\left(\mathbf{L}_{\mathrm{sensor}} - \mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})\right)}.$$

A.2.2 Application 2: Aerosol Size Distribution and Refractive Index Retrieval Equations

Let us examine Application 2; the retrieval of aerosol size distribution and refractive index, $\mathbf{x} = [\mathbf{n}^{\mathrm{T}}, \mathbf{m}^{\mathrm{T}}]^{\mathrm{T}}$.

Since, in equation (32), we converted the radiance equations into the general forms described in the Chapter 2 (eqn(4)), we can consequently include error terms and present the resulting linearised equations as our first information equations; $\boldsymbol{\tau}_{\mathrm{sensor}}^{\mathrm{SUN}} = \boldsymbol{\tau}_{\mathrm{RTE}}^{\mathrm{SUN}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SUN}}(\mathbf{x}-\mathbf{x0}) \pm \mathbf{El}_{\mathrm{SUN}}$ and $\mathbf{L}_{\mathrm{sensor}}^{\mathrm{SKY}} = \mathbf{L}_{\mathrm{RTE}}^{\mathrm{SKY}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SKY}}(\mathbf{x}-\mathbf{x0}) \pm \mathbf{El}_{\mathrm{SKY}}$. So that,

$$\mathbf{f}_0{*} = \boldsymbol{\tau}_{\mathrm{sensor}}^{\mathrm{SUN}} \text{ and } \mathbf{f}_0(\mathbf{x}) = \boldsymbol{\tau}_{\mathrm{RTE}}^{\mathrm{SUN}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SUN}}\left(\mathbf{x}-\mathbf{x0}\right),$$
$$\mathbf{f}_1{*} = \mathbf{L}_{\mathrm{sensor}}^{\mathrm{SKY}} \text{ and } \mathbf{f}_1(\mathbf{x}) = \mathbf{L}_{\mathrm{RTE}}^{\mathrm{SKY}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SKY}}\left(\mathbf{x}-\mathbf{x0}\right),$$

where $\mathbf{L}_{\mathrm{RTE}}(\mathbf{x0})$ and $\hat{\mathbf{J}}$ are calculated from the Sun and Sky radiance equations (eqn(29) and eqn(31)).

The second information equation involves the error in the "first guess" $\mathbf{x0} = [\mathbf{n0}^{\mathrm{T}}, \mathbf{m0}^{\mathrm{T}}]^{\mathrm{T}}$ which is stated in Chapter 2.3.2; $\mathbf{x0} = \mathbf{x} \pm \mathbf{Ex}$. So that,

$$\mathbf{f}_2{*} = \mathbf{x0} \text{ and } \mathbf{f}_2(\mathbf{x}) = \mathbf{x}.$$

In the case of the aerosol retrieval, it is also necessary that the retrieved solution be well behaved; that is, smooth and continuous. Let us then introduce another virtual information equation that will smooth the solution. As is explained in Appendix B.3 the appropriate smoothing matrix **B** is chosen such that $\mathbf{0} = \hat{\mathbf{B}}\mathbf{x} \pm \mathbf{Eb}$. So that,

$$\mathbf{f}_3{*} = \mathbf{0} \text{ and } \mathbf{f}_3(\mathbf{x}) = \hat{\mathbf{B}}\mathbf{x}.$$

For the case in which we are required to retrieve aerosol size distribution and refractive index there are four information equations ($k = \{0,\ldots,3\}$) to consider: Sun radiance and sky radiance as the observed, real data; "first guess" approximation and smoothing as the virtual information. Substituting these information equations into equation (35) gives;

$$\begin{gathered}
(\hat{\mathbf{J}}^{\mathrm{SUN}})^{\mathrm{T}}\left(\hat{\mathbf{C}}_{\mathrm{Elsun}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{Elsun}}{}^{-1})^{\mathrm{T}}\right)\left(\mathbf{L}_{\mathrm{RTE}}^{\mathrm{SUN}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SUN}}\left(\mathbf{x}-\mathbf{x0}\right) - \mathbf{L}_{\mathrm{sensor}}^{\mathrm{SUN}}\right) + \\
(\hat{\mathbf{J}}^{\mathrm{SKY}})^{\mathrm{T}}\left(\hat{\mathbf{C}}_{\mathrm{Elsky}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{Elsky}}{}^{-1})^{\mathrm{T}}\right)\left(\mathbf{L}_{\mathrm{RTE}}^{\mathrm{SKY}}(\mathbf{x0}) + \hat{\mathbf{J}}^{\mathrm{SKY}}\left(\mathbf{x}-\mathbf{x0}\right) - \mathbf{L}_{\mathrm{sensor}}^{\mathrm{SKY}}\right) + \\
\hat{\mathbf{I}}\left(\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1})^{\mathrm{T}}\right)\left(\mathbf{x}-\mathbf{x0}\right) + \hat{\mathbf{B}}^{\mathrm{T}}\left(\hat{\mathbf{C}}_{\mathrm{Eb}}{}^{-1} + (\hat{\mathbf{C}}_{\mathrm{Eb}}{}^{-1})^{\mathrm{T}}\right)\hat{\mathbf{B}}\mathbf{x} = \mathbf{0}.
\end{gathered}$$

Again, let us assume here that the errors are uncorrelated, such that the covariance matrices are diagonal. That is, $\hat{\mathbf{C}}^{\mathrm{T}} = \hat{\mathbf{C}}$ so that $(\hat{\mathbf{C}})^{-1} = (\hat{\mathbf{C}}^{\mathrm{T}})^{-1} = (\hat{\mathbf{C}}^{-1})^{\mathrm{T}}$.

Rearranged, we obtain the required retrieval equation;

$$\boxed{\begin{gathered}
\mathbf{x} = \mathbf{x0} + \left(\left(\hat{\mathbf{J}}_{\mathrm{SUN}}{}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{Elsun}}{}^{-1}\hat{\mathbf{J}}_{\mathrm{SUN}}\right) + \left(\hat{\mathbf{J}}_{\mathrm{SKY}}{}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{Elsky}}{}^{-1}\hat{\mathbf{J}}_{\mathrm{SKY}}\right) + \left(\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1}\right) + \left(\hat{\mathbf{B}}^{\mathrm{T}}\hat{\mathbf{C}}_{\mathrm{Ex}}{}^{-1}\hat{\mathbf{B}}\right)\right)^{-1} \times \\
\left(\left(\hat{\mathbf{J}}_{\mathrm{SUN}}{}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{Elsun}}{}^{-1}\left(\boldsymbol{\tau}_{\mathrm{sensor}}^{\mathrm{SUN}} - \boldsymbol{\tau}_{\mathrm{RTE}}^{\mathrm{SUN}}(\mathbf{x0})\right)\right) + \left(\hat{\mathbf{J}}_{\mathrm{SKY}}{}^{\mathrm{T}}\,\hat{\mathbf{C}}_{\mathrm{Elsky}}{}^{-1}\left(\mathbf{L}_{\mathrm{sensor}}^{\mathrm{SKY}} - \mathbf{L}_{\mathrm{RTE}}^{\mathrm{SKY}}(\mathbf{x0})\right)\right) - \left(\hat{\mathbf{B}}^{\mathrm{T}}\hat{\mathbf{C}}_{\mathrm{Eb}}{}^{-1}\hat{\mathbf{B}}\,\mathbf{x0}\right)\right)
\end{gathered}}$$

Appendix B: Retrieval Matrices

B.1. Jacobian Matrices, $\hat{\mathbf{J}}$

B.1.1 Jabobian of "Long-Wave Infrared" Radiance

The direct evaluation of the long-wave infrared Jacobian matrix, corresponding to the atmospheric temperature and humidity profiles, is complicated due to the unknown composition of the transmittance function. An approximation to the transmittance can be made by substituting $\mathbf{x0}$ into an appropriate atmospheric model. However, since we do not know the transmittance dependence on temperature and humidity analytically, we can therefore not calculate the required derivatives of transmittance and the radiance equation analytically.

Theriault [36] offers another method for calculating $\hat{\mathbf{J}}$, which treats the partial derivative as a small linear change, Δ.
That is,

$$\hat{\mathbf{J}}_{j,i} = \left.\frac{\partial \mathbf{L}_j^{\mathrm{RTE}}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \approx \left.\frac{\Delta \mathbf{L}_j^{\mathrm{RTE}}}{\Delta \mathbf{x}_i}\right|_{\mathbf{x0}} = \frac{\mathbf{L}_j^{\mathrm{RTE}}(\mathbf{x0}+\Delta\mathbf{x0}_i) - \mathbf{L}_j^{\mathrm{RTE}}(\mathbf{x0})}{\Delta \mathbf{x0}_i}.$$

For the calculation of each element of the Jacobian matrix we require the partial derivative of the total radiance, $\mathbf{L}^{\mathrm{RTE}}$, with respect to each layer's temperature or humidity value, evaluated for the "first guess" profile vector. Theriault's strategy involves using FASCODE or MODTRAN to produce $\mathbf{L}^{\mathrm{RTE}}$ with the original profile $\mathbf{x0}$, and then again with profile $\mathbf{x0}_k + \Delta\mathbf{x0}_k$ at layer k only. This forward-model run is performed with consecutive changes to the profile, until each layer has been tested (Theriault uses $\Delta\mathbf{x0} = (2\mathrm{K}, 0.1\mathrm{g/m}^3)$ [39]). After each "forward run" with an altered layer, the total atmospheric radiance is subtracted from the original total radiance, and the appropriate Jacobian is created by dividing by $\Delta\mathbf{x0}$.

This approximation of the partial derivative matrix can potentially introduce more error, as it assumes a degree of linearity of $\mathbf{L}^{\mathrm{RTE}}(\mathbf{x})$ around $\mathbf{x0}$. The preceding Taylor's approximation linearised the total radiance about $\mathbf{x0}$ for each atmospheric layer, and thus should negate the effects of this assumption, depending on the degree of the linearisation. The error associated with linearisation of the RTE should be incorporated into the covariance matrix $\hat{\mathbf{C}}_{\mathrm{El}}$. Thus, $\Delta\mathbf{x0}_k$ must be sufficiently small so as to not add too large a linear approximation, but also large enough so that a sufficient difference in value can be measured in $\mathbf{L}^{\mathrm{RTE}}(\mathbf{x0})$.

A combined numerical and analytic approach for calculating $\hat{\mathbf{J}}$ is to analytically differentiate the radiance equations (eqn(13)) with respect to optical depth, and numerically calculate the partial derivatives of the optical depth with respect to the profiles at each layer. These optical depth partial derivatives would be calculated via "Δ" changes as described above. This requires that the optical depth can be adequately represented by linear profile equations about each altitude, and it this assumption that prompts the use of optical depth rather than the transmittance function (which is an exponential function of path length).

Again, the specific application, scenario, *a priori* information and atmospheric modelling packages available will determine which method is used to calculate the Jacobian matrix.

$$\hat{\mathbf{J}} = \begin{bmatrix} \left.\frac{dL_{\text{RTE}}(\lambda_1)}{dT(z_1)}\right|_{\mathbf{x0}} & \cdots & \left.\frac{dL_{\text{RTE}}(\lambda_1)}{dT(z_N)}\right|_{\mathbf{x0}} & \left.\frac{dL_{\text{RTE}}(\lambda_1)}{d\rho(z_1)}\right|_{\mathbf{x0}} & \cdots & \left.\frac{dL_{\text{RTE}}(\lambda_1)}{d\rho(z_N)}\right|_{\mathbf{x0}} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \left.\frac{dL_{\text{RTE}}(\lambda_M)}{dT(z_1)}\right|_{\mathbf{x0}} & \cdots & \left.\frac{dL_{\text{RTE}}(\lambda_M)}{dT(z_N)}\right|_{\mathbf{x0}} & \left.\frac{dL_{\text{RTE}}(\lambda_M)}{d\rho(z_1)}\right|_{\mathbf{x0}} & \cdots & \left.\frac{dL_{\text{RTE}}(\lambda_M)}{d\rho(z_N)}\right|_{\mathbf{x0}} \end{bmatrix}$$

B.1.2 Jacobians of "Solar" Radiance

The "solar" radiance Jacobians, required for the aerosol characteristic retrieval equation, can be calculated through analytic differentiation of the radiance equations. This is presented below. However, the resulting matrices can have extremely large element values. This can cause singularities during inversion in the retrieval equation, and thus care in the application of the matrices must be taken, as specified in section 4.3.1.2.

For the retrieval of aerosol size distribution and refractive index we require two Jacobian matrices,

$$\hat{\mathbf{J}}^{\text{SUN}}_{j,i} = \left.\frac{\partial \boldsymbol{\tau}^{\text{SUN}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} \quad \text{and} \quad \hat{\mathbf{J}}^{\text{SKY}}_{j,i} = \left.\frac{\partial \mathbf{L}^{\text{SKY}}_{\text{RTE}\,j}}{\partial \mathbf{x}_i}\right|_{\mathbf{x0}} .$$

For the sky RTE, $\mathbf{L}_{\text{RTE}}$ is a function of radius (bins) r, wavelength λ, refractive index $\mathbf{m}$, atmospheric size distribution $\mathbf{n}$, and scattering angle Ω. We require the partial derivative of $\mathbf{L}_{\text{RTE}}$ with respect to size distribution, real part of the refractive index and imaginary part of the refractive index.

Now, since,

$$\begin{aligned} &\varpi(\lambda,\mathbf{n},\mathbf{m})P^{\Theta}(\lambda,\Omega,\mathbf{n},\mathbf{m}) \\ &\quad = \frac{\tau^{\text{total}}_{\text{scat}}(\lambda,\mathbf{n},\mathbf{m})}{\tau^{\text{total}}_{\text{ext}}(\lambda)}\left(\frac{\tau^{\text{gas}}_{\text{scat}}(\lambda)}{\tau^{\text{total}}_{\text{scat}}(\lambda,\mathbf{n},\mathbf{m})}P^{\text{gas}}(\lambda)+\frac{\tau^{\text{aerosol}}_{\text{scat}}(\lambda,\mathbf{n},\mathbf{m})}{\tau^{\text{total}}_{\text{scat}}(\lambda,\mathbf{n},\mathbf{m})}P^{\text{aerosol}}(\lambda,\Omega,\mathbf{n},\mathbf{m})\right) \\ &\quad = \frac{1}{\tau^{\text{total}}_{\text{ext}}(\lambda)}\left(\tau^{\text{gas}}_{\text{scat}}(\lambda)P^{\text{gas}}(\lambda)+\tau^{\text{aerosol}}_{\text{scat}}(\lambda,\mathbf{n},\mathbf{m})P^{\text{aerosol}}(\lambda,\Omega,\mathbf{n},\mathbf{m})\right) \end{aligned}$$

and

$$\tau^{\text{aerosol}}_{\text{scat}}(\lambda,\mathbf{m},\mathbf{n})P^{\text{aerosol}}(\lambda,\Omega,\mathbf{m},\mathbf{n}) = \frac{\lambda^2}{2\pi}\sum_{i\,=\,\text{radii bin 1}} Amp(\lambda,\Omega,r_i,m(\lambda))\;n(r_i)\;\Delta\log r_i \;,$$

we can express the integrated RTE as,

$$L_{\mathrm{RTE}}^{\mathrm{SKY}}(\lambda,\Omega,s0,\mathbf{m},\mathbf{n}) = F_0(\lambda)\frac{\cos(\theta_S)}{\cos(\theta_S)-\cos(\theta)}\left(e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda)}{\cos(\theta_S)}} - e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda)}{\cos(\theta)}}\right) \times$$

$$\frac{1}{4\pi}\frac{1}{\tau_{\mathrm{ext}}^{\mathrm{total}}(\lambda)}\left[\tau_{\mathrm{scat}}^{\mathrm{gas}}(\lambda)P^{\mathrm{gas}}(\lambda) + \frac{\lambda^2}{2\pi}\sum_{i\,=\,\text{radii bin 1}} Amp(\lambda,\Omega,r_i,m(\lambda))\; n(r_i)\,\Delta\log r_i\right].$$

And thus, the Jacobian for the sky RTE with respect to size distribution, $\mathbf{n}$, is easily calculated as,

$$\frac{\partial L_{\mathrm{RTE}}(\lambda_i,\Omega,s0,\mathbf{m},\mathbf{n})}{\partial n(r_j)} = F_0(\lambda_i)\frac{\cos(\theta_S)}{\cos(\theta_S)-\cos(\theta)}\left(e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda_i)}{\cos(\theta_S)}} - e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda_i)}{\cos(\theta)}}\right) \times$$

$$\frac{1}{4\pi}\frac{1}{\tau_{\mathrm{ext}}^{\mathrm{total}}(\lambda_i)}\left[\frac{\lambda_i^2}{2\pi}Amp(\lambda_i,\Omega,r_j,m(\lambda_i))\,\Delta\log r_j\right].$$

For the direct sun radiance,

$$\tau_{\mathrm{RTE}}^{\mathrm{SUN}}(\lambda,\mathbf{n},\mathbf{m}) = \tau_{\mathrm{ext}}^{\mathrm{gas}}(\lambda) + \sum_{i\,=\text{radius bin 1}} \beta_{\mathrm{ext}}(\lambda,r_i,m(\lambda))\,n(r_i)\,\Delta(\log r_i).$$

Again, the Jacobian elements are easily calculated with respect to the aerosol size distribution,

$$\frac{\partial \tau_{\mathrm{RTE}}^{\mathrm{SUN}}(\lambda_i,s0,\mathbf{n},\mathbf{m})}{\partial n(r_j)} = \beta_{\mathrm{ext}}(\lambda_i,r_j,m(\lambda_i))\,\Delta(\log r_i).$$

To calculate the analytic derivatives of the radiance equations with respect to aerosol size distribution, therefore, we required the Mie formulae for $Amp(\lambda,r)$ and $\beta(\lambda,r)$. These complex summation formulae are specified in Deirmendjian [39] for example.

For the Jacobians of the refractive index, the derivatives are not as simple to determine analytically. That is, since Amp is a function of $\mathbf{m}$, the partial derivatives of the real and imaginary parts of the refractive index are non-trivial.

For the real part of the complex refractive index function, the Jacobian elements are described by,

$$\left.\frac{\partial L_{\mathrm{RTE}}(\lambda_j,\Omega,s0,\mathbf{m},\mathbf{n})}{\partial\,\mathrm{Re}(m(\lambda_i))}\right|_{\mathbf{n0},\mathbf{m0}}$$

$$= F_0(\lambda_j)\frac{\cos(\theta_{\mathrm{S}})}{\cos(\theta_{\mathrm{S}})-\cos(\theta)}\left(e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda_j)}{\cos(\theta_{\mathrm{S}})}}-e^{\frac{-\tau_{\mathrm{ext}}^{\mathrm{tot}}(\lambda_j)}{\cos(\theta)}}\right)\times$$

$$\left.\frac{1}{4\pi}\frac{1}{\tau_{\mathrm{ext}}^{\mathrm{total}}(\lambda_j)}\left[\frac{\lambda_j^{\;2}}{2\pi}\sum_{k\,=\,\mathrm{radii\ bin\ 1}}\frac{\partial Amp(\lambda_j,\Omega,r_k,m(\lambda_j))}{\partial\,\mathrm{Re}(m(\lambda_i))}\,n(r_k)\,\Delta\log r_k\right]\right|_{\mathbf{n0},\mathbf{m0}}$$

and,

$$\left.\frac{\partial\,\tau_{\mathrm{RTE}}^{\mathrm{SUN}}(\lambda_j,s0,\mathbf{n},\mathbf{m})}{\partial\,\mathrm{Re}(m(\lambda_i))}\right|_{\mathbf{n0},\mathbf{m0}}=\left.\sum_{k\,=\mathrm{radius\ bin\ 1}}\frac{\partial\beta_{\mathrm{ext}}(\lambda_j,r_k,m(\lambda_j))}{\partial\,\mathrm{Re}(m(\lambda_i))}\,n(r_k)\,\Delta(\log r_k)\right|_{\mathbf{n0},\mathbf{m0}}.$$

Similar matrix elements can be derived for the imaginary part, $\mathrm{Im}(\mathbf{m})$, for both sun and sky Jacobians.

A useful construction of the derivatives of the $Amp(\lambda,r)$ and $\beta(\lambda,r)$ functions with respect to the refractive index is given in [41] and, with greater detail, in [42].

Below is the sky Jacobian, $\hat{\mathbf{J}}^{\mathrm{SKY}}=[\hat{\mathbf{J}}^{\mathbf{n}},\hat{\mathbf{J}}^{\mathbf{m}}]$,

$$\hat{\mathbf{J}}^{\mathbf{n}}=\begin{bmatrix}
\left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_1)}{dn(r_1)}\right|_{\mathbf{x0}_1} & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_1)}{dn(r_2)}\right|_{\mathbf{x0}_1} & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_1)}{dn(r_N)}\right|_{\mathbf{x0}_1}\\
\cdots & \cdots & \cdots & \cdots\\
\left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_1)}{dn(r_1)}\right|_{\mathbf{x0}_M} & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_1)}{dn(r_2)}\right|_{\mathbf{x0}_M} & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_1)}{dn(r_N)}\right|_{\mathbf{x0}_M}\\
\left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_2)}{dn(r_1)}\right|_{\mathbf{x0}_1} & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_2)}{dn(r_2)}\right|_{\mathbf{x0}_1} & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_2)}{dn(r_N)}\right|_{\mathbf{x0}_1}\\
\cdots & \cdots & \cdots & \cdots\\
\left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_P)}{dn(r_1)}\right|_{\mathbf{x0}_M} & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_P)}{dn(r_2)}\right|_{\mathbf{x0}_M} & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_P)}{dn(r_N)}\right|_{\mathbf{x0}_M}
\end{bmatrix}$$

$$\hat{\mathbf{J}}^{\mathbf{m}} = \begin{bmatrix} \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_1)}{d\,\mathrm{Re}(m(\lambda_1))}\right|_{\mathbf{x0}_1} & \cdots & 0 & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_1)}{d\,\mathrm{Im}(m(\lambda_1))}\right|_{\mathbf{x0}_1} & \cdots & 0 \\ \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_2,\Omega_1)}{d\,\mathrm{Re}(m(\lambda_2))}\right|_{\mathbf{x0}_2} & \cdots & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_2,\Omega_1)}{d\,\mathrm{Im}(m(\lambda_2))}\right|_{\mathbf{x0}_2} & \cdots \\ 0 & 0 & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_1)}{d\,\mathrm{Re}(m(\lambda_M))}\right|_{\mathbf{x0}_2} & 0 & 0 & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_1)}{d\,\mathrm{Im}(m(\lambda_M))}\right|_{\mathbf{x0}_M} \\ \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_2)}{d\,\mathrm{Re}(m(\lambda_1))}\right|_{\mathbf{x0}_1} & 0 & 0 & \left.\frac{dL_{\mathrm{RTE}}(\lambda_1,\Omega_2)}{d\,\mathrm{Im}(m(\lambda_1))}\right|_{\mathbf{x0}_1} & 0 & \cdots \\ \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_2,\Omega_2)}{d\,\mathrm{Re}(m(\lambda_2))}\right|_{\mathbf{x0}_2} & \cdots & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_2,\Omega_2)}{d\,\mathrm{Im}(m(\lambda_2))}\right|_{\mathbf{x0}_2} & \cdots \\ 0 & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_P)}{d\,\mathrm{Re}(m(\lambda_M))}\right|_{\mathbf{x0}_M} & 0 & \cdots & \left.\frac{dL_{\mathrm{RTE}}(\lambda_M,\Omega_P)}{d\,\mathrm{Im}(m(\lambda_M))}\right|_{\mathbf{x0}_M} \end{bmatrix}.$$

A similar Jacobian matrix can be obtained for the direct sun radiance (without reference to the scattering angle, Ω).

B.2. Covariance Matrices, $\hat{\mathbf{C}}$

The covariance matrices, $\hat{\mathbf{C}}_k$, are introduced as the error variance parameters in the probability formulae used to optimise the solution (Appendix A.1). The diagonal elements of $\hat{\mathbf{C}}_k$ are defined by the square of the error in the information equations, $\mathbf{E}_k$. It is through setting the covariance parameters suitably that the solution can be constrained (section 3.3.1).

The application of probability theory is used to maximise the probability of obtaining $\mathbf{f}_k(\mathbf{x})$ given $\mathbf{f}_k{}^*$, in order to extract an accurate value for $\mathbf{x}$ with minimum error. We define this error as $\mathbf{E}_k$, such that $\mathbf{f}_k{}^* - \mathbf{f}_k(\mathbf{x}) = \mathbf{E}_k$. The error is simply the difference between the true solution and the approximation. The diagonal elements of the covariance matrices are then defined by the appropriate error variances, $\hat{\mathbf{C}}_k(i,i) = \mathbf{E}_k(i) \cdot \mathbf{E}_k(i)$.

The covariances are firstly assumed to be the result of independent errors, such that the matrices are diagonal (*i.e.* all non-diagonal elements are zero). With Newtonian iteration of the solution, it is also possible to iteratively improve the covariance matrix, $\hat{\mathbf{C}}_{\mathrm{Ex}}$, for a more accurate solution. See [43], [44] and [45] for greater mathematical detail, in retrieving different scenarios.

For the first, real information equation $\mathbf{f}_0{}^* = \mathbf{L}_{\text{sensor}} = \mathbf{L}_{\text{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0}) \pm \mathbf{El}$, so that the variance is $\left(\mathbf{L}_{\text{sensor}} - \left(\mathbf{L}_{\text{RTE}}(\mathbf{x0}) + \hat{\mathbf{J}}(\mathbf{x} - \mathbf{x0})\right)\right)^2 = \left(\pm\mathbf{El}\right)^2$. The diagonal covariance matrix is then defined by $\hat{\mathbf{C}}_{\text{El}}(i,i) = \mathbf{El}(i) \cdot \mathbf{El}(i)$. As can be similarly shown for total optical depth, $\boldsymbol{\tau}^{\text{RTE}}$.

The error $\mathbf{El}$ is a combination of the sensor error and the error in the linearised radiance equation, $\mathbf{El} = \mathbf{E}_{\text{formula}} + \mathbf{E}_{\text{instrument}}$. These values must be estimated from the known sensor sensitivity and variability, and the consideration of the *a priori* model known for the atmosphere. Setting an appropriate covariance matrix $\hat{\mathbf{C}}_{\text{El}}$ can help stabilize the retrieval by including the "actual limit" of the measurement and the uncertainty in the atmospheric model.

For "first guess" virtual information we have $\mathbf{f}_2{}^* = \mathbf{x0} = \mathbf{x} \pm \mathbf{Ex}$, so that the variance is $(\mathbf{x0} - \mathbf{x})^2 = (\pm\mathbf{Ex})^2$. The diagonal covariance matrix is then defined by $\hat{\mathbf{C}}_{\text{Ex}}(i,i) = \mathbf{Ex}(i) \cdot \mathbf{Ex}(i)$.

The covariance matrix of the first guess of the solution, $\hat{\mathbf{C}}_{\text{Ex}}$, is often referred to as the "damping factor". The elements of the matrix are arbitrarily chosen in order to stabilise the retrieval by confining the solution to within a chosen "error" degree of the "first guess". A better estimation of the covariance elements can then be gained by iterating the solution, as described above. This is not possible for all scenarios, and since the covariance matrix is ultimately determined by "chosen" values, this parameter of the retrieval equation is not a robust variable.

For the smoothing we have, $\mathbf{f}_4{}^* = \mathbf{0} = \hat{\mathbf{B}}\,\mathbf{x} \pm \mathbf{Eb}$, so that the variance is $(\mathbf{0} - \hat{\mathbf{B}}\,\mathbf{x})^2 = (\pm\mathbf{Eb})^2$. The diagonal covariance matrix is $\hat{\mathbf{C}}_{\text{Eb}}(i,i) = \mathbf{Eb}(i) \cdot \mathbf{Eb}(i)$.

B.3. Smoothing Matrix, $\hat{\mathbf{B}}$

The retrieved solution for the aerosol size distribution is known to be a smooth function. This 'smoothness' can be used as virtual information to obtain a more accurate inversion [46]. The degree to which the function is to be smoothed determines the form of $\hat{\mathbf{B}}$. The curvature of a function is defined by its second derivative, and thus restrictions on this can influence the smoothness. That is, by minimising the curvature or the change in curvature (third derivative), the function should appear to become smoother. Dubovick and King [47] describe the smoothing parameter, $\hat{\mathbf{B}}$, as a matrix operator of "second differences" on the profile $\mathbf{x}$ (*ie.* the coefficients of recurrent difference equations, as an approximation to derivative functions). Within the inversion equation it is this product, $\hat{\mathbf{B}}\,\mathbf{x}$, that is minimised. That is, we require the second derivative of the solution to tend to zero, with minimum error, and thus give a smoother solution, $\mathbf{x}$.

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for Long-Wave Infrared and Solar Radiance Scenarios

Michelle Hackett

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19. ABSTRACT
Atmospheric retrieval is the extraction of atmospheric data from spectral radiance, as observed at a remote sensor. In particular, consider the retrieval of temperature and humidity profiles, and aerosol size distribution and the scattering refractive index from long-wave infrared and solar radiance spectra, respectively. The application of retrieval, in this report, primarily involves inversion of a radiative transfer equation (RTE). However, due to the ill-posed nature of the problem and the inherent errors involved, such inversions are non-trivial. This report presents a combined, generalised approach to retrieval via statistical inversion, which is derived in detail for the atmospheric parameters mentioned above.

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