EVALUATING RADIANCE AND RETRIEVAL ASSIMILATION OF MARS THERMAL EMISSION SPECTROMETER SPACECRAFT OBSERVATIONS

A Thesis in
Meteorology
by
Petros K. Kalogeras

© 2015 Petros K. Kalogeras

Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Master of Science

August 2015
The thesis of Petros K. Kalogeras was reviewed and approved* by the following:

Steven J. Greybush  
Assistant Professor of Meteorology  
Thesis Advisor

Eugene E. Clothiaux  
Professor of Meteorology

Fuqing Zhang  
Professor of Meteorology

Johannes Verlinde  
Professor of Meteorology  
Associate Head, Graduate Program in Meteorology

*Signatures are on file in the Graduate School.
Abstract

In the current study two types of data assimilation approaches for updating atmospheric temperature profiles on Mars are explored. Namely, we investigate a retrieval and a radiance data assimilation, where in each case the assimilated observations are atmospheric temperature profiles and satellite spectra respectively. Temperature profiles alongside pressure distributions are simulated by utilizing the Mars Global Climate Model (MGCM). In particular, these temperature profiles serve as the prior to the applied filtering technique, an ensemble Kalman filter (EnKF). Direct satellite measurements in the form of Thermal Emission Spectrometer (TES) spectra of radiance available from the Planetary Data System (PDS), as well as Optimal Spectral Sampling (OSS) temperature retrievals deduced from PDS TES radiance spectra, are considered as the observations to be assimilated. Temperature retrievals, which are not direct observations, depend upon their respective acquisition procedures and in this sense are not unique. On the other hand, observed spectra cannot be compared directly with a weather model. Nevertheless, both geophysical quantities can be considered as observations and in this lies the focus of the current project.

The findings suggest that both types of observations can yield physically sensible Kalman filtering analysis results. However, the quality of the results depends profoundly on how the filtering approach is carried out, with vertical and spectral localizations having the greatest impact.

Comparing retrieval and radiance assimilations for the Martian atmosphere is also relevant to NWP on Earth; the Martian observations network is limited to satellite observations, whereas the terrestrial observations include satellite measurements, atmospheric soundings, and data procured from ground weather stations. Considering the paucity of data directly usable in a Martian weather model, the Martian case may then serve as suitable test bed being in the position to highlight viable assimilation procedures, in the context of operating only with such observed spectra.
# Table of Contents

List of Figures ................................................................. vi

List of Tables ................................................................. xiv

Chapter 1

Introduction ........................................................................ 1
  1.1 Literature Review ....................................................... 3
  1.2 Study Objective ......................................................... 5

Chapter 2

Methodology ....................................................................... 7
  2.1 Mars Global Climate Model (MGCM) ............................... 7
  2.2 Filtering Methodology .................................................. 10
  2.3 Retrieval Data Assimilation .......................................... 14
    2.3.1 Retrieval Model and Observation Spaces .................... 15
    2.3.2 Retrieval Global Approach ..................................... 19
    2.3.3 Retrieval Local Approach ..................................... 19
    2.3.4 Retrieval R Modulation ....................................... 29
  2.4 Radiance Data Assimilation .......................................... 31
    2.4.1 Radiance Observation Space ................................... 33
    2.4.2 Radiance Global Approach .................................... 43
    2.4.3 Radiance Local Assimilation .................................. 44
    2.4.4 Radiance per Pressure Levels Localization ................. 52
    2.4.5 Radiance per Spectral Channels Localization ............... 57

Chapter 3

Results ............................................................................. 63
  3.1 Pressure Versus Temperature ....................................... 70
  3.2 Signed Differences ..................................................... 84
  3.3 Radiance Spectral Distributions .................................... 96
Chapter 4
4.1 Discussion ........................................................................................................ 98
4.2 Summary and Conclusions ............................................................................. 106

Appendix A
MGCM Resolution and Pressure–Sigma Schemes .............................................. 111

Appendix B
Longitudinal–Latitudinal Interpolation ................................................................. 123

Appendix C
Retrieval Forward Model Operator ..................................................................... 135

Appendix D
TES Spectra Inversion .......................................................................................... 139

Appendix E
Scale Analysis ....................................................................................................... 146

References ............................................................................................................. 155
List of Figures

Figure 2.1. Model space error covariance matrix $P_b$ for the profile case of 1374/8664 of 000155700. ................................................................. 22

Figure 2.2. Model space error covariance matrix $P_b$ for the profile case of 7600/7952 of 000239506. ................................................................. 23

Figure 2.3. Conceptual draft outlining the establishment of the local domain of the assimilation model space (for both retrieval and radiance). ........................................ 25

Figure 2.4. Conceptual draft outlining the first valid observation to be used in the localized retrieval data assimilation. ................................................................. 26

Figure 2.5. For a histogram portraying the accounted observations, per model space grid point k, in a localized retrieval data assimilation. The corresponding profile is 7600/7952 of 000239506. The orange bars are for localization coefficient value $c = 0.030$, while the blue bars for a smaller value $c = 0.015$, signifying the spatially reduced local neighborhood, in model space. ................................................................. 28

Figure 2.6. Spectral distribution of a satellite observed radiance, for the profile 7600/7952 of 000239506. ................................................................. 40

Figure 2.7. Partial spectral distribution of the satellite observed radiance, for the profile 7600/7952 of 000239506. Negative radiance values are present and therefore excluded from the valid radiance observation space. ................................................................. 40

Figure 2.8. Spectral distribution of the background observations (radiance), of profile 7600/7952 of 000239506, evaluated from the OSS forward model operator. ................. 41

Figure 2.9. Partial spectral distribution of the background observations (radiance) from the OSS forward model operator, for the profile 7600/7952 of 000239506. Non negative values are recorded in this case. ................................................................. 41
Figure 2.10. Spectral distribution of the signed difference between background observation ensemble member 1, and the satellite observations. The light blue domains denote the spectral range of potential exclusion of that information content, from the filtering process. ............ 42

Figure 2.11. Spectral distribution of the signed difference between background observations ensemble mean, and the satellite observations. The light blue domains denote the spectral range of potential exclusion of that information content, from the filtering process. ............ 42

Figure 2.12. Jacobian matrix graphical representation for profile 0001/8664 of 000155700. The vertical axis is for the reference pressure levels (table 2.1), while the horizontal axis for the radiance to temperature differences, explicating the radiance to temperature sensitivity for each spectral channel, out of 143. ................................................................. 49

Figure 2.13. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 0001/8664 of 000155700, for the full spectral case. .............. 58

Figure 2.14. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 0001/8664 of 000155700, for the partial spectral case. ............ 59

Figure 2.15. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 1374/8664 of 000155700, for the full spectral case. ............ 61

Figure 2.16. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 7600/7952 of 000239506, for the full spectral case. .............. 62

Figure 3.1. Examined profiles topographic locations. Profiles 0001/8664 of 000155700 (yellow dots), 1374/8664 of 000155700 (cyan dots), and 7600/7952 of 000239506 (white dots) are presented in their respective satellite locations. ............................................................. 64

Figure 3.2. Analysis temperature profiles for the retrieval global assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a and b) For profile 0001/8664 of 00155700. (c and d) For profile 1374/8664 of 00155700. (e and f) For profile 7600/7952 of 000239506. Sub plots (a), (c), and (e) are for observational standard deviation $\sigma_o=3.0$ K, and (b), (d), and (f) for $\sigma_o=5.0$ K. .......................................................................................................................... 70
Figure 3.3. Analysis temperature profiles for the radiance global assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a and b) For profile 0001/8664 of 00155700. (c and d) For profile 1374/8664 of 00155700. (e and f) For profile 7600/7952 of 00239506. Sub plots (a), (c), and (e) are for the full spectral case, where every channel is accounted for. For sub plot (b), the excluded channels are the first 5 and the last 9, for (d) the first 8 and the last 43, and for (f) the first 7 and the last 66.

Figure 3.4. Analysis temperature profiles for the retrieval local assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue, magenta, green) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a, b, c, and d) For profile 0001/8664 of 000155700. (e, f, g, and h) For profile 1374/8664 of 000155700. (i, j, k, and l) For profile 7600/7952 of 000239506. Sub plots (a), (e), and (i) correspond to observational standard deviation $\sigma_o=3.0$ K with localization coefficient $c = 0.015$. Sub plots (b), (f), and (j) are for $\sigma_o=3.0$ K with $c = 0.030$. Sub plots (c), (g), and (k) are for $\sigma_o=5.0$ K with $c = 0.015$ and (d), (h), and (l) for $\sigma_o=5.0$ K with $c = 0.030$.

Figure 3.5. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 0001/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.

Figure 3.6. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 0001/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 129 out of 143. Excluded channels are the first 5 and the last 9. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
Figure 3.7. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 1374/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels. ... 80

Figure 3.8. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 1374/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 129 out of 143. Excluded channels are the first 5 and the last 9. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels. ... 81

Figure 3.9. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 7600/7952 of 000239506. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels. ... 82

Figure 3.10. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 7600/7952 of 000239506. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 129 out of 143. Excluded channels are the first 5 and the last 9. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels. ... 83

Figure 3.11. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both sub plots are for the profile 0001/8664 of 000155700. (a) For the global assimilation; $\sigma_o=3.0$ K (orange line) and $\sigma_o=5.0$ K (blue line). (b) For the local assimilation; $\sigma_o=3.0$ K with $c = 0.015$ (orange line),
Figure 3.12. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both subplots are for the profile 1374/8664 of 000155700. (a) For the global assimilation; $\sigma_o=3.0$ K (orange line) and $\sigma_o=5.0$ K (blue line). (b) For the local assimilation; $\sigma_o=3.0$ K with $c = 0.015$ (orange line), $\sigma_o=3.0$ K with $c = 0.030$ (blue line), $\sigma_o=5.0$ K with $c = 0.015$ (magenta line), and $\sigma_o=5.0$ K with $c = 0.030$ (green line).

Figure 3.13. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both subplots are for the profile 7600/7952 of 000239506. (a) For the global assimilation; $\sigma_o=3.0$ K (orange line) and $\sigma_o=5.0$ K (blue line). (b) For the local assimilation; $\sigma_o=3.0$ K with $c = 0.015$ (orange line), $\sigma_o=3.0$ K with $c = 0.030$ (blue line), $\sigma_o=5.0$ K with $c = 0.015$ (magenta line), and $\sigma_o=5.0$ K with $c = 0.030$ (green line).

Figure 3.14. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 5 and the last 9 channels have been excluded from the analysis, thus rendering the valid channels 129 out of 143.

Figure 3.15. Signed differences between analysis mean and background mean for the radiance local per pressure level assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from all available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 129 out of 143 channels, excluding the first 5 and the last 9.

Figure 3.16. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 8 and the last 43 channels have been excluded from the analysis, thus rendering the valid channels 92 out of 143.
Figure 3.17. Signed differences between analysis mean and background mean for the radiance local per pressure level assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from the available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 92 out of 143 channels, excluding the first 8 and the last 43.

Figure 3.18. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 7 and the last 66 channels have been excluded from the analysis, thus rendering the valid channels 70 out of 143.

Figure 3.19. Signed differences between analysis mean and background mean for the radiance local per pressure level assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from the available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 70 out of 143 channels, excluding the first 7 and the last 66.

Figure 3.20. Signed differences between analysis mean and background mean for the radiance local per spectral channel assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 5 and the last 9 channels from the analysis.

Figure 3.21. Signed differences between analysis mean and background mean for the radiance local per spectral channel assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 8 and the last 43 channels from the analysis.

Figure 3.22. Signed differences between analysis mean and background mean for the radiance local per spectral channel assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 7 and the last 66 channels from the analysis.
Figure 3.23. PDS TES 0001/8664 of 000155700 profile spectral distributions of the observed spectra $y_0$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30. ................................................................. 96

Figure 3.24. PDS TES 1374/8664 of 000155700 profile spectral distributions of the observed spectra $y_0$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30. ................................................................. 97

Figure 3.25. PDS TES 7600/8664 of 000239506 profile spectral distributions of the observed spectra $y_0$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30. ................................................................. 97

Figure A.1. The Martian topography from a top view. The geographic coordinates, longitude $\lambda$ and latitude $\phi$ are in degrees. The Southern and Northern polar caps are not included in the analysis. ................................................................. 118

Figure A.2. Surface plot of the Martian topography from a front right view point. ........... 119

Figure A.3. Surface plot of the Martian topography from a top left view point. ........... 119

Figure A.4. Surface plot of the $\phi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 26$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution. ........... 120

Figure A.5. Surface plot of the $\phi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 13$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution. ........... 120

Figure A.6. Surface plot of the $\phi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 8$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution. ........... 121
Figure A.7. Density – contour plot of the φ – λ horizontally interpolated ensemble mean MGCM pressure, for model level k = 26. ................................................................. 121

Figure A.8. Density – contour plot of the φ – λ horizontally interpolated ensemble mean MGCM pressure, for model level k = 13. ................................................................. 122

Figure A.9. Density – contour plot of the φ – λ horizontally interpolated ensemble mean MGCM pressure, for model level k = 8. ................................................................. 122

Figure B.1. Conceptual draft outlining the scripting approach for a two dimensional known images set, locally. ................................................................. 127

Figure B.2. Conceptual draft outlining an one dimensional local regime of interpolation. .. 129

Figure B.3. Conceptual draft emphasizing script discrepancies arising from an one dimensional interpolation in a regime with periodicity. ................................................................. 132

Figure C.1. Conceptual draft showing 9 model space values ξ_k, for k ={1, 2, ..... , 9}, and 6 observation space values ζ_r, for r ={1, 2, ..... , 6}. This draft is to be viewed vertically. .... 136
List of Tables

Table 2.1. Fixed (spatially and temporally independent) reference pressure values, defining the full observation space in the retrieval data assimilation, in Pascal. The data are to be read per row, from left to right. ................................................................. 14

Table 2.2. Thermal emission spectrometer (TES) spectral resolution, in inverse centimeters. The data are to be read per row, from left to right. ........................................... 32

Table 2.3. OSS forward model operator input vector of one ensemble member, for profile 0001/8664 of 000155700. The data are to be read per row, from left to right. ................. 37

Table 2.4. OSS forward model operator input vector of one ensemble member, for profile 1374/8664 of 000155700. The data are to be read per row, from left to right. ................. 37

Table 2.5. OSS forward model operator input vector of one ensemble member, for profile 7600/7952 of 000239506. The data are to be read per row, from left to right. ................. 37

Table A.1. Latitudinal MGCM discretization values, defining the parallel circles locations, in degrees North. The data are to read per row, from left to right, in ascending order. ......... 111

Table A.2. Definition of the coefficients a and b for the hybrid pressure – sigma MGCM coordinate system, in the vertical direction. ......................................................... 116

Table E.1. Analysis increments $\mathbf{x}_a - \mathbf{x}_b$ for a performed data assimilation on profile 7600/7952 of 000239506. Column 1 pertains to the model space levels. Column 2 is for the case of retrieval global assimilation with $\sigma_o = 3.0 \text{ K}$ and column 3 for the radiance global assimilation of the partial spectral space with used channels 70/143, where the neglected channels are the first 7 and the last 66. ......................................................... 147

Table E.2. Retrieval global assimilation of profile 7600/7952 of 000239506 with $\sigma_o = 3.0 \text{ K}$ relevant numerical figures. Column 1 is for the enumeration of the valid reference pressure levels. Column 2 is for the numerical values of those levels. Column 3 presents the innovations, and column 4 the background standard deviation in observation space. ......................... 148
Table E.3. Radiance global assimilation of the partial spectral space innovations data set for profile 7600/7952 of 000239506. The data are to be read per row, from left to right, for a total number of elements equal to 70, excluding the first 7 and the last 66 spectral channels. Physical units in $\text{mW (cm}^{-1}\text{)}^{-1} \text{m}^{-2} \text{sr}^{-1}$, for included channels 8 to 77 out of 143. ................................. 149

Table E.4. Radiance global assimilation of the partial spectral space background standard deviations in observation space for profile 7600/7952 of 000239506. The data are to be read per row, from left to right, for a total number of elements equal to 70, excluding the first 7 and the last 66 spectral channels. Physical units in $\text{mW (cm}^{-1}\text{)}^{-1} \text{m}^{-2} \text{sr}^{-1}$, for included channels 8 to 77 out of 143. ............................................................................................................. 149

Table E.5. Transpose of the background perturbation matrix in observation space of the retrieval global assimilation (7600/7952 of 000239506). The rows pertain to select ensemble members and the columns to select cases of valid reference pressure levels. Physical units in K. ....................................................................................................................... 150

Table E.6. Transpose of the background perturbation matrix in observation space of the radiance global and partial spectral space assimilation (7600/7952 of 000239506). The rows pertain to select ensemble members and the columns to select cases of valid spectral channels. Physical units in $\text{mW (cm}^{-1}\text{)}^{-1} \text{m}^{-2} \text{sr}^{-1}$. ................................................................. 151

Table E.7. Background perturbation matrix of the retrieval global and radiance global of the partial spectral space assimilations (7600/7952 of 000239506). The rows pertain to select model space levels and the columns to select ensemble members. Physical units in K. .... 151

Table E.8. Kalman gain (dimensionless) for the retrieval global assimilation of 7600/7952 of 000239506, with $\sigma_o = 3.0$ K. The rows pertain to select model space levels and the columns to select cases of valid reference pressure levels. ................................................................. 151

Table E.9. Kalman gain (K $\text{mW (cm}^{-1}\text{)}^{-1} \text{m}^{-2} \text{sr}^{-1}$) for the radiance global assimilation of the partial spectral space of 7600/7952 of 000239506 (70/143 used channels). The rows pertain to select model space levels and the columns to select cases of valid spectral channels. .... 152
Chapter 1

Introduction

Meteorology is the discipline engaging itself with the study of the atmosphere, from a dynamical, thermodynamical, and radiative perspective. In the applied sense, most associate this field with concepts such as predictability and forecasting because from a societal point of view interest lies primarily in the ability to discern beforehand regional weather patterns that may have vital implications for the public, financially or for its wellbeing. Additionally, vocational fields like agriculture, aviation, the shipping industry, and government, among others, rely to some extent on the knowledge of those forecasts for the sake of assessing infrequent eventualities or for well-grounded decision making.

From a technical standpoint, these forecasts are realized in the context of Numerical Weather Prediction (NWP). As the name suggests, NWP involves the application of computers, given the fact that the volume of calculations to be performed is rather immense. Across the various countries of the world there exist several operational weather systems, which employ numerical weather models stemming from the physics describing the atmosphere. At the same time, observational networks are accounted for; these networks may refer to ground – weather stations, atmospheric soundings, or to instruments pertaining to remote sensing like satellites and radars.

At the heart of the notion of predictability lies data assimilation. In data assimilation the information acquired from the aforementioned observational networks is incorporated in the weather models, so that these observations will serve as the driver of those models that produce the forecasts. In other words, contemporary observational information is used to update the initial conditions of the weather models, so that the forecasts may stay relevant to any given state of the atmosphere, within a reasonable time window.

The key elements that comprise a weather operational system are the following: the known physics, the numerical application of those in modeling, observational networks, and data assimilation schemes. In the current study we focus our attention to one particular observational network and the ramifications its appliance may have in data assimilation. Specifically, we deal with satellite measurements procured from the Thermal Emission
Spectrometer (TES) which orbited planet Mars during the years 1997–2006 being mounted on the Mars Global Surveyor spacecraft (MGS).

Thus, the current study revolves around the topic of a Martian NWP. Mars, compared to Earth, has a different topography, atmospheric climatology and chemical composition, and a more distant orbit around the Sun, yet has a similar axial tilt and length of day to the Earth. There are no oceans so that certain thermodynamical processes like phase changes occur differently from Earth; evaporation and condensation are limited while fusion and sublimation are more prevalent given the seasonal cycles of the available molecular CO₂ and H₂O atmospheric content. During the Martian winter certain amounts of those atmospheric vapors freeze in the polar cap regions, which are then released via sublimation back in the atmosphere during spring and summer. Furthermore, unlike Earth on Mars dust storms are more common, have a greater spatial scale, and can last for prolonged periods of time. So, the amounts of dust and aerosols in conjunction with the other gaseous constituents in a Martial annual cycle (approximately 668 sols) or more, also lead to microphysical processes which are diversified compared to the terrestrial case, and also impact the radiative properties of this atmosphere accordingly. Mars is not so dissimilar to Earth, with regards to its dynamics. However, different ranges in atmospheric variables such as density, pressure, or temperature are encountered. Typical pressure ranges are for \( p \in (0, 1 \times 10^3) \text{ Pa} \), while temperatures are typically for \( T \in [150, 250] \text{ K} \), even though there are seasonal extremes for \( T \) around 300 K. It then follows that the Martian climatology, parameterization, and scaling will be correspondingly different compared to the terrestrial case. A Martian forecasting and the constitution of pertinent models demand a robust understanding of the relevant physics and parameterizations, and from these studies improvements for the terrestrial models may arise.

Studying Mars meteorology offers certain benefits of an academical and practical nature. The advantages are multi fold; one is related to the overall technological effort put to produce and be able to test equipment oriented to function in an extra terrestrial environment, as that relates to space engineering and to remote sensing. The MGS spacecraft and the TES represent products of such labor, which in future times may lead to improved characterization of the Martian atmospheric thermodynamic state, while allowing for more precise spacecraft landings and the facilitation of future exploration of the red planet. Of course, these instruments are but means to an end, which is to explore and assess methods related in particular to NWP and how we may further the accuracy and
applicability of the used approaches. Weather forecasting using satellites already takes
place in the terrestrial atmosphere, and pertinent remote sensing methodologies are already
being explored and applied. Nevertheless, the study of a different climatology, like the
Martian, simpler compared to the terrestrial, may yield theoretical studies which then can
be used for comparison purposes for investigating techniques relevant to NWP on Earth.

1.1 Literature Review

A key component of any operational weather system aspiring to deduce information on the
state of the atmosphere, is the model. The model incorporates the known physics in
numerical fashion. The known physics pertaining to the atmosphere involve the three
equations of motion (the Navier–Stokes momentum equations), the first law of
Thermodynamics, the equation of mass continuity, one equation of state relating
thermodynamic variables such as pressure, density, and temperature, and one additional
equation tracking the water vapor content of the atmospheric fluid, a measure of which can
typically be the specific humidity. We have a system of seven equations in which six are
partial differential equations (PDE's) and one equation, that of state, an algebraic one. The
unknown variables are the three components of the velocity, pressure, density, temperature,
and specific humidity. Additional features are also incorporated, such as spatial scaling, or
the inclusion of cloud microphysical processes. Analytically, initial and boundary value
problems such as this are not solvable, considering the mathematical complexity and the
fact that the boundary conditions typically are not known. Therefore, we resolve to
numerical solutions. A model or numerical solver, is in the position to simulate atmospheric
states, given initial and boundary conditions of a subjective nature, essentially by
implementing prognostic equations and equations of state pertaining to the scope of the
physical phenomena at hand. In the current study and for the case of the Martian
atmosphere, this numerical solver is the Mars Global Climate Model (MGCM) [19], given
appropriate adaptations [13].

TES Mars observations were mostly nadir radiance spectral distributions in a
waveband 6 – 50 μm, where the applicable frequency range was selected as such in an
effort to capture information in the CO₂ absorption band, given that carbon dioxide is the
dominant chemical constituent in the Martian atmosphere [4]. Since in the current study the
used spectral coordinate is inverse centimeters, the relevant spectral resolution of the TES
can also be found in table 2.2 (section 2.4). The TES was a surface oriented instrument [1], [2], as the observed spectra were intended for the analysis of the chemical composition of the Martian surface. Despite that, the presence of the atmosphere, which may not have been favorable to the geologists, contributed to the observations and pertinent data sets arose [2], [3], that have been used from atmospheric scientists for the study of a plentitude of atmospheric phenomena.

Several studies using the TES observed spectra have already been performed [6], [10], [12]. A central concept that is of a profound significance in the current study is that of the temperature retrievals. On one hand, we have spectral radiances as the direct observations, and on the other hand we wish to reach to other variables related to the dynamical or the thermodynamical state of the Martian atmosphere. In this regard, there exists a field focusing on the conversion of radiative variables to thermodynamic ones, among others. Specifically in the current context, retrieval methodologies elucidate how we may obtain temperatures from spectral radiances. There are retrieval approaches and algorithms performing this task, and pertinent data sets have been produced accordingly. In particular, we have the Planetary Data System (PDS TES) retrievals [18], and the Optimal Spectral Sampling (OSS) retrievals [6], both of which give atmospheric temperature profiles, among other results, accounting the TES observed spectra. The used data set currently is of the OSS TES retrievals, while several other studies previously used the PDS TES temperature retrievals [10], which were formerly estimated [18], and therefore available longer. The theoretical basis of the OSS method can be found in [15]. The specifics of the modeling of this approach are attributed to [5], [14], and [17].

There are several retrieval algorithms whose results do not necessarily coincide. Accordingly, there may be discrepancies within the relevant data sets, stemming from each applied method. A comparison between the PDS TES and the OSS TES retrievals has been performed [12]. A sensitivity analysis has been carried out, examining the impact on the retrievals of factors such as the algorithm per se, the forward model used, vertical smoothing, or the temperature prior (in the context of the retrievals).

The inversion methodologies essentially are mappings that estimate temperatures from radiance distributions, so that these temperatures may then be used in the procurement of a model posterior in an assimilation approach. However, the infrared inversion problems exhibit one deficiency; the temperature retrievals are not attainable should we attempt to estimate all elements of such atmospheric temperature profiles. To circumvent this issue, typically we reduce the dimensionality of the problem by projecting the solutions
(temperature profiles) to appropriate subspaces, in the form of empirical orthogonal functions [6]. This subject is highlighted in detail in appendix D. Practically, if a temperature retrieval is comprised from 21 elements, we are in the position to estimate no more than three to six elements of it, thus representing only a truncated version of it. Even if the satellite spectra are very accurate, we are bound to relinquish some accuracy from the application of such IR inversion algorithms.

In order to carry out a data assimilation, we require the model prior and the observations. At the same time, we also need to evaluate the observational increments (innovations). The observations can either be satellite spectra, in the form of spectral distributions of radiance, or retrieved temperatures. Assimilating directly retrieved temperatures is more straightforward than assimilating radiances, which currently is not fully explored but has been suggested. If we use retrieved temperatures, first we have to estimate those from a retrieval algorithm. For the innovations we also need to evaluate the background in observation space. The observation space here will either be altitude, pressure levels, or otherwise directly related to the $E^3$ space. This background in observation space can typically be estimated from simpler interpolation schemes, obviating any additional inversions. On the other hand, if we assimilate directly radiances, we probably are more certain of the direct observations, given a small observational standard deviation, but the evaluation of the background in observation space will involve additional inversions. Consequently, there is a certain trade off, which the current study sets out to shed some light on.

1.2 Study Objective

Considering the closing remarks of section 1.1, the problem at hand consists of whether we wish to directly incorporate satellite spectra in a data assimilation method, or conversely to use retrieved atmospheric temperature profiles, procured from these observed spectra.

In the current study we wish to implement two types of data assimilation schemes. Throughout, we refer to those two schemes as the retrieval and radiance data assimilation. In both cases, the same filtering equations are being applied. A generic ensemble Kalman filter (EnKF) is used [7], where the model prior is comprised of an ensemble of 16 temperature profiles derived from the MGCM, [19]. From this prior, its ensemble mean is evaluated and is then used for the calculation of the posterior mean. We do not perform a
cycling data assimilation, which is reserved for future work, and in this regard the consideration ends with the evaluation of the analysis mean, so that an updated prior of ensembles is not generated anew afterwards. The focus is not in understanding the overall performance of the full data assimilation system, but rather assessing the impact of radiance versus retrieval upon the analysis. This one dimensional study (we note that "1DVAR" experiments are also used in Earth NWP) is an important prerequisite for implementing radiance assimilation in an operational Mars NWP [20], [21].

In the retrieval data assimilation, the observations, and therefore the background in observation space as well, are temperatures. In this case we use the OSS TES temperature retrievals for our observations [6], and we evaluate the background ones with an applicable retrieval forward model operator (implementation specifics in appendix C).

On the other hand, in the radiance data assimilation, the observations are direct satellite measurements, given from the PDS TES data sets [2], [3]. There exist PDS TES temperature retrievals as well [18], which are not used here, however. Instead, only the OSS TES temperature retrievals are used [6]. In this case, the background in observation space is evaluated by using a forward model operator [5], [14], [17], applicable for this case. Additional information can be found in section 2.4.1 as well as in appendix D.

Reflecting on the remarks made in section 1.1, we implement those two data assimilation approaches given specific representative atmospheric profiles, and the objective is to determine the impact each approach has on the evaluated posterior ensemble mean.
Chapter 2

Methodology

In chapter 2 the methodology of the current study is presented. This chapter consists of four parts. In section 2.1 we present pertinent information regarding the MGCM, which is also accompanied by appendix A, where further details of the climate model resolution, the used Martian topography by the model, and the hybrid pressure sigma coordinate scheme in the vertical direction are also expounded. In the second part, in section 2.2, we have the applied Kalman filtering approach employed herein. In the third part of chapter 2, namely in sections 2.3 – 2.3.4, we explain how the retrieval data assimilation is carried out. More specifically, in section 2.3.1 we have the constitution of the assimilation model space, which is equally used in the retrieval and the radiance assimilation, followed by section 2.3.2 for the retrieval global assimilation, and sections 2.3.3 and 2.3.4 for the retrieval local assimilation. Then we have sections 2.4 – 2.4.5 for the radiance assimilation, as the fourth part of chapter 2. In section 2.4.1 we analyze the establishment of the radiance observation space, in like manner to section 2.3.1 where the retrieval observation space is also being founded. In section 2.4.2 we have the examination of the radiance global assimilation, in section 2.4.3 clarifications on the use and meaning of jacobian matrices, in section 2.4.4 the first of the two applied radiance localization assimilations, and in 2.4.5 the second radiance localization implementation.

2.1 Mars Global Climate Model (MGCM)

In data assimilation implementations, we incorporate observations to prior (background) model states in order to generate a posterior (analysis) which is then used to drive a used numerical solver forward in time, while maintaining these numerical solutions relevant to the observed state of the physical system at hand. In view of that, we discern the two corner stones of data assimilation, namely the observation networks, which provide the observations, and the numerical solver, which provides the prior state. In this section we present an insight on the climate model used in the current study.
Currently, we perform a study related to the Martian atmosphere and its case specific characteristics, some of which involve its composition as that relates to the dominant chemical constituents encountered in this physical system, the topographic features of Mars and how those may impact relevant physical variables like pressure or temperature and their vertical structures at specific geographic locations, the presence of aerosols, weather phenomena like tides and planetary waves, or radiative effects which are also closely related to the composition of the atmospheric fluid. In the Martian atmosphere, the most prevalent constituent is carbon dioxide \( \text{CO}_2 \), even though \( \text{H}_2\text{O} \) exists in traceable amounts including vapor, liquid, and solid phases. The time of the Martian year as well as the latitude are important factors determining whether we may or may not encounter solid \( \text{H}_2\text{O} \) for example, so time and geographic locations are more often than not pivotal in targeted studies [6]. A typical range for surface pressures is \[ 250, 950 \, \text{Pa} \] closely related to the topography of the planet, while a typical temperature range is \[ 150, 250 \, \text{K} \]. From a dynamical perspective, representative atmospheric states of Mars are largely different from those encountered on Earth and in this regard the applied climate models which are used for the generation of pertinent priors need to account for the specific parameterization and climatology of the Martian atmosphere.

Like stated in section 1.1, herein we apply the GFDL Mars Global Climate Model (MGCM) [19]. This model is adapted to operate on the Martian atmosphere and it describes physical processes like the dynamics, dust cycles, \( \text{CO}_2 \) cycles, while accounting for the presence of water ice clouds [10]. However, in the current study the focus lies primarily in the dynamics of the model. Relevant generated priors from the MGCM involve zonal and meridional velocities, temperatures, and pressures following the discretization of the solver. Specific details on the MGCM discretization and topography are also found in appendix A. The attention falls on pressure and temperature priors exclusively, due to the fact that these are the only two pertinent variables appearing in the present analysis in view of the available data sets, namely the PDS TES data set which offers observations as spectral distributions of radiance at given TES spectral channel wavebands, and the OSS TES data set of the temperature retrievals at prescribed reference pressure levels. Considering that we explore two different types of data assimilation schemes, that is a retrieval and a radiance data assimilation, the MGCM simulated outputs will serve as the prior, equally in both applied assimilation techniques.
For a first quantification of the subsequent analysis we mention here some essential aspects of the climate model resolution. Vertically, we have 28 pressure levels (p), while in the horizontal direction we have 36 parallel circles (φ), and 60 meridians (λ). This coordinate system is posed (p,φ,λ). In the zonal direction, the longitudes λ are in degrees East, in the meridional direction the latitudes φ in degrees North, while in the vertical the positive direction is taken downwards so that the first pressure level is at a high altitude, or around 0.02 Pa and the 28th pressure level just above the surface for a value contingent upon each specific (φ,λ) location, as that relates to the topography of the planet. In the vertical direction, the used coordinate is a flow dependent hybrid pressure sigma, denoted no less simply as p. The climate model does not give directly pressure outputs, but pressure differences at given interfaces. In order to reach to required pressure priors for the ensuing analysis, a relevant mathematical treatment takes place, and is presented in appendix A. In any event, these pressures at the 28 vertical levels are known quantities, which in turn allow us to perform the presented methodologies of sections 2.3 – 2.4.5.

We also introduce the pertinent notation that will be used throughout the current study. For the vertical direction we introduce index k, for the meridional direction index j, and for the zonal direction index i. The index ranges are k = {1, 2, ..., 28}, j = {1, 2, ..., 36}, and i = {1, 2, ..., 60}. An equivalent notation pertaining to the climate model resolution is also (p_k,φ_j,λ_i), giving one location in the MGCM grid, out of the 28×36×60 = 60480 available ones. Additionally, we introduce sets giving coordinate values per direction; in the vertical we have D_p = {p_k}^{K}_{k=1}, in the meridional D_φ = {φ_j}^{J}_{j=1}, and in the zonal D_λ = {λ_i}^{I}_{i=1}, with k_max = K = 28 , j_max = J = 36 , and i_max = I = 60 as the maximum index values per direction. The focus lies in assimilating PDS TES radiances and OSS TES temperatures in the vertical direction, so from the three corresponding ranges the one that will be of a particular use to us is for index k.

Analytically, given the current assimilation problem, we also make a distinction between model and observation spaces. Given the fact that the climate model produces priors in the "sensible" $\mathbb{E}^3$ Euclidian space, then the corresponding pressures and temperatures abut on such a space. The climate model variables have a given spatiotemporal dependence and in view of that are regarded at one spatial position r at one time frame t. The position vector r denotes position measured from a global origin O (as
the point in space where we measure distances from), which is not explicitly defined herein but can be at the center of planet Mars (considering a more simplified spherical planetary geometry and not that of an oblate spheroid). One temperature value can then be posed \( T(\mathbf{r}, t) \), while a pressure value \( p(\mathbf{r}, t) \). Upon spatial discretization, the indices \((k, j, i)\) can be used to describe position. Similarly a temporal discretization \( t^n \) is introduced, with index \( n \) enumerating discrete time frames. One discretized temperature value can now be posed \( T(p_k, \varphi_j, \lambda_i, t^n) \equiv T_{k,j,i}^{n} \), giving one such climate model output at one vertical level, one parallel circle, and one meridian. For pressure values we have a similar notation involving a symbol \( p_{k,j,i}^{n} \). This symbol describes one pressure value at the same location as the temperature, following the same climate model evaluations, at the same time frame. Implicitly, we consider a mapping between the geographical coordinates \((\lambda, \varphi, r)\) and the current hybrid system \((p, \varphi, \lambda)\), where one pressure \( p \) is also related to an altitudinal level \( r \), given an applicable hypsometric equation.

As a closing remark of the current section, we have that the current study implements an ensemble Kalman filter (EnKF) assimilation approach [7], thereby involving ensemble members. An index \( m \) is introduced and used all through the current study, in order to enumerate ensemble members, originating from separate applications of the climate model. Therefore, we also introduce a more appropriate notation for the MGCM temperatures and pressures \( T_{k,j,i}^{n,(m)} \) and \( p_{k,j,i}^{n,(m)} \), in order to fully specify for which ensemble member we may refer to, its spatial location, and the corresponding time frame. The ensemble size herein is fixed at \( m_{\text{max}} = M = 16 \), with an index range \( m = \{1, 2, \ldots, 16\} \).

2.2 Filtering Methodology

The applied data assimilation scheme for both the retrieval and radiance cases stems from the ensemble Kalman filter (EnKF) [7]. Currently, for the prior (background), the background in observation space, and the posterior (analysis) only the ensemble means are taken into account. In the current section, the general equations being applied for both cases are presented.
For the analysis ensemble mean, we have equation

\[ \mathbf{x}_a = \mathbf{x}_b + \mathbf{K} (\mathbf{y}_o - \mathbf{y}_b) . \]  

(1)

In equation (1), \( \mathbf{x}_a \) is the analysis ensemble mean, \( \mathbf{x}_b \) the background ensemble mean, \( \mathbf{y}_b \) the background ensemble mean in observation space, \( \mathbf{y}_o \) the observations pertaining to each case, and \( \mathbf{K} \) the Kalman gain matrix. Generally, the overbars here denote such ensemble mean statistical estimations.

For both the retrieval and radiance data assimilation, the background states are the same. The process of how to obtain them is presented in section 2.3.1. For each case, these background states are derived from a horizontal interpolation of MGCM temperature outputs to a given satellite location \((\phi_s, \lambda_s)\), so that, per ensemble member \( m \), the background states \( \mathbf{x}_b^{(m)} \) are temperatures in \( \mathbf{K} \). An equivalent representation of the background ensemble state \( \mathbf{x}_b^{(m)} \) used herein is in matrix form as \( \mathbf{X}_b \). By construction, \( \mathbf{X}_b \) is a \( \mathbf{K} \times \mathbf{M} = 28 \times 16 \) matrix, so that in each column of it, we have one background ensemble member \( \mathbf{x}_b^{(m)} \), considered as a \( 128 \times 1 \) column vector.

Conversely, the observations \( \mathbf{y}_o \) and the background in observation space \( \mathbf{y}_b^{(m)} \), \( \forall m \), are different in each analysis case. In the retrieval data assimilation they are temperatures in \( \mathbf{K} \), whereas in the radiance data assimilation are spectral radiances in \( \text{mW} (\text{cm}^{-1})^{-1} \text{m}^{-2} \text{sr}^{-1} \). The observations \( \mathbf{y}_o \) are directly known; for the retrieval assimilation we have \( \mathbf{y}_o \) from the OSS TES temperature retrievals [6] and for the radiance assimilation \( \mathbf{y}_o \) from the PDS TES datasets respectively [18]. The background in observation space is evaluated from the general formulation \( \tilde{h}(\mathbf{x}_b^{(m)}) = \mathbf{y}_b^{(m)} \) in order to then evaluate \( \mathbf{y}_b \), or directly from \( \tilde{h}(\mathbf{x}_b) = \mathbf{y}_b \). A detailed explanation follows in sections 2.3.1 for the retrieval and in 2.4.1 for the radiance case. At this point it suffices to say that the forward model operator \( \tilde{h} \) for the retrieval assimilation performs one dimensional interpolation in the vertical direction on each \( \mathbf{x}_b^{(m)} \) in order to project it to observation space and thus yield \( \mathbf{y}_b^{(m)} \). For the radiance case, the argument of \( \tilde{h} \) is still temperatures \( \mathbf{x}_b^{(m)} \), the output though will be \( \mathbf{y}_b^{(m)} \) as spectral radiances. In the latter case, we have the
application of an atmospheric forward model operator modeled using the OSS method [15], not related to interpolation.

Similarly to the construction of $X_b$, for the background ensemble state in observation space we introduce matrix $Y_b$, with each column being one background ensemble member $y_b^{(m)}$ in observation space. The number of rows depends on implementation factors analyzed in the following sections. At this point we can mention that the number of rows for $Y_b$ follows the following classification; in sections 2.3.1 and 2.4.1 there is a separation if full and partial or valid observation space. The details appear in these two sections, yet necessity has it that portions of the full observation space for both the retrieval and the radiance assimilation need to be obviated. In the retrieval assimilation, the full observation space consists of 21 reference pressure levels, and in the radiance of 143 spectral channels, following the TES spectral resolution. From those 21 and 143 records, some are neglected so that only the remaining number of reference pressure levels and spectral channels will actually be used in the filtering process, a fact that is also viewed from the number of rows this $Y_b$ matrix will have.

The ensemble means are evaluated following the equations

$$
\bar{x}_b = \frac{1}{M} \sum_{m=1}^{M} x_b^{(m)} \Rightarrow (\bar{x}_b)_k = \frac{1}{M} \sum_{m=1}^{M} (x_b^{(m)})_k , \quad (2.a)
$$

$$
\bar{y}_b = \frac{1}{M} \sum_{m=1}^{M} y_b^{(m)} \Rightarrow (\bar{y}_b)_r = \frac{1}{M} \sum_{m=1}^{M} (y_b^{(m)})_r , \quad (2.b)
$$

where $m$ enumerates ensemble members, $k$ model space elements, and $r$ the elements of the appropriate observation space (full or partial, depending on the case).

The evaluation of the Kalman gain is achieved from

$$
K = \frac{1}{M-1} X_p Y_p^{tr} (R_o + R_b)^{-1} . \quad (3)
$$

In the formulation of equation (3), $R_o$ is the observations error covariance matrix, $R_b$ the background error covariance matrix in observation space, $X_p$ the background perturbations matrix, and $Y_p$ the background perturbation matrix in observation space. We may denote, tentatively, $R$ to be the number of elements of the applicable observation space. Then, the
dimensions of these sets are $\mathbb{R} \times \mathbb{R}$ for $\mathbf{R}_o$ and $\mathbf{R}_b$, $\mathbb{K} \times \mathbb{M}$ for $\mathbf{X}_p$, $\mathbb{R} \times \mathbb{M}$ for $\mathbf{Y}_p$, and $\mathbb{K} \times \mathbb{R}$ for $\mathbf{K}$. The evaluation of $\mathbf{R}_b$ follows

$$\mathbf{R}_b = \frac{1}{\mathbb{M} - 1} \mathbf{Y}_p \mathbf{Y}_p^\text{tr}.$$

(4)

For the perturbation matrices, we have a subtraction from each row of $\mathbf{X}_b$ the corresponding value of the background ensemble mean $\mathbf{x}_b$, and from each row of $\mathbf{Y}_b$ the background ensemble mean in observation space $\mathbf{y}_b$. Formalistically, we have

$$(\mathbf{X}_p)_{k,m} = (\mathbf{X}_b)_{k,m} - \bar{x}_k,$$

(5.a)

$$(\mathbf{Y}_p)_{r,m} = (\mathbf{Y}_b)_{r,m} - \bar{y}_r,$$

(5.b)

for the element $(k,m)$ of $\mathbf{X}_p$, and similarly for $(r,m)$ of $\mathbf{Y}_p$.

As a closing remark, from equation (3) we have the inversion of matrix $\mathbf{R}_o + \mathbf{R}_b$. It may be so that $\mathbf{R}_b$ will not be full rank, yet $\mathbf{R}_o$ is always set by construction diagonal, with main diagonal elements equal to $\sigma_o^2$, where $\sigma_o$ is the standard deviation of the observations, in the same physical units as the observations. According to this formulation of $\mathbf{R}_o$, which will be full rank, the same applies to $\mathbf{R}_o + \mathbf{R}_b$, thus rendered invertible so that in the current study we do not face any dimensionality issues.

Regarding the application of the ensemble Kalman filter described in the current section, we also offer two additional remarks; equation (3) for the evaluation of the Kalman gain matrix differs from the equation that was historically first introduced for $\mathbf{K}$. This equation was posed originally as

$$\mathbf{K} = \mathbf{P}_b \mathbf{H}^\text{tr}(\mathbf{R}_o + \mathbf{H} \mathbf{P}_b \mathbf{H}^\text{tr})^{-1}.$$

(6)

Equations (3) or (6) are both for the evaluation of $\mathbf{K}$. In equation (6), matrix $\mathbf{P}_b$ is the model space error covariance matrix, and $\mathbf{H}$ is the applicable forward model operator in matrix form. However, in order to be able to formulate $\mathbf{H}$ in the first place, the mapping of model to observation space typically needs to follow some spatial interpolation scheme, like in the retrieval assimilation. Theoretically, for the retrieval assimilation equation (6) is directly applicable, but not for the radiance assimilation. In the latter case, the mapping of
model to observation space, that is the process of mapping atmospheric temperature profiles to spectral distributions of radiance, does not follow interpolation schemes, so that \( H \) is not even extant. Eventually, we apply equation (3) for both assimilations for conformity and for the bypassing of the evaluation of \( P_b \), which is not a prerequisite for the filtering application. The second remark is in relation to the fact that this EnKF includes flow dependent covariances obtained from the climate model ensemble member outputs.

### 2.3 Retrieval Data Assimilation

The first main consideration of this study involves the retrieval data assimilation. In this case the background originates from the MGCM outputs. The assimilation model space is expressed in terms of the natural logarithm of a horizontally \( \varphi - \lambda \) interpolated ensemble mean pressure of the climate model at a satellite location \((\varphi_s, \lambda_s)\), across all 28 model levels, as that relates to the discretization of the MGCM. The background ensemble state \( x_b^{(m)} \), \( \forall m \), is represented in terms of MGCM temperature outputs, again interpolated to the satellite location in a manner identical as for the pressures. The observation space is given from the natural logarithm of a spatiotemporal fixed reference pressure profile given from table 2.1, presented below. The observations \( y_o \) are temperatures, directly available from the OSS TES temperature retrievals, assumed at the reference pressure levels. The reference pressure levels are in total 21, and so are the observations, as opposed to the 28 background pressure levels and temperatures (per ensemble member).

<table>
<thead>
<tr>
<th>Fixed (spatially and temporally independent) reference pressure values, defining the full observation space in the retrieval data assimilation, in Pascal. The data are to be read per row, from left to right.</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.072</td>
</tr>
<tr>
<td>224.407</td>
</tr>
<tr>
<td>1005.720</td>
</tr>
</tbody>
</table>
2.3.1 Retrieval Model and Observation Spaces

In the context of the retrieval data assimilation, on one hand we consider the OSS TES temperature retrievals [6], as the observations $y_o$ at the corresponding reference pressure levels (table 2.1), and on the other hand climate model outputs for temperature and pressure as well. The observed temperatures are always related to a satellite position, denoted $(\varphi_s, \lambda_s)$, whereas the gridded MGCM output temperatures are given originally $T_{k,j,i}^{n,m}$, as in section 2.1. With regards to the spatial consideration, we have that the satellite position does not coincide with any horizontal $(\varphi_j, \lambda_i)$ MGCM discretized location. According to that, in order to evaluate the retrieval innovations $y_o - \overline{y}_b$ we need to perform a series of interpolations on the $T_{k,j,i}^{n,m}$ climate model profiles. Additionally, the time frame $n$ of a given MGCM output may not exactly correspond to the time frame of when the satellite measurement occurred. The MGCM outputs exist within a $\pm 1 \ h$ time window, centered at the time of the satellite measurements, yet that does not inhibit us from performing the data assimilation given the fact that one background is but a subjective first guess, presumably close to the system state of when the observations are taken.

In general, we may write for a background temperature $T_b(r_b,t)$ and for an observed temperature $T_0(r_o,t)$. These variables abut on one point in the sensible space $\mathbb{E}^3$, where $r_b, r_o \in \mathbb{E}^3$, are the corresponding position vectors. Commonly, it may be so that the positions $r_b$ are different from $r_o$, so that the model and observation spaces may not coincide.

In this particular case, given the procurement nature of the observations, we may write $T_0(p_q, \varphi_s, \lambda_s, t)$. Given the fact that the exact time frame is not exactly a crucial aspect of the analysis, we completely obviate the presence of $t$, and thus write $T_0(p_q, \varphi_s, \lambda_s)$. The coordinate $\lambda_s$ is the satellite longitude, $\varphi_s$ is the satellite latitude, and $p_q$ is the reference pressure level coordinate, in $\text{Pa}$. In table 2.1 we have the fixed and time independent values for $p_q$, with a corresponding index range $q = \{1, 2, \ldots, 21\}$, so that $q_{\text{max}} = Q = 21$ is the total number of reference pressure levels, as that relates intrinsically to the PDS TES or OSS TES data sets. Then, at the satellite position, the observations are in total 21.
On the other hand, from any MGCM output we have for the background temperature profiles \( T_b(p_k, \varphi_j, \lambda_i; m) \). Per ensemble member \( m \), the total number of these temperatures are \( K \times J \times I = 28 \times 36 \times 60 = 60480 \). As a result, from the entire repertoire of the background information, we need to take into account only the most relevant subset which is at first achieved by interpolating \( T_b \) or \( T_{k,j,i}^{(m)} \) horizontally, in the \( \varphi - \lambda \) domain, at the satellite position \((\varphi_s, \lambda_s)\) (index \( n \) is dropped).

A similar reasoning stands for the MGCM pressures as well. From equation (A.6) of appendix A, we have a profile \( p_{k,j,i}^n \) or \( p_{k,j,i} \), with a total number of elements equal to 60480, stemming from the ensemble mean of the \( M = 16 \) ensemble members of the MGCM outputs (given originally in terms of the pressure differences at the interfaces). A two dimensional \( \varphi - \lambda \) interpolation is to be performed here as well, in order to estimate, along with the background temperatures, the inferred (interpolated) MGCM outputs at the satellite position \((\varphi_s, \lambda_s)\).

The technical details of a two dimensional interpolation are given in appendix B. From the analysis unveiled there, several key points arise, the most important of which for here are that this \( \varphi - \lambda \) interpolation is performed locally and in a domain that exhibits periodicity in the longitudinal direction, close to the prime meridian, at \( \lambda = 0^\circ \).

Assuming some of the notation of appendix B, here we write for the local regime of interpolation a Cartesian product \( D^{(L)}_{\varphi} \times D^{(L)}_{\lambda} \), where the superscript \( (L) \) denotes the local nature of the global sets \( D_{\varphi} = \{ \varphi_j \}_{j=1}^J \) and \( D_{\lambda} = \{ \lambda_i \}_{i=1}^I \), given in section 2.1. If the local regime of interpolation has two elements per direction, that is the two closest neighbors of \( \varphi_s \) in the \( \varphi \) direction from \( D_{\varphi} \), and the two closest of \( \lambda_s \) in the \( \lambda \) direction from \( D_{\lambda} \), the interpolation is bilinear. We may extend that to include up to 5 to 7 closest latitudinal and up to 7 to 12 longitudinal neighbors to \( \varphi_s \) and \( \lambda_s \) respectively, for a better estimation of the horizontally interpolated MGCM pressures and temperatures. Of course, the evaluation of those closest neighbors that formulate \( D^{(L)}_{\varphi} \) and \( D^{(L)}_{\lambda} \) is a part of the interpolation procedure. A noteworthy detail is related to some interesting satellite positions. Extra care must be put when the value of \( \varphi_s \) is very close to the southern most or
northern most parallel circles (close to the polar caps), or when \( \lambda_s \) is very close to the prime meridian due to the periodicity of the domain in the zonal direction.

Following appendix B, from the performed \( \varphi - \lambda \) interpolation we estimate 28 values for pressure, and \( 28 \times 16 \) for temperature, that is 28 temperature values for the 16 ensemble members. At this point, we denote these horizontally interpolated variables \((p_b)_k\) and \((T_b^{(m)})_k\), for pressure and temperature respectively. The subscript "b" denotes the background, stemming originally from an MGCM output. Index \( k \) continues to enumerate vertical levels as in the MGCM grid, but since currently the profiles of \((p_b)_k\) and \((T_b^{(m)})_k\) pertain not on a \((\varphi, \lambda)\) but on the \((\varphi_s, \lambda_s)\) location, this index \( k \) will hereafter be dubbed the model space index for both retrieval and radiance data assimilations. For the observations at \((\varphi_s, \lambda_s)\), we introduce the notation \((p_o)_q\) and \((T_o)_q\), where the subscript "o" denotes the OSS TES observations (temperature retrievals).

For the retrieval data assimilation, to make the connection with the nomenclature of section 2.2, we have for the background ensemble state \(x_b^{(m)}\), \( \forall m \), the profiles \((T_b^{(m)})_k\), and for the observations \(y_o\), the profile \((T_o)_q\). Essentially, \(x_b^{(m)}\) is represented by matrix \(\mathbf{X}_b\) with dimensions \(K \times M = 28 \times 16\), and \(y_o\) is represented as a column vector, originally with \(Q = 21\) elements.

The next step of the process involves the definitions of the assimilation model and observation spaces, numerically. Innately, we always have 21 elements for \((p_o)_q\). However, there are two constraints here that limit these reference pressure levels to a maximum of 21, but almost never equal to 21. The first constraint is a physical one; some \((p_o)_q\) values may be greater than the skin pressure and so go below the ground. The other constraint is that below \((p_b)_{28}\), there is no additional information related to the background. Primarily due to the second constraint, from the 21 reference pressure levels we are to consider only those for which \((p_o)_q < (p_b)_{28}\). From this inequality, we obtain a value \(r_{\text{max}} \leq q_{\text{max}}\), where index \( r \) specifies the valid reference pressure levels, and so the valid retrieval observation space. As explained later on in the current section, we also need to evaluate the retrieval forward model operator \(\mathbf{H}\), for which calculation we need the
model and valid observation space coordinates so that no extrapolation is performed in the evaluation of $\mathbf{H}$. In spite of the fact that we use the notation $\mathbf{H}$, pertaining to a linearized version of the formulation $\mathbf{h}(\mathbf{x}^{(m)})$, for the retrieval assimilation that is still applicable, considering section 2.2. Rewriting $(p_o)_q$ and $(T_o)_q$, to $(p_o)_r$ and $(T_o)_r$, hence we will refer to the valid reference pressure levels and observations.

The model and valid observation spaces, are defined

$$\xi_k \equiv \ln((p_b)_k),$$

$$\zeta_r \equiv \ln((p_o)_r),$$

for each $k$, $r$ model and valid observation space index values. This generalized coordinate $\xi_k$ is the natural logarithm of the horizontally interpolated MGCM pressure taken from the ensemble mean, for each model space index value $k$. The other one $\zeta_r$ is the natural logarithm of the valid reference pressure levels. Both coordinates have units in $\ln(\text{Pa})$.

These spaces are also given in terms of $D_\xi = \{\xi_k\}_{k=1}^{K}$ and $D_\zeta = \{\zeta_r\}_{r=1}^{R}$, like in appendix B. Consequently, the observations column vector $\mathbf{y}_o$ will only have its first $r_{\text{max}} = R \leq 21$ elements, with the rest dropped.

In the beginning of this section we had general notations $T_b(\mathbf{r}_b, t)$ and $T_o(\mathbf{r}_o, t)$. Given the previous analysis, at this point we may also write $(T^{(m)}_b)_k = T^{(m)}_b(\xi_k)$ for the background ensemble state, and $(T_o)_r = T_o(\zeta_r)$ for the valid observations, pertaining to $\mathbf{x}^{(m)}_b$ and $\mathbf{y}_o$ respectively. The last performed step involves the evaluation of the background in observation space $\mathbf{y}^{(m)}_b$, corresponding to matrix $\mathbf{Y}_b$ of section 2.2, with dimensions $R \times M$. Appendix C analyzes this very process. From equation (C.1), $\mathbf{h}(\mathbf{x}^{(m)}_b) = \mathbf{y}^{(m)}_b$, which can be put equivalently in terms of $\mathbf{H} \mathbf{x}_b = \mathbf{Y}_b$, we have the necessary operation illustrated. After the evaluation of the retrieval forward model operator $\mathbf{H}$, and the evaluation of the retrieval background ensemble state in observation space $\mathbf{y}^{(m)}_b$ or $\mathbf{Y}_b$, we have all the required components to perform the retrieval data assimilation at the satellite position.
2.3.2 Retrieval Global Approach

In the retrieval global data assimilation approach, every available observation, from the valid ones, is taken into account when we perform the analysis at each model space grid point \( k \). In this regard the value of \( r_{\text{max}} = R \) will be the greatest possible, for each examined case (from section 2.3.1). For the retrieval global approach we then have the application of the equations of section 2.2 for the evaluation of \( X_p, Y_p, R_b, \) and \( K \), and the analysis is performed in one step, from \( x_a = x_b + K \bar{d} \), where \( \bar{d} = y_o - y_b \) the observation increments (innovations), represented as an \( R \times 1 \) column vector.

For a performed sensitivity analysis, the observation standard deviations are taken \( \sigma_o = 3.0 \) \( \mathbf{K} \) and \( \sigma_o = 5.0 \) \( \mathbf{K} \), when we construct the diagonal form of matrix \( R_o \). In the first case, where the observations procurement error is assumed less, the filter is expected to trust the observations \( y_o \) more than in the second case and that is expected to be reflected in the results as well.

2.3.3 Retrieval Local Approach

Data assimilation implementations may be treated in terms of a global or a local approach. The term *global* data assimilation refers to the fact that for every model space grid point we incorporate *every* available observation existing within the model space domain. Even if there are observations outside of the model space, these will be neglected, so that spatial extrapolations will never be performed. In the Martian case we never consider the two polar caps or in the vertical direction those reference pressure levels than fall outside of the retrieval assimilation model space (see section 2.3.1). Therefore, otherwise existing observations that fail to exist within the assimilation model are excluded from the filtering process, leaving us with only the *valid* observations, as a subset of the available ones.

These valid observations alongside the model space variables are deemed to be stochastic variables. The total number of stochastic variables are as many as the number of model space grid points times the plentitude of physical variables we consider per ensemble member, plus the total number of valid observations. A very pertinent statistical quantity used in the context of data assimilation is the correlation coefficient or a proxy measure of it, which may be an appropriate covariance matrix, pertaining to the assimilation model or
observation spaces. For a simple scalar case involving two stochastic variables $x$ and $y$, the correlation coefficient is defined

$$\rho(x, y) = \frac{\text{COV}(x, y)}{\sigma(x) \sigma(y)},$$

(8)

where $\text{COV}(x, y)$ is the covariance between $x$ and $y$, with $\sigma(x)$ and $\sigma(y)$ being the standard deviations of those two variables. The denominator terms are essentially normalization factors so that $|\rho(x, y)| \leq 1$. In practice, despite whatever statistical assumptions we make for the stochastic variables we deal with, moments of unknown probability density functions like the standard deviations or the covariances are always estimated statistically. From equation (3) we have for instance $R_o$ and $R_b$, as the statistical estimates of the covariances of the observations $y_o$ and the background ensemble state in observation space $y_b^{(m)}$, which also present a measure for the correlations between these variables, following equation (8). Considering the formulation of Kalman gain $K$ from equation (3) and its presence in the analysis equation (1) it follows that the correlations or the covariance matrices play an important role in the execution of the assimilation as they impact the analysis ensemble mean vector $x_a$.

From a physical standpoint, if the absolute valued correlation coefficient between two variables is close to unity that means that one stochastic variable is related to the other, so that changes in one entail changes in the other and vice versa. From a dynamical perspective, in a case such as this, it would then be irrelevant what the spatial distance between those two variables would be, as one would be in the position to influence the other. Therefore, the correlations or the covariance matrices in data assimilation offer a means with which we may ascertain the statistical importance of each involved stochastic variable in the analysis. For the retrieval assimilation performed in this study that is true, considering that both spaces are natural logarithms of pressure; pressure can be mapped to altitude given an appropriate hypsometric equation, so that the concept of the physical distance can be then substantiated.

Estimating covariance matrices offers insights in the spatial distribution of the correlation structures of the variables, and also points to their statistical importance. Nevertheless, these statistical estimations stem from a limited sample size, that is how many variables we can afford to consider in the analysis. Sample size is governed by ensemble
size. Equations (2.a), (2.b), or (4) involve summations over the ensemble index \( m \); for greater ensemble sizes we may then estimate statistical moments more accurately and in turn the spatial correlation structures may then be more dependable. In practice, the sample size is limited so that we cannot be entirely certain of the estimated moments, and thereby of the statistical importance of the involved variables. If a limited sample, due to a limited ensemble size, is characterized by sampling errors, this may give rise to the estimation of spurious correlations, which may be misleading and give erroneous spatial correlation structures. In a case such as this the potential dynamical, thermodynamical, or radiative impact of the valid observations to the performed assimilation at one model space grid point may result to fraudulent posterior results.

To bypass the issue of the spurious correlations we resort to a local data assimilation. It is a method that forcefully neglects observations that are farther away from one model space node where the assimilation is performed, considering that it is more likely that local observations will be correctly correlated to that node, than observations that are more distanced. If the model and observation spaces are linked to space \( \mathbb{E}^3 \), like in the retrieval assimilation, we then may say that the local approach involves a distance related criterion that cuts off remote observations, the statistical importance of which in the analysis is not exactly certain. The local approach is not the most optimal way to perform the analysis, but given the limited sample size of these stochastic processes it offers a more reliable course of action. Ideally, for very large sample sizes we would not need to localize, were we convinced of the accuracy of the correlation structures, but due to the computational cost involved in greater ensemble sizes the localization offers a reliable alternative.

Before proceeding to the implementation specifics of the retrieval local assimilation, we present examples highlighting correlation structures as in equation (8), only in terms of the model space error covariance matrix \( P_p \), appearing in equation (6). This form of the Kalman gain formulation is not used here, but it is an alternative way to perform the analysis. Matrix \( P_p \) is evaluated from

\[
P_p = \frac{1}{M-1} X_p X_p^\text{tr},
\]

a form that is also related to the ensemble size, and through that the sample that we have available. The following two figures 2.1 and 2.2 are a graphical representation of this
K × K = 28 × 28 matrix for two examined profile cases, 1374/8664 of 000155700 and 7600/7952 of 000239506.

**Figure 2.1.** Model space error covariance matrix $P_b$ for the profile case of 1374/8664 of 000155700.
From figures 2.1 and 2.2 we have the spatial distributions of the statistical estimations of the error covariances of the model space, for here given in terms of pressures in Pa. The ensemble size is \( M = 16 \), with the model space resolution fixed at \( K = 28 \). Through the background perturbation matrix \( \mathbf{X}_p \), we have the statistical estimation of the background ensemble mean \( \mathbf{x}_b \), which for greater ensemble sizes becomes more accurate, and so do the covariances. For greater model space resolutions, the results become finer. Similar reasoning applies to the observation space for matrix \( \mathbf{R}_b \) for instance. Greater ensemble sizes and more dense observations will be conducive to better analysis estimates while further obviating the need for localization. For more modest sample sizes and sparser resolutions in either space, the localization is then deemed more significant.

In the context of the current study now, we have equation (3) which is eligible to modifications so that it can be applied individually for each model space node in a process explained hereafter. Let the total number of valid observations be \( r_{\text{max}} = R \). In the retrieval data assimilation (from section 2.3.1) it is \( R \leq Q = 21 \), where the total number of
model space grid points is fixed at $K = 28$. In a global data assimilation approach, for each model space node $k$, we incorporate information from all $R$ valid observations, as in section 2.3.2.

In order to bypass the global assimilation approach, we apply localization techniques that are case specific to each consideration. In the retrieval case, at node $k$ we have coordinate $\xi_k$ and the model variable $(\bar{x}_b)_k$, that is $\overline{T_b}(\xi_k)$, where $\bar{\quad}$ overbar denotes the background ensemble mean (temperature). We wish to evaluate $\overline{T_a}(\xi_k)$, namely $(\bar{x}_a)_k$ at $\xi_k$ in such a manner that we do not implement $\bar{x}_a = \bar{x}_b + K(y_o - \bar{y}_b)$ in its entirety but only for a proper local subset of the innovations $y_o - \bar{y}_b$, and $K$. In the retrieval case where the background and the background in observation space are both temperatures abutting on pressure levels, we may apply a localization criterion based on distance in model and observation spaces $D_{\xi}$ and $D_{\zeta}$, [9], [11]. We then consider for every $\xi_k$, a local regime of assimilation so that the valid observations $(y_o)_r$ taken into account in the analysis need to exist within that local subset of $D_{\xi}$, and an ad hoc vertical localization cut off distance is then introduced.

Following section 2.3.1 we have for the horizontally interpolated MGCM ensemble mean pressures at the satellite position the symbol $(p_b)_k$, the natural logarithm of which gives $\xi_k$, following equation (7.a). The numerical figures are such that $(p_b)_1 = 0.02$ Pa and $(p_b)_{28}$ in the range $300 - 800$ Pa (also seen in appendix A). Correspondingly, $\xi_1 \sim -4 \ln(\text{Pa})$ and $\xi_{28} \sim 6.5 \ln(\text{Pa})$, so that $\xi_{28} - \xi_1 \equiv (\Delta \xi)_{\text{max}} - 10 \ln(\text{Pa})$. As we proceed from lower pressure levels towards the ground, these $(p_b)_k$ values become more dense so that $\xi_{k+1} - \xi_k$ becomes less and less until it reaches a value of $\sim 0.01$. At the same time, the reference pressure levels (table 2.1) start at $(p_o)_r = 11.173$ Pa until typically between $(p_o)_r = 369.984$ Pa and $(p_o)_r = 783.255$ Pa, for a total number of valid observations in the range $15 - 18$, out of 21. The majority of the $\zeta_r$ values are for $k > 15$, so that if we apply a constant distance criterion, for certain $k$ values closer to the ground we will incorporate almost every observation. In a case such as this there would be no effective localization. Instead, we introduce a localization distance that is $k$ dependent, in other words is related to each location of the model space where we localize.
We introduce a local factor $f_f$

\[ f_f = c (\Delta \xi)_{\text{max}}, \quad (10) \]

where $c = \{0.015, 0.030\}$ is an ad hoc dimensionless parameter whose values scale $(\Delta \xi)_{\text{max}}$ appropriately. Coefficient $c$ assumes these two values for sensitivity analysis reasons, as that relates to the numerical figures encountered in this specific problem. The greater the value of $c$, the larger the local domain for each $\xi_k$ is, so that more $(y_o)_f$ observations are taken into account in the analysis. A left $\xi_{lb}$ and right $\xi_{rb}$ bounds are introduced from

\[ \xi_{lb} = \xi_k - f_f \xi_k, \quad (11.a) \]
\[ \xi_{rb} = \xi_k + f_f \xi_k, \quad (11.b) \]

so that $\xi_k$ is the median $\xi_k = \frac{\xi_{rb} - \xi_{lb}}{2}$. Visually, we have the following figure 2.3.

**Figure 2.3.** Conceptual draft outlining the establishment of the local domain of the assimilation model space (for both retrieval and radiance).

For every model space grid point $\xi_k$, we introduce a local subset of the global model space $D_\xi$, like $D_\xi^{(f)} : \xi \in [\xi_{lb}, \xi_{rb}]$, so that if an observation $(y_o)_f$ abutting on the observation space grid point $\xi_r$ is to be taken into account in the analysis, then it needs to be $\xi_r \in D_\xi^{(f)}$. This set $D_\xi^{(f)}$ is then the local regime of assimilation.

During an analysis cycle we then have three possible cases; one is for when no observations exist within $D_\xi^{(f)}$, the second being for when only one observation exists in
D(ξ)\(^{(f)}\), and the third is for when more than one observation is in \(D(ξ)\(^{(f)}\). This distinction is made for technical reasons, as that impacts the dimensions of the ordered sets used in the analysis filtering equations.

In the first case (no local observations) no analysis is performed. The analysis ensemble mean \((\bar{x}_a)_k\) at \(ξ_k\), is evaluated \((\bar{x}_a)_k = (\bar{x}_b)_k\). In the second case, we have only one observation in \(D(ξ)\(^{(f)}\). We may visualize this from the following figure 2.4.

![Figure 2.4](image)

**Figure 2.4.** Conceptual draft outlining the first valid observation to be used in the localized retrieval data assimilation.

From the set of the valid observations \(y_o = \{ (y_o)_r \}_{r=1}^R\), we first need to locate the one existing within \(D(ξ)\(^{(f)}\). If we denote \(r'\) that \(r\) index value, out of \(\{1, 2, ..., R\}\), for which it is \(ξ_{r'} \in D(ξ)\(^{(f)}\), then the analysis proceeds as follows; the global perturbation matrices \(X_p, Y_p\), with global dimensions \(K \times M, R \times M\), are now rendered local. We introduce the symbols \(X_p\(^{(f)}\) and \(Y_p\(^{(f)}\) in order to represent these local arrays with local dimensions \(1 \times M\) for both, that is they are now treated as row vectors. For \(X_p\(^{(f)}\) we have the \(k\)–th row of \(X_p\), like \((X_p\(^{(f)}\))_m = (X_p)_k,m, \forall m\), and for \(Y_p\(^{(f)}\) the \(r'\)–th row of \(Y_p\), like \((Y_p\(^{(f)}\))_m = (Y_p)_r',m, \forall m\). Computationally, the global sets \(X_p, Y_p\) are pre evaluated only once, for each examined case. For Kalman gain, it will be

\[
K\(^{(f)}\) = \frac{1}{M-1} X_p\(^{(f)}\) Y_p\(^{(f)}\)^{tr} (R_o\(^{(f)}\) + R_b\(^{(f)}\))^{-1}, \quad (12)
\]

with

\[
R_b\(^{(f)}\) = \frac{1}{M-1} Y_p\(^{(f)}\) Y_p\(^{(f)}\)^{tr}. \quad (13)
\]
The transpose $\mathbf{Y}_p^{(f)\text{tr}}$ will have dimensions $M \times 1$ (column vector), the observation error covariance matrix $\mathbf{R}_o^{(f)}$ now is $1 \times 1$ (scalar), as is the case for the background error covariance matrix $\mathbf{R}_b^{(f)}$ in observation space. From equation (12) we then have that $\mathbf{K}^{(f)}$ is a scalar, so that the performed analysis assumes the form

$$\left(\mathbf{X}_a\right)_k = \left(\mathbf{X}_b\right)_k + \mathbf{K}^{(f)} \left(\mathbf{Y}_o^{(f)} - \mathbf{Y}_b^{(f)}\right). \quad (14)$$

The background observation at location $r'$, is obtained directly from the $r'$-th row of the already evaluated $\mathbf{y}_b$, given from $\mathbf{H} \mathbf{x}_b$, or $\mathbf{H} \mathbf{X}_b$.

The last case is for a total population of local observations more than one. Here we need to find the very first $r'$ value for which it is $\zeta_r' > \zeta_{\text{lb}}$ and construct the local observation space $\mathbf{D}_\zeta^{(f)}$, with index values $\{r', r'+1, r'+2, \ldots\}$ from the global $\mathbf{D}_\zeta$, with a total number of elements equal to the number of the observations that are within $\mathbf{D}_\zeta^{(f)}$.

For the evaluation of the Kalman gain we have a similar reasoning as previously, with a few differences; the set $\mathbf{X}_p^{(f)}$ is as in the second case (row vector), whereas the set $\mathbf{Y}_p^{(f)}$ now has dimensions $R' \times M$, where $R'$ can be 2, 3, or more depending on the number of the local observations. Similarly, for $\mathbf{Y}_p^{(f)\text{tr}}$ we have $M \times R'$, and for $\mathbf{R}_o^{(f)}$, $\mathbf{R}_b^{(f)}$ dimensions $R' \times R'$, so that $\mathbf{K}^{(f)}$ becomes $1 \times R'$ (row vector). For the elements of $\mathbf{Y}_p^{(f)}$ we have in its first row the corresponding $r'$-th row of the global $\mathbf{Y}_p$, in its second row the corresponding $r'+1$ row of $\mathbf{Y}_p$, and so on, $\forall m$. Matrix $\mathbf{R}_o^{(f)}$ is still diagonal, as in the global case, with diagonal elements $\sigma_o^2$, and $\mathbf{R}_b^{(f)}$ follows equation (13).

After the evaluation of the elements of $\mathbf{K}^{(f)}$, we implement the analysis equation

$$\left(\mathbf{X}_a\right)_k = \left(\mathbf{X}_b\right)_k + \mathbf{K}^{(f)} \left(\mathbf{Y}_o^{(f)} - \mathbf{Y}_b^{(f)}\right), \quad (15)$$

where the local subsets of the observations and the background in observation space have dimensions $R' \times 1$, with elements in their respective first rows $(\mathbf{y}_o)_{t'}$, $(\mathbf{y}_b)_{t'}$, in their second record $(\mathbf{y}_o)_{t'+1}$, $(\mathbf{y}_b)_{t'+1}$, and so on. The above process loops over the entire
model space, for each model node \( k \), thus updating each analysis ensemble mean individually.

The following histogram visualizes the local observations counter, per model space node, for an examined profile 7600/7952 of 000239506. In the absence of a spatial localization scheme, the applied analysis equation is (1). In this case, it can be seen that per \( k \) value, every valid observation will be used in the analysis, whereas in the presence of a spatial localization scheme we use only an appropriate sub set of the valid observations.

From figure 2.5, for low pressure levels there are no observations in the domain \( D^{(f)}_\xi \) thus no data assimilation is performed. For pressure levels closer to the surface the used observations are certainly less than the total (in this case 14), with populations that are sensitive to the value of the coefficient \( c \), as that relates to the aforementioned analysis.

![Figure 2.5](image_url)

**Figure 2.5.** For a histogram portraying the accounted observations, per model space grid point \( k \), in a localized retrieval data assimilation. The corresponding profile is 7600/7952 of 000239506. The orange bars are for localization coefficient value \( c = 0.030 \), while the blue bars for a smaller value \( c = 0.015 \), signifying the spatially reduced local neighborhood, in model space.
2.3.4 Retrieval R Modulation

In the retrieval data assimilation alone, we perform one additional step in the analysis process. This step involves an $R_o$ – localization, or modulation [9]. From the one dimensional (scalar) Kalman filtering equations, the Kalman gain is given

$$K = \frac{H \sigma_b^2}{H^2 \sigma_b^2 + R_o},$$

(16)

where $\sigma_b^2$ is the background (model space) variance, $H$ the forward model operator, and $R_o$ the observation space variance (all scalar). From equation (16) the greater the value of $R_o$, the less $K$ becomes. From the analysis equation of the scalar case it also is

$$\bar{x}_a = \bar{x}_b + K (y_o - \bar{y}_b),$$

so that as $R_o$ becomes greater, the contribution of the observational increment $y_o - \bar{y}_b$ becomes less significant. Since the reciprocal of any variance is the corresponding accuracy, in this regard a value of $R_o$ is reversely proportional to the accuracy of an observation, so that this observation becomes less important in the Kalman filtering process as the values of $R_o$ increase. This is generalized for the multi-dimensional case as well.

The modulation of the elements of $R_o$ involves a practice which renders some observations, in an artificial manner, less important in the filtering process. Considering the previous paragraph and equation (16) in conjunction with the fact that in a localized approach we only consider those valid observations falling within the local regime of assimilation, we perform this extra step in order to lessen ever more the importance of the used local observations being farther away from the model space node where the assimilation is performed. Valid observations within the local regime of assimilation are not equally distanced from the assimilation model node, so within this local regime $D^{(f)}_\xi$ we 

modulate ever further as one additional fail safe measure, again in hopes that the evaluated posterior may be better. In the current context we introduce a function

$$\rho(k,r) = \rho_{k,r} \equiv \exp \left[ \frac{(\xi_k - \xi_r)^2}{2 \left( \mu \xi_k^2 \right)^2} \right],$$

(17)
stemming from the more general structure of $\exp\left(\frac{d^2}{2L^2}\right)$, where $d$ is the distance between a given model space node and some other observation location and $L$ a fixed parameter as the model space modulation distance. In this case we have $L = \mu \xi_k$, with $\mu = 0.32$, $\forall k$. This value of $\mu$ is of an ad hoc nature, and is obtained practically, given the numerical figures and their range, of the current retrieval assimilation problem.

For the case in which we have only one observation in the local domain $D_{\xi}^{(f)}$, $R_o^{(f)}$ is a scalar. Like stated in section 2.3.3, by evaluating the index value $r'$, we ascertain the location of the observation $(y_o)_{r'}$, at $\zeta_{r'}$. By introducing the modulated matrix $\tilde{R}_o^{(f)}$, its one element is then given $\rho_{k,r'} \sigma_o^2$, with $\sigma_o = \{3.0, 5.0\} K$, evaluated for that particular model space node $k$.

For the case where we have more than one observations $R_o^{(f)}$ is an $R' \times R'$ matrix. If for example the locations of the observations are given from $\{r', r'+1, r'+2\}$, then $R' = 3$. We introduce another diagonal matrix $\mathcal{P}$ with dimensions $R' \times R'$, with its main diagonal elements being $\mathcal{P}_{1,1} = \rho_{k,r'}$, $\mathcal{P}_{2,2} = \rho_{k,r'+1}$, and $\mathcal{P}_{3,3} = \rho_{k,r'+2}$ (similarly for a generalization), so that the main diagonal elements of $\tilde{R}_o^{(f)}$ are calculated from $\rho_{k,r'} \sigma_o^2$, $\rho_{k,r'+1} \sigma_o^2$, and $\rho_{k,r'+2} \sigma_o^2$. This operation can be put in terms of a Schur product, $\tilde{R}_o^{(f)} = \mathcal{P} \circ R_o^{(f)}$, and past that point we implement the previous steps of section 2.3.3, where instead of the original matrix $R_o^{(f)}$, will now have the modulated $\tilde{R}_o^{(f)}$. 
2.4 Radiance Data Assimilation

The second focal point of this study is engaged with the radiance data assimilation. This case shares some similarities with the retrieval assimilation; the background is the same as before as in section 2.3.1, meaning we still assume the satellite location \((\phi_s, \lambda_s)\) and the model space \(D_z\) on which the background temperatures \(x_b^{(m)}, \forall m\), exist upon. That being said, in the radiance case we do not perform the same interpolations applied in the retrieval assimilation, rather we use these already evaluated results in the radiance assimilation as well. The objective is to evaluate the analysis ensemble mean \(\bar{x}_a\) using the exact same equations of section 2.2, where now the differentiation is that the observation space is a portion of the electromagnetic spectrum (a spectral space) and the observations \(y_o\) are spectral radiances at prescribed channels of that spectral space.

With regards to a clarification pertaining to the terminology "spectral" radiance, we have that radiance alone, as a term, is insufficient. That is because we may have the spectral distribution of radiance, or a spectrally integrated radiance. In the first case, a typical notation of the distribution of radiance with respect to a spectral coordinate, is \(L_{dv}\). In the second case we have \(L_{\Delta v}\), where the two are related:

\[
L_{\Delta v} = \int L_{dv} \, dv. \tag{18}
\]

In the following we will speak of a spectral radiance value at one spectral channel, \(n\). Originally, this index \(n\) was used as a temporal index for MGCM outputs, yet hereon it will denote a channel in spectral space. Even though the used notation is \(L_n\), a symbol like that pertains only to \(L_{dv}\). In table 2.2 at the end of the current section we have the relevant values of the spectral coordinate used in the current study. An exact "monochromatic" channel does not exist. When we consider a value for \(L_n\), that is perceived in a very narrow waveband centered at that \(n\)–th channel value. What is mentioned here can also be seen from the physical units of the spectral radiance; they are \(\text{mW} (\text{cm}^{-1})^{-1} \text{m}^{-2} \text{sr}^{-1}\), where \(\text{cm}^{-1}\) is the unit of the spectral coordinate used, namely inverse centimeters, \(\nu_{cm}^{-1}\).

Unaltered ordered sets in the Kalman filtering process are the background ensemble mean \(x_b\) and the background ensemble state \(X_b\). At a technical level, every other ordered
set, namely $y_o$, $y_b$, $Y_p$, $R_o$, $R_b$, and $K$ will have values and dimensions that follow the case of the radiance assimilation. The process of obtaining the background in observation space $y_b^{(m)}$ via a formulation $\tilde{h}(x_b^{(m)}) = y_b^{(m)}$ is not related to interpolation schemes rather stems from an Optimal Spectral Sampling (OSS) method [14], [15], which can be seen from the fact that $x_b^{(m)}$ are temperatures and $y_b^{(m)}$ spectral radiances. Another point of interest is that the localization methodology in the radiance assimilation is partially related to a distance criterion in pressure space, yet uses additionally jacobian matrices stating the sensitivity of radiance at each spectral channel, to temperature changes.

In section 2.4.1 the specifics of the radiance assimilation observation space are presented. In section 2.4.2 there is a brief treatment on the global filtering methodology, followed by section 2.4.3 where the significance of the jacobian matrices is elucidated. Then we have sections 2.4.4 and 2.4.5 describing how the two applied localization approaches in the radiance assimilation are carried out.

### Table 2.2. Thermal emission spectrometer (TES) spectral resolution, in inverse centimeters.
The data are to be read per row, from left to right.

| 149.23 | 159.81 | 170.39 | 180.98 | 191.56 | 202.14 |
| 212.72 | 223.30 | 233.88 | 244.46 | 255.04 | 265.62 |
| 276.20 | 286.78 | 297.37 | 307.95 | 318.53 | 329.11 |
| 339.69 | 350.27 | 360.85 | 371.43 | 382.01 | 392.59 |
| 403.17 | 413.75 | 424.33 | 434.92 | 445.50 | 456.08 |
| 466.66 | 477.24 | 487.82 | 498.40 | 508.98 | 519.56 |
| 530.14 | 540.72 | 551.31 | 561.89 | 572.47 | 583.05 |
| 593.63 | 604.21 | 614.79 | 625.37 | 635.95 | 646.53 |
| 657.11 | 667.70 | 678.28 | 688.86 | 699.44 | 710.02 |
| 720.60 | 731.18 | 741.76 | 752.34 | 762.92 | 773.50 |
| 784.08 | 794.67 | 805.25 | 815.83 | 826.41 | 836.99 |
| 847.57 | 858.15 | 868.73 | 879.31 | 889.89 | 900.47 |
| 911.06 | 921.64 | 932.22 | 942.80 | 953.38 | 963.96 |
| 974.54 | 985.12 | 995.70 | 1006.28 | 1016.86 | 1027.45 |
| 1038.03 | 1048.61 | 1059.19 | 1069.77 | 1080.35 | 1090.93 |
| 1101.51 | 1112.09 | 1122.67 | 1133.25 | 1143.84 | 1154.42 |
| 1165.00 | 1175.58 | 1186.16 | 1196.74 | 1207.32 | 1217.90 |
| 1228.48 | 1239.06 | 1249.64 | 1260.22 | 1270.81 | 1281.39 |
| 1391.97 | 1302.55 | 1313.13 | 1323.71 | 1334.29 | 1344.87 |
| 1355.45 | 1366.03 | 1376.61 | 1387.20 | 1397.78 | 1408.36 |
| 1418.94 | 1429.52 | 1440.10 | 1450.68 | 1461.26 | 1471.84 |
| 1545.91 | 1556.49 | 1567.07 | 1577.65 | 1588.23 | 1598.81 |
| 1609.39 | 1619.97 | 1630.56 | 1641.14 | 1651.72 |
2.4.1 Radiance Observation Space

The objective of the current section is to describe the radiance observation space, the separation of it to full spectral space and partial or valid spectral space, and to portray the process of obtaining the background in this observation space.

In the retrieval assimilation given section 2.3.1, in order to quantify the analysis we introduce certain indices, each pertaining to one particular space. Namely, we have index \( k \) in the range \( k = \{1, 2, ..., 28\} \), with \( K = 28 \), giving position in the assimilation model space \( D_\xi = \{\xi_k\}_{k=1}^{K} \), which stems from the climate model vertical resolution. For the retrieval observation space, originally we have index \( q \) in the range \( q = \{1, 2, ..., 21\} \), with \( Q = 21 \), giving position in the assimilation observation space, following table 2.1. Ultimately, we retain only a partial, or valid, subset of this \( q \) range and we introduce index \( r \) in the range \( r = \{1, 2, ..., R\} \), with \( R \leq Q \), signifying the fact that the last \( Q - R \) of the 21 reference pressure levels are ignored, thus reaching to the set \( D_\zeta = \{\zeta_r\}_{r=1}^{R} \). In spite of the fact that we use coordinates \( \xi_k \) and \( \zeta_r \), following equations (7.a) and (7.b), these two spaces \( D_\xi \) and \( D_\zeta \) can also be dubbed "pressure" spaces, although their physical dimensions are in \( \ln(\text{Pa}) \).

In the radiance assimilation, the model space is equally \( D_\zeta \), and the background here is as in the retrieval case. For the radiance case, starting from the constitution of the full observation space, or full spectral space, we introduce index \( n \) with a corresponding range \( n = \{1, 2, ..., 143\} \), with \( N = 143 \). We then have all 143 TES spectral channels, following table 2.2, each one for a given value of index \( n \) in ascending order, so that for \( n = 1 \) it is \( \nu_{cm}^{-1} = 149.23 \ \text{cm}^{-1} \), and for \( n = 143 \) it is \( \nu_{cm}^{-1} = 1651.72 \ \text{cm}^{-1} \).

In the retrieval assimilation, the reasoning behind the obviation of the last \( Q - R \) reference pressure levels was that some \( q \) levels may had values greater than the background pressure level at \( k = 28 \) and the assimilation would not have been possible, unless extrapolations were to be performed. In the radiance case the reasoning behind the exclusion of certain spectral channels out of the 143 follows a different rationale. The full waveband of the TES is from 149.23 cm\(^{-1}\) to 1651.72 cm\(^{-1}\), yet in the beginning and the end of this waveband due to low signal to noise ratio [6] the information content is not
reliable. On top of that, from the observed spectra it is also possible to encounter negative radiance values, typically for $v_{\text{cm}}^{-1} > 900$ cm$^{-1}$, so that the first 5 to 15, and the last 10 to 60 spectral channels are always under question, with regards to the given observations in those channels.

The valid spectral channels selection method is presented later on in the current section. At this point, for the further quantification of the radiance assimilation, we introduce one additional index $s$, pertaining to the radiance valid or partial observation space, with a corresponding range that is case specific to each examined PDS TES profile. For example, if we neglect the first 10 and the last 30 spectral channels, the partial channels range will become $\{11, 12, \ldots, 113\}$. In this case, index $s$ will have values from a minimum of $s_{\text{min}}$ up to a maximum $s_{\text{max}} = S$, with these $s_{\text{min}}$ and $s_{\text{max}}$ values being contingent upon the valid channels selection choice.

The terminology valid observation space is not related to a global or local Kalman filtering approach. It only signifies from which observations subset we will draw information during the analysis process. In this regard, we have results classified as radiance global assimilation for the full or partial spectral space, or radiance local assimilation, again for the full or partial spectral space. Similarly, for the retrieval assimilation.

During a data assimilation implementation, we encounter closed form Kalman filtering symbols, such as $x_b^{(m)}$, $\bar{x}_b$, $y_o$, $y_b^{(m)}$, or $\bar{y}_b$. In the retrieval case, the correspondence between these symbols and the actual physical quantities that we currently use, has been established in section 2.3.1. Here, we are to perform a similar task, for the radiance case.

For the background ensemble state $x_b^{(m)}$, we still have for each ensemble member $m$ the physical values of $(T_b^{(m)})_k$ (see section 2.3.1), which are the horizontally interpolated climate model temperature outputs at the satellite location, abutting on the $\xi_k$ model space pressure levels. The background ensemble mean $\bar{x}_b$ is obtained by application of equation (2.a). The $y_o$ will now represent the satellite observed spectra. If we are referring to the full spectral case, we will have $y_o$ to be a $N \times 1$ column vector, while for the partial spectral case it will be a $S \times 1$, excluding certain channels. In order to represent the spectral radiances which are the elements of vector $y_o$ we introduce the symbol $L_o$, in physical
units $\text{mW}(\text{cm}^{-1})^{-1}\text{m}^{-2}\text{sr}^{-1}$. The subscript "o" pertains to the observations. For the full spectral case, an element wise notation involves $\mathbf{y}_o = \{(L_{o,n})_n\}_{n=1}^N$, for the full range of index $n$. For the partial spectral case we will have $\mathbf{y}_o = \{(L_{o,s})_{s\max}\}_{s=\min}^{s\max}$.

Spectral radiances pertaining to each ensemble member $m$ are not known and therefore need to be evaluated. In order to carry out this task, we implement an atmospheric forward model operator applying the Optimal Spectral Sampling (OSS) method [8], [15]. This operator is related to the radiance data assimilation and is used to convert temperatures to spectral radiances, considering that a forward model operator maps model to observation space. In the retrieval case, we had the formulation of $\hat{h}(\mathbb{x}_{b}^{(m)}) = \mathbb{y}_{b}^{(m)}$, where this notation $\hat{h}(\mathbb{x}_{b}^{(m)})$ is for the forward model operator described in appendix C, with its input being the temperatures $\mathbb{x}_{b}^{(m)}$, $\forall m$, at the $\xi_k$ model space pressure levels, and its output the retrieval background in retrieval observation space $\mathbb{D}_{\zeta}$. This section 2.3.1 operator $\hat{h}(\mathbb{x}_{b}^{(m)})$ converts temperatures of space $\mathbb{D}_{\xi}$ to temperatures of space $\mathbb{D}_{\zeta}$. The symbols above pertain to section 2.3.1.

For the radiance assimilation and for notation separation reasons, we introduce a formulation $\hat{h}_{L}(\mathbb{y}_{b,\text{ret}}^{(m)}) = \mathbb{y}_{b}^{(m)}$ as that relates to this section 2.4.1. The used notation $\hat{h}_{L}(\mathbb{y}_{b,\text{ret}}^{(m)})$ is for the OSS forward model operator. The subscript "L" pertains semantically to the radiance case. One of the inputs to this operator is the retrieval background in retrieval observation space $\mathbb{D}_{\zeta}$. In other words, originally we have temperatures $\mathbb{x}_{b}^{(m)}$ at the 28 model space $\xi_k$ levels. Then we apply the appendix C retrieval forward model operator and we map those to the $\mathbb{R}$ retrieval observation space $\zeta_f$ levels. The symbol $\mathbb{y}_{b,\text{ret}}^{(m)}$ is for the output of the retrieval forward model operator. If we then apply the OSS operator $\hat{h}_{L}(\mathbb{y}_{b,\text{ret}}^{(m)})$, for each individual ensemble member, we obtain spectral radiances $\mathbb{y}_{b}^{(m)}$, which constitute the background in the radiance observation space. That is how the supplied OSS operator works, in practice. Given the 28 pressure levels temperatures, we map those to the $\mathbb{R}$ pressure levels. Then, we apply the OSS
operator and we map those $R$ temperatures always to the full spectral space, following table 2.2.

This particular formulation $\tilde{h}_t(y^{(m)}_{b, \text{ret}}) = y^{(m)}_t$ is only used to convey the general idea of the OSS forward model operator. In reality, the input vector to operator $\tilde{h}_t$ is not only temperatures at the reference pressure levels, but involves other physical variables as well. The input vectors per examined profile are presented in the three following tables, 2.3, 2.4, and 2.5. These tables have a total number of elements equal to 67. The data are to read per row, from left to right. In this order, the first 21 elements of the input vector are the temperatures $y^{(m)}_{b, \text{ret}}$ at the reference pressure levels, in $K$. Upon closer observation, we notice that the last $Q-(R+1)$ elements of those 21 first values, are the same. Specifically, for profile 0001/8664 of 000155700, out of the 21 reference pressure levels, the valid ones are the first 17, for 1374/8664 of 000155700 we have the first 15, and for 7600/7952 of 000239506 the first 14. Consequently, in table 2.3, from the first 21 elements, the last 5 are the same, in table 2.4 the last 7, and in table 2.5 the last 8. That is how this OSS implementation works in practice. The 22nd element of the input vector is the skin temperature in $K$, while the 23rd is the skin pressure in mb. Then, from element 24 to 44 we have the molecular $H_2O$ in $g/g$, and from element 45 to 65 the molecular $CO_2$ in $g/g$, as the primary constituents of the Martian atmosphere accounted for in the OSS operator. Element 66 is the total opacity (optical thickness) for dust (the PDS retrieved dust absorption optical depth) at the reference spectral coordinate in which the instrument line shape function is equal to unity, at $v_{cm}^{-1} = 1075 \text{ cm}^{-1}$, as is the case for element 67 giving the total opacity for ice. The basic mapping from atmospheric variables to the input vector of the OSS forward model operator is provided by global attributes.
### Table 2.3. OSS forward model operator input vector of one ensemble member, for profile 0001/8664 of 000155700. The data are to be read per row, from left to right.

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>166.75</td>
<td>169.19</td>
<td>171.32</td>
<td>173.26</td>
<td>174.69</td>
<td>175.22</td>
</tr>
<tr>
<td>175.81</td>
<td>176.77</td>
<td>177.98</td>
<td>179.72</td>
<td>182.25</td>
<td>185.49</td>
</tr>
<tr>
<td>188.94</td>
<td>192.49</td>
<td>195.93</td>
<td>200.35</td>
<td>204.21</td>
<td>204.21</td>
</tr>
<tr>
<td>204.21</td>
<td>204.21</td>
<td>204.21</td>
<td>204.21</td>
<td>204.21</td>
<td>204.21</td>
</tr>
<tr>
<td>5.650×10⁻⁶</td>
<td>6.927×10⁻⁶</td>
<td>8.655×10⁻⁶</td>
<td>1.054×10⁻⁶</td>
<td>1.260×10⁻⁶</td>
<td>1.572×10⁻⁶</td>
</tr>
<tr>
<td>1.892×10⁻⁶</td>
<td>2.278×10⁻⁶</td>
<td>2.675×10⁻⁶</td>
<td>3.067×10⁻⁶</td>
<td>3.226×10⁻⁶</td>
<td>3.358×10⁻⁶</td>
</tr>
<tr>
<td>3.169×10⁻⁶</td>
<td>3.026×10⁻⁶</td>
<td>2.988×10⁻⁶</td>
<td>2.883×10⁻⁶</td>
<td>2.703×10⁻⁶</td>
<td>2.670×10⁻⁶</td>
</tr>
<tr>
<td>2.670×10⁻⁷</td>
<td>2.670×10⁻⁷</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>9.820×10⁻⁴</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2.4. OSS forward model operator input vector of one ensemble member, for profile 1374/8664 of 000155700. The data are to be read per row, from left to right.

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>166.37</td>
<td>167.88</td>
<td>169.64</td>
<td>172.05</td>
<td>174.58</td>
<td>177.39</td>
</tr>
<tr>
<td>181.10</td>
<td>184.92</td>
<td>188.51</td>
<td>192.08</td>
<td>196.17</td>
<td>202.66</td>
</tr>
<tr>
<td>208.50</td>
<td>214.76</td>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
</tr>
<tr>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
<td>217.30</td>
</tr>
<tr>
<td>5.650×10⁻⁶</td>
<td>6.927×10⁻⁶</td>
<td>8.655×10⁻⁶</td>
<td>1.054×10⁻⁶</td>
<td>1.260×10⁻⁶</td>
<td>1.572×10⁻⁶</td>
</tr>
<tr>
<td>1.892×10⁻⁶</td>
<td>2.278×10⁻⁶</td>
<td>2.675×10⁻⁶</td>
<td>3.067×10⁻⁶</td>
<td>3.226×10⁻⁶</td>
<td>3.358×10⁻⁶</td>
</tr>
<tr>
<td>3.169×10⁻⁶</td>
<td>3.026×10⁻⁶</td>
<td>2.988×10⁻⁶</td>
<td>2.883×10⁻⁶</td>
<td>2.703×10⁻⁶</td>
<td>2.670×10⁻⁶</td>
</tr>
<tr>
<td>2.670×10⁻⁷</td>
<td>2.670×10⁻⁷</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>-8.60×10⁻⁴</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2.5. OSS forward model operator input vector of one ensemble member, for profile 7600/7952 of 000239506. The data are to be read per row, from left to right.

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>149.21</td>
<td>152.31</td>
<td>153.62</td>
<td>155.68</td>
<td>158.73</td>
<td>162.15</td>
</tr>
<tr>
<td>165.50</td>
<td>167.18</td>
<td>165.62</td>
<td>164.95</td>
<td>171.11</td>
<td>178.64</td>
</tr>
<tr>
<td>184.08</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
</tr>
<tr>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
<td>180.83</td>
</tr>
<tr>
<td>5.651×10⁻⁶</td>
<td>6.927×10⁻⁶</td>
<td>8.656×10⁻⁶</td>
<td>1.054×10⁻⁶</td>
<td>1.261×10⁻⁶</td>
<td>1.572×10⁻⁶</td>
</tr>
<tr>
<td>1.892×10⁻⁶</td>
<td>2.279×10⁻⁶</td>
<td>2.676×10⁻⁶</td>
<td>3.067×10⁻⁶</td>
<td>3.226×10⁻⁶</td>
<td>3.358×10⁻⁶</td>
</tr>
<tr>
<td>3.169×10⁻⁶</td>
<td>3.026×10⁻⁶</td>
<td>2.988×10⁻⁶</td>
<td>2.884×10⁻⁶</td>
<td>2.704×10⁻⁶</td>
<td>2.671×10⁻⁶</td>
</tr>
<tr>
<td>2.670×10⁻⁷</td>
<td>2.671×10⁻⁷</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1.812×10⁻⁴</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
What is important here is that by a combined application of the retrieval and the radiance assimilation forward model operators, we evaluate the background in spectral space, denoted in closed form \( y_b^{(m)} \), \( \forall m \), following the current section. To assign a symbol with a physical connotation, we have \( L_b^{(m)} \); an element wise representation of this background in spectral space is \( y_b^{(m)} = \{(L_b^{(m)})_n\}_{n=1}^N \), specifically for the full spectral case. The OSS operator always points to that, so if we are to implement a partial spectral case assimilation, and consequently speak of \( y_b^{(m)} = \{(L_b^{(m)})_s\}_{s=1}^{s_{\text{max}}} \), we only neglect the appropriate spectral channels.

Next follows the description of how we establish the partial (or valid) observation space in the radiance assimilation. The OSS forward model operator produces the background radiances \( y_b^{(m)} = \{(L_b^{(m)})_n\}_{n=1}^N \) in the full spectral space in a process that also incorporates the observations \( y_o = \{(L_o)_n\}_{n=1}^N \). The used criterion in the determination of whether a spectral channel specifically from the first 10 and the last 60 will be used in any radiance partial space assimilation or not, is derived from an absolute valued difference \( |y_b - y_o| \). First we evaluate the background ensemble mean in spectral space \( y_b \), using an equation like (2.b), then we subtract from each element of \( y_b \) the corresponding element of \( y_o \), and if this difference is greater than a fixed ad hoc value, for example \( 1.0 \text{ mWcm}^{-1}\text{m}^{-2}\text{sr}^{-1} \), then that channel is ignored. This process only applies in the beginning and the end of the TES waveband, not in-between. Even if the in-between absolute valued differences are greater than the threshold, these channels are never neglected.

This process is in close relation to how the OSS TES temperature retrievals are produced originally [6]. In the OSS TES retrieved temperatures, observations in wavebands greater than \( \nu_{\text{cm}}^{-1} = 900 \text{ cm}^{-1} \) and less than \( \nu_{\text{cm}}^{-1} = 200 \text{ cm}^{-1} \) are neglected due to the low signal to noise ratio of the observed spectra. So intrinsically, almost half of the data of the observed spectra are not used in practice either in the temperature retrievals or in a radiance assimilation.

For a performed sensitivity analysis, in order to ascertain the impact of this choice in the radiance data assimilation results, both cases are considered. In the first, the full spectral case, we perform the data assimilation by incorporating information from every channel,
whereas in the partial spectral case we take into account the previous criterion. Again, this feature is not related to localization, where in a local radiance data assimilation we may perform the previous criterion on top of the localization implementation.

The following figures are related to the analysis of the current section. Every figure below pertains to a used profile 7600/7952 of 000239506. Figure 2.6 shows the spectral distribution of satellite observed radiances for the used profile. Roughly, in the spectral range $1000 - 1200 \text{ cm}^{-1}$, upon closer inspection of figure 2.7, we see the presence of negative radiance values, which is not physically acceptable. Figure 2.7 is a partial close up to figure 2.6 in the given waveband. In figure 2.8 we have the background in observation space obtained by the OSS forward model. Upon comparison of figure 2.6 with 2.8, we note that in the beginning of the waveband, close to $200 \text{ cm}^{-1}$, there are significant differences. That is attributed to technical limitations of the spectrometer, with regards to how the observations are obtained. In the partial range $1000 - 1200 \text{ cm}^{-1}$ of figure 2.8, which is presented in figure 2.9, we have positive radiance values for the background observations. In figures 2.10 and 2.11 we have the signed differences $y^{(1)}_b - y_o$ and $y_b - y_o$. In these two figures 2.10 and 2.11 the light blue background is a graphical representation of the spectral range where one needs to be careful when establishing the radiance valid observation space, since in these partial wavebands the satellite observations are not always trustworthy.
Figure 2.6. Spectral distribution of a satellite observed radiance, for the profile 7600/7952 of 000239506.

Figure 2.7. Partial spectral distribution of the satellite observed radiance, for the profile 7600/7952 of 000239506. Negative radiance values are present and therefore excluded from the valid radiance observation space.
Figure 2.8. Spectral distribution of the background observations (radiance), of profile 7600/7952 of 000239506, evaluated from the OSS forward model operator.

Figure 2.9. Partial spectral distribution of the background observations (radiance) from the OSS forward model operator, for the profile 7600/7952 of 000239506. Non negative values are recorded in this case.
Figure 2.10. Spectral distribution of the signed difference between background observation ensemble member 1, and the satellite observations. The light blue domains denote the spectral range of potential exclusion of that information content, from the filtering process.

Figure 2.11. Spectral distribution of the signed difference between background observations ensemble mean, and the satellite observations. The light blue domains denote the spectral range of potential exclusion of that information content, from the filtering process.
2.4.2 Radiance Global Approach

In the radiance data assimilation, the term global indicates that in the filtering equation (1) we employ, for each model space node, information from every available spectral channel, out of either all 143 or a subset, as that relates to the full or partial spectral case.

Like stated, the model space given in terms of $\{\xi_k\}_{k=1}^K$ (see section 2.3.1) is the same as in the retrieval data assimilation, so that symbols like $x_b^{(m)}$, $\bar{x}_b$, $X_b$, and $X_p$ follow the nomenclature of sections 2.2 or 2.3.1. On the other hand, in the radiance data assimilation we have the observations $y_o$ now being satellite observed spectra (PDS TES data sets), the background in observation space $y_b^{(m)}$, $\forall m$, also spectral radiances evaluated from the OSS forward model operator, the corresponding ensemble mean $\bar{y}_b$ of the background in observation space, and also the matrices $Y_b$, $Y_p$, $R_o$, $R_b$, and $K$, defined in section 2.2.

Specifically, for the background in observation space ensemble mean $\bar{y}_b$, we still have equation (2.b), where the summation is for $n = \{1, 2, ..., 143\}$, or for an appropriate subset, following index $s$ (section 2.4.1), so that it is

$$ (\bar{y}_b)_n = \frac{1}{M} \sum_{m=1}^{M} (y_b^{(m)})_n, \quad (19.a) $$

or

$$ (\bar{y}_b)_s = \frac{1}{M} \sum_{m=1}^{M} (y_b^{(m)})_s, \quad (19.b) $$

where the element-wise notations for $(\bar{y}_b)_n$ and $(\bar{y}_b)_s$, pertain respectively to either $(\bar{L}_b)_n$ or $(\bar{L}_b)_s$ (section 2.4.1), signifying when we consider the full or partial observation space, in the radiance case. In this regard, $\bar{y}_b$ is now represented by a column vector, either $N \times 1$ or $S \times 1$, and the same applies for the observations $y_o$.

The background ensemble state matrix in observation space $Y_b$ will be either $N \times M$ or $S \times M$, with every $m$-th column still containing each individual ensemble member $y_b^{(m)}$ of the background in observation space, so that element-wise it is
(Y_b)_{n,m} = (y_b^{(m)})_n \text{ or } (Y_b)_{s,m} = (y_b^{(m)})_s, \text{ for its } (n,m) \text{ or } (s,m) \text{ element respectively, following the full or partial radiance observation space. The background perturbation matrix in observation space } Y_p \text{ has the same dimensions with, where the initialization of its elements follow equation (5.b), given here from }

(Y_p)_{n,m} = (Y_b)_{n,m} - \bar{y}_n, \quad (20.a)

or

(Y_p)_{s,m} = (Y_b)_{s,m} - \bar{y}_s. \quad (20.b)

The background error covariance matrix in observation space R_b follows equation (4). In the radiance global assimilation is either N × N or S × S. The observations error covariance matrix R_o, has the same dimensions with R_b. It is assumed diagonal, with its main diagonal elements equal to \(\sigma_o^2\), where the observational standard deviation is fixed at \(\sigma_o = 1.5 \text{ mW cm}^{-1} \text{ m}^{-2} \text{ sr}^{-1}\) across every spectral channel. The evaluation of Kalman gain K follows equation (3). Matrix K is either K × N or K × S, for the global case. From the global implementation, we evaluate once \(X_p\), \(Y_p\), \(R_o\), and \(R_b\). In the local implementation, which follows in the next section, we draw information as necessary from those already evaluated matrices.

### 2.4.3 Radiance Local Assimilation

In order to carry out a localized radiance data assimilation, additional information from jacobian matrices is taken into account in two approaches elucidated in the following sections 2.4.4 and 2.4.5. Section 2.4.4 is titled radiance per pressure levels localization while section 2.4.5 radiance per spectral channels localization, in order to separate these two implemented computational approaches.

The data sets used currently are the PDS TES from which we obtain the observed satellite radiances and the OSS TES which give the temperature retrievals. Primarily, these data sets supply us with the observations used in the retrieval and the radiance data assimilations, which for both cases are denoted \(y_o\). However, the dimensionalities of the two cases are different; in the retrieval assimilation the observations, being temperatures,
abut on the 21 reference pressure levels (table 2.1, section 2.3) whereas in the radiance assimilation abut on 143 spectral channels, being spectral radiances (table 2.2, section 2.4). One additional data set conveys information on the sensitivity of the spectral radiances at each spectral channel, to temperature changes, and that is given in the form of jacobian matrices, whose dimensions are $143 \times 21$, pertaining to each examined profile of this study.

With regards to the dimensions of the jacobians we have that each row of these matrices corresponds to one TES spectral channel, and each column to one reference pressure level. Specifically, the fist row of the jacobians is for spectral channel $n = 1$ or $\nu_{cm} = 149.23 \text{ cm}^{-1}$ and the last row for $n = 143$ or $\nu_{cm}^{-1} = 1651.72 \text{ cm}^{-1}$, given table 2.2, from section 2.4. The first column is for reference pressure level $q = 1$ or $p = 11.173 \text{ Pa}$, and the 21st column for reference pressure level $q = 21$ or $p = 1658.15 \text{ Pa}$, given table 2.1 from section 2.3.

In a radiance global assimilation, as described in section 2.4.2, the jacobian matrices are not used. In an approach such as that, one applies equation (1) $x_a = x_b + K(y_o - y_b)$ in such a manner so that for every model space grid point $k$, the analysis ensemble mean $(\overline{x}_a)_k$ is evaluated from the superposition of the background ensemble mean $(\overline{x}_b)_k$ with the $k$–th element of the term $K(y_o - y_b)$, where the Kalman gain $K$ is a matrix with dimensions either $K \times N = 28 \times 143$ or $K \times S$, for the full or partial spectral case respectively, and the innovations $y_o - y_b$ are correspondingly either $N \times 1 = 143 \times 1$, or $S \times 1$. In this respect, for each $(\overline{x}_a)_k$ we incorporate information from every available spectral channel, either from all 143, or a subset of those (see section 2.4.1).

Conversely, in a radiance local assimilation equation (1) is to be implemented again only in this case the term $K(y_o - y_b)$ contains information only from the most relevant spectral channels, determined for each reference pressure level as those channels in which the radiance to temperature sensitivity is at a maximum (as an absolute value), or close to a maximum. This verbal distinction at a maximum and close to a maximum is key in the separation of sections 2.4.4 and 2.4.5.

From a physical standpoint, the rationale behind the detection of the channels of the maximum radiance to temperature sensitivity is related to the fact that we try to recognize, for each reference pressure level, the correlation between the spectral distribution of the observed satellite radiance and the vertical structure of the atmosphere. Theoretically, for a
true state of the atmosphere $\mathbf{x}_t$ (at one $(\varphi, \lambda)$ location), as that relates exclusively to atmospheric temperature profiles, we assume $\mathbf{x}_t$ to be a $21 \times 1$ column vector, giving temperature at each reference pressure level $q = \{1, 2, \ldots, 21\}$, following table 2.1. Given the notation of section 2.4.1 we have that the observed radiances are $\mathbf{y}_o$, translated to $(L_o)_n$, for $n = \{1, 2, \ldots, 143\}$. These $(L_o)_n$ radiances, spectrometer instrumentation deficiencies included, point to $\mathbf{x}_t$. Considering a non zero observational standard deviation, e.g. $\sigma_o = 1.5$ mW(cm$^{-1}$)$^{-1}$m$^{-2}$sr$^{-1}$ and an inversion methodology, from the known values $(L_o)_n$ and a temperature prior (see appendix D) we estimate a state, currently denoted $\tilde{\mathbf{x}}_t$. The tilde separates $\mathbf{x}_t$ from $\tilde{\mathbf{x}}_t$ in the sense that the latter is but an estimation. Were the true state $\mathbf{x}_t$ to be altered, that would also impact the observations, so that the satellite would measure a differentiated $(L_o)_n$ profile. For simplicity, let us assume that at one reference pressure level alone there is a change $\Delta T$ between two $\mathbf{x}_t$ states. Physically, in one atmospheric layer the chemical composition could change, impacting the emissivity of that layer so that the profile $\mathbf{x}_t$ would change accordingly. A $\Delta T$ perturbation in one pressure level can be recorded and diagnosed in two satellite radiance observations, which otherwise may be realized via simulations. In the following, we explore the constitution of jacobian matrices given such simulations.

From appendix D we have equation (D.11), which is repeated here as well:

$$\mathbf{J} = \frac{\partial \hat{h}_n}{\partial \mathbf{x}_q} \mathbf{\hat{e}}_n \otimes \mathbf{\hat{e}}_q,$$

following the notation of appendix D. The unit vectors $\mathbf{\hat{e}}_n$, $\mathbf{\hat{e}}_q$ are basis vectors of the rectangular coordinate system. Indices $n$, $q$ follow section 2.4.1, where $n$ enumerates spectral channels and $q$ reference pressure levels. The symbol $\mathbf{x}_q$ appearing on the denominator pertains semantically to the $q$–th element of a state vector like $\tilde{\mathbf{x}}_t$. In the numerator, $\hat{h}_n$ corresponds to spectral radiances evaluated with a forward model operator, like the OSS one, given an input $\tilde{\mathbf{x}}_t$. From the stand point of inversions, this $\tilde{\mathbf{x}}_t$ state can be an OSS TES atmospheric temperature profile, so that for an input $\tilde{\mathbf{x}}_t$ to a forward model operator, the output will be a spectral distribution of radiance, like $\hat{h}_n$. 

For the \((n,q)\) element of a jacobian, we have

\[
J_{n,q} = \frac{\partial f_n}{\partial x_q} = \frac{\partial L_n}{\partial T_q},
\]

in units \(m W (cm^{-1})^{-1} m^{-2} sr^{-1} K^{-1}\). Jacobian matrices include the information of the radiance to temperature sensitivity, a fact which can be illustrated from a simplified formulation

\[
J_{n,q} \approx \frac{L_n(T_q + \Delta T) - L_n(T_q)}{\Delta T},
\]

accounting for temperature perturbations \(\Delta T\) at each reference pressure level \(q\). We rewrite the estimated state vector \(\bar{x}_t\) like \(T = \{T_q\}_{q=1}^Q\), with \(Q = 21\). The radiance state vector, pertaining to one such atmospheric temperature profile \(T\), is now posed \(L = \{L_n(T)\}_{n=1}^N\), with \(N = 143\). Given the application of a forward model operator that maps temperature to radiance (appendix D), for one profile \(T\) we may estimate \(L\). On another run of the simulation, we may change \(T\) only in its first element, for \(q = 1\), by adding a temperature increment \(\Delta T\). Some spectral channels may respond to this change, while others may not. We apply equation (23) between the two simulation runs thereby estimating the jacobian matrix elements \((n,q = 1)\), for each channel \(n\). The process is repeated for every \(q\), so that the initial \(T\) input only changes at the corresponding \(q\) pressure level. In this regard all \((n,q)\) elements of a jacobian are computable.

Physically, this process offers insights to the vertical structure of the atmosphere. Given the broader field of the radiative transfer, if for example a change in pressure level \(q = 1\) impacts significantly the radiance in some spectral channels, then reversely if we were to have satellite observed spectra that were different to each other in these spectral channels, we would have an idea that, roughly, at that altitude (given a hypsometric equation) the atmosphere would have a different state, attributed for example to chemical composition. The association of satellite observations with vertical atmospheric structures is not straightforward. Nevertheless, the point here is that in the context of the localized radiance data assimilation we wish to take into account, at the reference pressure levels, only those spectral channels that are strongly related with those levels of the atmosphere, in terms of statistical importance estimation and in view of the correlation structures.
Another relevant reason, more of a computational nuance, is related to the evaluation of the innovations $\mathbf{y}_o - \tilde{\mathbf{y}}_b$. If we consider a scenario, not physically realizable, so that the atmospheric contribution to the radiance at one pressure level were to be absent, then the temperature of that particular pressure level would have no impact on the observed spectra and the corresponding column of the jacobians would only have exact zeros. Given different $\mathbf{T} = \{ T_q \}_{q=1}^Q$ inputs to a forward model operator in order to evaluate the radiances $\{ \mathbf{L}_n(\mathbf{T}) \}_{n=1}^N$, and from those their ensemble mean $\mathbf{y}_b$, in light of the reduced dependence of radiance to temperature, this $\tilde{\mathbf{y}}_b$ profile could be for some channels close to the observations $\mathbf{y}_o$. If there were no correlation at all between radiance and temperature, then the innovations $\mathbf{y}_o - \tilde{\mathbf{y}}_b$ would always be exact zeros. Considering that the temperature priors for the observations $\mathbf{y}_o$ and the background ensemble mean in observation space $\tilde{\mathbf{y}}_b$ stem from different temperature states, then it is to our benefit to exclude from the analysis those channels in which the radiance to temperature sensitivity is weak, since in these cases the innovations will have an insignificant impact in the evaluation of $\mathbf{x}_a$. We then have one additional reason not wishing to include in the analysis those channels for which the jacobians have values closer to zero.

Given the previous analysis, in the localized radiance data assimilation, one part is to locate from the jacobians those channels of maximum radiance to temperature sensitivity, for each reference pressure level. At the same time, considering that the model space in the retrieval and the radiance assimilations is the same, in the radiance assimilation we are to perform one additional spatial localization, in pressure space, as was the case in the retrieval assimilation (see section 2.3.3). For example, at model space level $k = 24$, if the reference pressure levels that are in the local domain of assimilation $D_{\xi}^{(r)}$ are $\{8, 9, 10, 11, 12, 13\}$, then in the implementation of $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y}_o - \tilde{\mathbf{y}}_b)$, for that level $k$, the Kalman gain and the innovations will pertain only to spectral channels of maximum radiance to temperature sensitivity from these six columns of matrix $\mathbf{J}$.

In section 2.4.4, where we treat the radiance per pressure levels localization approach, we search in the jacobians per column $q$. Given the previous example, we would search for those channels $n$ of maximum $\mathbf{L}$ to $\mathbf{T}$ sensitivity in columns $\{8, 9, 10, 11, 12, 13\}$ out of the $R \leq Q$ valid ones (see section 2.4.1), and the retained channels, per column $r$ (instead
of index $q$), are of a user defined choice. If we wish to retain 5 channels, per applicable column, then we will have a maximum of $6 \times 5 = 30$ channels to be used in equation (1). If some channels appear more than once, then we will take the union of this index information to perform the analysis equation (1). Another choice may be so that we wish to retain 30 channels, per applicable column. In this case, the total number of used spectral channels in the analysis equation (1) would be from the minimum amount of 30 (assuming that in every column of $J$ we have the exact same channels of maximum $L$ to $T$ sensitivity) up to a case specific maximum.

In section 2.4.5, for the radiance per spectral channels localization, we search in the jacobians per row $n$. For each spectral channel $n$ we locate the one and only one pressure level $r$ (of the valid ones, as in section 2.3.1) where we have the maximum $L$ to $T$ sensitivity. In the application of the analysis equation (1), if this pressure level $r$ is among those existing within $D^{(f)}_{\xi}$, then the spectral channels that will be accounted for in the data assimilation will be all those in which this level $r$ maximizes the aforementioned sensitivity. For example, for a pressure level $r = 11$, the channels of the maximum $L$ to $T$ sensitivity may be $n = \{17, 23, 28, 58, 90, 121, 122, 139\}$. For those channels to appear in the analysis equation, or in the evaluation of the Kalman gain, or the innovations, then this $r = 11$ will need to be in the local regime of assimilation $D^{(f)}_{\xi}$, for those applicable model space pressure levels $k$.

The following figure 2.11 is presenting visually a jacobian matrix for one of the examined profiles of the current study, that of 0001/8664 of 000155700. The reference pressure levels, given table 2.1, are from the first for $p = 11.173$ Pa until the 15th for $p = 369.984$ Pa, with the last six columns of that particular jacobian having zero elements.

**Figure 2.12.** Jacobian matrix graphical representation for profile 0001/8664 of 000155700. The vertical axis is for the reference pressure levels (table 2.1), while the horizontal axis for the radiance to temperature differences, explicating the radiance to temperature sensitivity for each spectral channel, out of 143.
2.4.4 Radiance per Pressure Levels Localization

The first of the two implemented radiance localized data assimilation techniques is presented in the following. In the previous section is mentioned that in order to carry out such a localization, we need to combine the spatial localization of the retrieval data assimilation in pressure space, as in section 2.3.3, with a method that determines which spectral channels will be used, out of the considered available.

With regards to the dimensionality of the problem as that relates to the ordered sets appearing in the analysis and their dimensions, we repeat a number of essential features; following section 2.3.1, the model space is posed $D_\xi = \{\xi_k\}_{k=1}^K$, with the generalized coordinate $\xi_k$ defined in equation (7.a) giving the natural logarithm of the horizontally interpolated at the satellite location ensemble mean climate model pressures, with $K = 28$ the total number of grid points of the assumed model space. The background and analysis ensemble means $\bar{x}_b$, $\bar{x}_a$, are $K \times 1$ column vectors abutting on this $D_\xi$ pressure space.

The observation space in the radiance assimilation, given section 2.4.1, is distinguished between the full and the partial spectral space, where the latter is also called the valid observation space. The full spectral space accounts for every one of all $N = 143$ TES channels, whereas the partial one for a subset of those with a corresponding population denoted $S$, where some of the first and some of the last spectral channels are neglected. The assigned notation to these two spaces is for the full $D_v = \{v_n\}_{n=1}^N$, and for the partial $D_v = \{v_n\}_{n=\min}^{\max}$, following section 2.4.1 and table 2.2. In view of that, the observations $\mathbf{y}_o$ (satellite observed spectra) will be represented by either a $N \times 1$ or a $S \times 1$ column vector.

This separation in full and partial spectral spaces also impacts the dimensions of the considered jacobians. These $\mathbf{J}$ matrices are by construction $N \times Q = 143 \times 21$. However, only a curtailed jacobian will actually be considered, given the following facts; out of the $Q = 21$ reference pressure levels (table 2.1, following section 2.3.1), ultimately we only consider a subset $R \leq Q$, where $R$ is typically from 14 to 17 accounting for the reference pressure levels from the first at $p = 11.173$ Pa until the element $R$ of table 2.1.

According to that, we neglect the last $Q - R$ columns of the jacobians, since these related pressure levels are not a part of the assimilation process itself. Consequently, if we apply the full spectral space radiance assimilation, the jacobians will have dimensions $N \times R$,
while for the partial spectral space assimilation, dimensions $S \times R$. For example, one of the examined profiles is $7600/7952$ of $000239506$. In this case for the partial spectral case we neglect the first $7$ and the last $66$ spectral channels, while it also is $R = 14$. The value of $S$ is $143 - (7 + 66) = 70$, with a valid jacobian subset being a $S \times R = 70 \times 14$ matrix, where we account for jacobian rows from $8$ until $77$, and jacobian columns from $1$ until $14$, with the rest of its elements ignored. Similarly for every other partial spectral case.

For the assimilation process itself, we follow the following equations

$$R^{(f)}_b = \frac{1}{M-1} Y^{(f)}_p Y^{(f)tr}_p,$$  \hfill (24.a)

$$K^{(f)} = \frac{1}{M-1} X^{(f)}_p Y^{(f)tr}_p (R^{(f)}_o + R^{(f)}_b)^{-1}.$$  \hfill (24.b)

$$(x_{ak})_k = (x_{bk})_k + K^{(f)} (y_o - y_b).$$  \hfill (24.c)

In the symbols of equations (24.a), (24.b), and (24.c) the superscript $(f)$ denotes a local subset of the ordered sets, otherwise used in section 2.4.2 for the radiance global assimilation.

The first step of the process involves the construction of the background ensemble state matrix $X_b$, being $K \times M = 28 \times 16$, with $M = 16$ the ensemble size. The individual background ensemble members $x^{(m)}_b$ are evaluated like in the retrieval assimilation of section 2.3.1, and $X_b$, by construction, contains in every column one $x^{(m)}_b$ vector. The construction of the background perturbations matrix $X_p$ follows equation (5.a), producing a $K \times M$ set in the process. The background ensemble mean $\bar{x}_b$ follows equation (2.a), and all things considered the background sets for the radiance assimilation are the very same as in the retrieval assimilation.

The second step is for the evaluation of the background in observation space for every ensemble member $m$, $y^{(m)}_b$. This step is covered in section 2.4.1 where we speak of the OSS forward model operator in the context of the radiance assimilation. In section 2.4.1 for the full spectral case we had a notation $y^{(m)}_b = \{(L^{(m)}_b)_{n}\}_{n=1}^N$, and for the partial spectral case $y^{(m)}_b = \{(L^{(m)}_b)_s\}_{s=1}^S$, following that nomenclature. With the state $y^{(m)}_b$, $\forall m$
known, we also construct the background ensemble state matrix $Y_b$ in observation space, whose dimensions will be either $N \times M = 143 \times 16$ or $S \times M$, with every column of it containing one member $y_{b(\cdot)}$. The background ensemble mean in observation space $\bar{Y}_b$ follows equation (19.a) or (19.b), the background perturbations matrix in observation space $\mathcal{Y}_p$ follows equation (20.a) or (20.b), and the observed spectra $y_o$ are given from the known $N \times 1$ or $S \times 1$ column vector.

In this regard, every global set $y_o$, $\bar{Y}_b$, $\bar{X}_b$, $\mathcal{X}_p$, and $\mathcal{Y}_p$ is known with the next part focusing on which elements of the sets $y_o$, $\bar{Y}_b$, and $\mathcal{Y}_p$ will actually be used in the realization of the equations (24.a), (24.b), and (24.c). At first, we consider a jacobian pertaining to one examined PDS TES profile. The *relevant* dimensions of such a set will be $N \times R$ or $S \times R$ in relation to which observation space we have under consideration. We then create an absolute valued jacobian so that from such a set we may find the channels of the maximum radiance to temperature sensitivity *from a given subset of it*. In the radiance per pressure levels localization we search this absolute valued jacobian per column $r$.

At a technical level, first we need to locate those columns in which we will search for the greatest elements of this absolute valued jacobian. That is achieved from the retrieval localization methodology; from section 2.3.3 and equation (10) we have the definition of the used distance related localization criterion in pressure space, $\ell_f = c \left( \Delta \xi \right)_{\text{max}}$, which is used equally for here as well, with a fixed value $c = 0.030$, and $(\Delta \xi)_{\text{max}} = \xi_{28} - \xi_1$. A local regime of assimilation in model space $D_{\xi}^{(f)}: \xi \in [\xi_{lb}, \xi_{rb}]$ is also established, in like manner as in section 2.3.3, with $\xi_{lb} = \xi_k - \ell_f \xi_k$ and $\xi_{rb} = \xi_k + \ell_f \xi_k$. If we are at model space level $k$, the relevant *retrieval observation space* pressure levels $D_{\zeta} = \{\zeta_r\}_{r=1}^R$ to be considered need to be within that $D_{\xi}^{(f)}$ set. For example, if at $k = 14$ there is only one $\zeta_r \in D_{\xi}^{(f)}$ value, we then evaluate the value of index $r'$ pertaining to that pressure $\zeta_r$. This $r'$ value will be one of $\{1, 2, ..., R\}$, giving the one and only $r'$ column of the absolute valued jacobian where the search will commence. It may be so that within $D_{\xi}^{(f)}$ there are more than one $\zeta_r$ pressures. At a different model level $k$, if we have for instance
four $\zeta_r$ levels close to the $\xi_k$ one, with corresponding indices \{r', r'+1, r'+2, r'+3\}, these will be the columns of the searching in the absolute valued jacobian, and so on.

Given the previous analysis, the subset of the absolute valued jacobian where the searching will occur will be for all those pertinent r' columns across every row, either all $N = 143$ or just the $S$. The radiance per pressure levels localization approach offers the following computational flexibility; assume for example that at one model level k we have four local $\zeta_r$ levels and that we consider a partial spectral case with e.g. $S = 97$, in which we neglect the first 7 and the last 39 channels. Assume also that for one particular PDS TES profile the value of $R$ is 16. From the total number of absolute valued jacobian elements $S \times R = 97 \times 16$, we search in a subset with total number of elements $97 \times 4 = 388$. It is our prerogative as to how many spectral channels we will ultimately consider in the Kalman filtering process. This number can be from 1 up to $S = 97$.

We introduce a proxy index $V$ denoting the plentitude of the retained spectral channels per r' column. If for instance it is $V = 5$, given the current example for that particular model level k, from each one of the columns $\{r', r'+1, r'+2, r'+3\}$ initially we will retain 5 channels. Assume that it is $k = 25$ and $\{r', r'+1, r'+2, r'+3\} = \{8, 9, 10, 11\}$. Since we neglect the first 7 and the last 39 channels, the remaining valid ones will be in the range $\{8, 9, 10, ..., 103, 104\}$ so that spectral indices for $s \leq 7$ or $s \geq 105$ will not appear. For column $r' = 8$ the channels of the maximum radiance to temperature sensitivity may be $\{23, 40, 58, 70, 89\}$, for column $r' + 1 = 9$ it may be for $\{11, 40, 58, 100, 101\}$, for column $r' + 2 = 10$ for $\{11, 32, 58, 63, 97\}$, and for column $r' + 3 = 11$ for channels $\{11, 32, 40, 63, 70\}$. Given the value of $V$, the total number of retained channels can be from $V \times 1 = V$ up to $V$ times the number of relevant absolute valued jacobian columns, for here four. We denote this upper value for the retained spectral channels as $V'$. In general, if a channel from this search appears more than one, we will take the logical union of this index information. For the current example, we would have an analytical formalism like $\{23, 40, 58, 70, 89\} \cup \{11, 40, 58, 100, 101\} \cup \{11, 32, 58, 63, 97\} \cup \{11, 32, 40, 63, 70\}$, yielding a set $\{11, 23, 32, 40, 58, 63, 70, 89, 97, 100, 101\}$. These are the indices that would then be used in the Kalman filtering process.

The other two possibilities in this approach are similar to those of section 2.3.3. It is possible that no local $\zeta_r$ levels are in close proximity to a given $\xi_k$ one, or it may be so
that only one \( \zeta_r \) level is within this \( D_{\zeta}^{(f)} \) set. If no local observations are found, then no Kalman filtering equation is being applied. We only overwrite the \( k \)-th element of the analysis ensemble mean \( (\tilde{x}_a)_k \) from the corresponding element of the background ensemble mean, following

\[
(\tilde{x}_a)_k = (\tilde{x}_b)_k. \tag{25}
\]

The other two cases are treated similarly. Only for those we apply equations (24.a), (24.b), and (24.c). If we have only one local \( \zeta_r \) level, then the total number of spectral channels to be used is equal to our \( V \) value choice. If we have more than one \( \zeta_r \) levels, we might as well follow the previous example in order to clarify how the filtering process is actually implemented.

We consider still the channels \( \{11, 23, 32, 40, 58, 63, 70, 89, 97, 100, 101\} \). We are also at one given model space level \( k \) anticipating to implement equation (24.c). The global set \( Y_p \) at this point is known so that the local \( Y_p^{(f)} \) may be evaluated as follows; the dimensions of \( Y_p \) are in general \( S \times M \). Given what was previously mentioned about the upper number of retained spectral channels, for here this value is \( V' = 11 \), between the limits 5 and \( 5 \times 4 = 20 \). The dimensions of \( Y_p^{(f)} \) will then be \( V' \times M \) and its rows will be equal to \( Y_p^{(f)}(1,m) = Y_p(11,m) \), \( Y_p^{(f)}(2,m) = Y_p(23,m) \), and so on until the last for \( Y_p^{(f)}(11,m) = Y_p(101,m) \), for each column \( m \), pertaining to each ensemble member. Having evaluated \( Y_p^{(f)} \), we then apply equation (24.a) for \( R_b^{(f)} \), giving the local background error covariance matrix in observation space, with dimensions \( V' \times V' \). The local observations error covariance matrix \( R_o^{(f)} \), with dimensions \( V' \times V' \), is assumed diagonal with main diagonal elements equal to \( \sigma_o^2 \), where the observational standard deviation is assumed still \( \sigma_o = 1.5 \) mW cm m\(^{-2}\) sr\(^{-1}\). The \( X_p^{(f)} \) set follows equation (5.a) in an implementation identical to the one of section 2.3.3, so that equation (24.b) for the evaluation of the local Kalman gain may be implemented. The dimensions of \( K^{(f)} \) will then be \( 1 \times V' \). Given the analysis equation (24.c) the innovations \( y_o - \bar{y}_b \) for here are perceived as follows; we assign a symbol \( \bar{d} \equiv y_o - \bar{y}_b \) for a \( V' \times 1 \) column vector. Its first
element will be \( \bar{d}(1) = y_o(11) - \bar{y}_b(11) \), its second \( \bar{d}(2) = y_o(23) - \bar{y}_b(23) \), and so on until its last for \( \bar{d}(11) = y_o(101) - \bar{y}_b(101) \), given the example at hand. We then apply equation (24.c) in a looping process for every model space grid point \( k \).

As a closing remark, we mention that the applicable sensitivity analysis in the radiance per pressure levels local assimilation involves several choices of the value \( V \). Specifically, for \( V = \{5, 20, 30, 40, 60\} \). The more channels we have (but not too many), the more information we incorporate from the spectral space, and that should be reflected in the data assimilation results in accordance. Additionally, on one occasion we include all \( N \) spectral channels, and at another only the proper \( S \), by using the radiance valid observation space (see section 2.4.1). The findings are recorded in the results section in chapter 3, even more so in section 3.2.

### 2.4.5 Radiance per Spectral Channels Localization

In this approach, the applied Kalman filtering equations and methodology are the same as in the radiance per pressure levels localization, notwithstanding the method with which we choose the spectral channels to be used in the pertinent sets \( y_o, \bar{y}_b, \) and \( Y_p \) in order to carry out the analysis, in terms of the equations (24.a), (24.b), and (24.c).

In this computational approach we search in the absolute valued jacobian matrices \textit{per spectral channel}, or otherwise per row \( n \). Given the analysis of the sections 2.4.3 and 2.4.4 we have that the jacobians have dimensions, at maximum, \( N \times Q = 143 \times 21 \). In practice, the last \( Q - R \) columns are neglected in this method as well, and whether we consider the full or partial spectral case is a user prerogative.

This approach can best be illustrated with a practical example. From the following figure 2.13, we have a graphical representation of such a per spectral channels search in an absolute valued jacobian, pertaining to profile 0001/8664 of 000155700, for the full spectral case, followed by figure 2.14 for the partial spectral case of the same PDS TES profile. Figure 2.14 is evaluated separately, but still is almost identical to figure 2.13 only for an abridged range of channel values. In this particular profile, for the partial spectral case we neglect the first 5 and the last 9 channels, thus leaving 129 out of 143, whereas in the full spectral case we account for all 143 TES channels. In these two figures 2.13,
In the horizontal axis we have index \( n \) and some \( v_{\text{cm}}^{-1} \) values, taken from table 2.2 of section 2.4. In figure 2.13 the inverse centimeter values are for channel indices \( n = \{1, 20, 40, 60, 80, 100, 120, 140\} \). The vertical axis in these section 2.4.5 figures conveys the information regarding at which \( \zeta \) reference pressure level we have the \textit{one and only one} maximum for that particular channel \( n \). In other words, if we are to start searching in an absolute valued jacobian per row \( n \), then we have to discover for each such row, at which column \( r \) we have a maximization and \textit{only one} column index, or reference pressure level, is retained for the subsequent analysis. At this point we have a clear separation between this method and the one of section 2.4.4, since here the retained channels are going to be in number, equal to the considered spectral channels, whereas in the per pressure levels localization at each column \( r \) we could retain any number of channels, typically from 5 to 40.

![Figure 2.13](image-url)

**Figure 2.13.** Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 0001/8664 of 000155700, for the full spectral case.
Figure 2.14. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 0001/8664 of 000155700, for the partial spectral case.

From figure 2.13 for example, we have that for \( n = \{50\} \) the reference pressure level where the radiance to temperature sensitivity is at a maximum occurs in level \( r = 7 \). For channels \( n = \{49, 51\} \) we have \( r = 8 \). Similarly, we establish a many to one mapping between a spectral channel \( n \) and an \( r \) value, as it can be seen from these section 2.4.5 figures.

In order to carry out the analysis, at first we have to fill the set \( Y_p^{(f)} \) from the already evaluated \( Y_p \). If we consider the full spectral case, these sets have dimensions \( N \times M \), otherwise \( S \times M \), following section 2.4.1. The local data assimilation occurs for every model space pressure level \( k \) separately, which is also view by how equation (24.c) is posed. For one particular level \( k \), we apply the same distance related criterion in pressure space as in sections 2.3.3 and 2.4.4 and we discover all those \( \zeta_r \) values existing within the local regime of assimilation \( D_{\zeta}^{(f)} \). In turn, this will give us the information on those \( r' \) indices, in an approach equal to the one from sections 2.3.3, 2.4.4. If, for instance, these \( \zeta_r \) levels, close to \( \xi_k \), are \( \{r', r'+1, r'+2, r'+3, r'+4, r'+5, r'+6\} = \{6, 7, 8, 9, 10, 11, 12\} \), then if we consider figure 2.13, or the many to one mapping between channel \( n \) and reference
pressure level \( r \), we take into account in the Kalman filtering process only those spectral channels for which there is a corresponding maximization, given those \( r' \) indices existing within \( D_{\xi}^{(f)} \).

Visually, following the current example, from figure 2.13 we have that at reference pressure level \( r = 6 \) there is no such absolute valued jacobian elements maximization, as is the case for level \( r = 9 \). For level \( r = 7 \) we have one channel \( n = \{ 50 \} \), for \( r = 8 \) channels \( \{ 49, 51 \} \), for \( r = 10 \) channels \( \{ 45, 48 \} \), for \( r = 11 \) channels \( \{ 47, 52, 53 \} \), and for \( r = 12 \) channels \( \{ 41, 44, 46, 63, 124 \} \). For that model space pressure level \( k \), the spectral channels to be used in the analysis are \( \{ 41, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 63, 124 \} \), which is the logical union of the previous channel indices information. The total number of these channels for here is 13 which gives one dimension for the local sets of equations (24.a), (24.b), and (24.c). The error covariance matrices \( R_{b}^{(f)} \) and \( R_{o}^{(f)} \) will be \( 13 \times 13 \), the innovations vector \( \bar{d} = y_{o} - \bar{y}_{b} \) will be \( 13 \times 1 \), the local Kalman gain \( K^{(f)} \) will be \( 1 \times 13 \), and the local background perturbations matrix in observation space \( Y_{p}^{(f)} \) will be \( 13 \times M \) with its transpose \( M \times 13 \), where \( M = 16 \) the fixed ensemble size. Following section 2.4.4, we will then have for the elements of \( Y_{p}^{(f)} \) values \( Y_{p}^{(f)}(1, m) = Y_{p}(41, m) \), \( Y_{p}^{(f)}(2, m) = Y_{p}(44, m) \) and so on until \( Y_{p}^{(f)}(13, m) = Y_{p}(124, m) \). For the innovations, similarly it will be \( \bar{d}(1) = y_{o}(41) - \bar{y}_{b}(41) \), \( \bar{d}(2) = y_{o}(44) - \bar{y}_{b}(44) \) and so on until \( \bar{d}(13) = y_{o}(124) - \bar{y}_{b}(124) \). From equation (24.a) we then evaluate \( R_{b}^{(f)} \). Matrix \( R_{o}^{(f)} \) is diagonal with the exact same formulation as in section 2.4.4. The local Kalman gain \( K^{(f)} \) is evaluated from equation (24.b) with the local background perturbations matrix \( X_{p}^{(f)} \) following computationally section 2.4.4, and from equation (24.c) we then evaluate the analysis ensemble mean \( ( \bar{x}_{a} )_{k} \), which is also the objective.

We notice that for one value of channel \( n \) to participate in the assimilation process, the corresponding \( \zeta_{r} \) level needs to be within \( D_{\xi}^{(f)} \). Given the PDS TES profiles, in general the levels of the radiance to temperature maximization occur for \( r > 6 \). What is more, the vast majority of jacobian maximizations occurs at one specific \( \zeta_{r} \) reference
pressure level, so that for this 2.4.5 section approach to start incorporating a significant amount of information from spectral space, we need to be in model space typically for \( k > 18 \). Otherwise, we only account for no more than 15 spectral channels, at maximum, for model space pressure levels at a higher altitude. Conversely, in the section 2.4.4 approach the information from the spectral space is more spread out, allowing us to consider for each \( k \geq 15 \) model level a greater amount of spectral channels. Computationally the per spectral channels localization, for pressure levels very close to the surface, is more expensive. From every figure of the current section, we observe that for one particular reference pressure level, be it \( r = 13 \) or \( r = 14 \) we have more than 90\% of the channels in this many to one mapping. If we assimilate close to the surface, where these \( r \) levels appear within \( D_{\xi}^{(f)} \), the dimensions of the ordered sets from equations (24.a) and (24.b) will be correspondingly greater than the dimensions of the sets if we apply the per pressure levels localization. Given the matrix inversions alone and the overall content of information from spectral space, we conclude that the per spectral channels is less optimal than the per pressure levels localization.

The following figures 2.15 and 2.16 are for the full spectral cases of the other two examined PDS TES profiles 1374/8664 of 000155700 and 7600/7952 of 000239506.

![Figure 2.15](image_url)

**Figure 2.15.** Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 1374/8664 of 000155700, for the full spectral case.
Figure 2.16. Pressure levels of maximum spectral radiance to temperature sensitivity, per spectral channel, for profile 7600/7952 of 000239506, for the full spectral case.
Chapter 3

Results

The results presented herein pertain to the three profiles under consideration. These profiles are 0001/8664 and 1374/8664 of 000155700, and 7600/7952 of 000239506 of the PDS TES observed radiances and OSS TES retrieved temperatures data sets respectively. Primarily, these profiles provide the observations used in the retrieval and the radiance data assimilation as described previously in the methodology sections 2.3 and 2.4.

In section 3.1 the results in a space pressure versus temperature are presented. In every figure of section 3.1 the vertical axis is the horizontally interpolated MGCM ensemble mean pressure, denoted previously \((p_b)_k\) (see section 2.3.1), and the horizontal axis the applicable temperature range of the plotted curves. For every examined case, vertically there always are 28 model space levels, for \(k = \{1, 2, \ldots, 28\}\), starting from \(k = 1\) at a pressure value \((p_b)_1 = 0.02 \text{ Pa}\) until just above the planetary surface, at \(k = 28\). It can be seen across the examined cases that for the pressure levels at \(k = 28\), these values are around 800 Pa, 500 Pa, and 300 Pa, indicative of the locations of the horizontal interpolation, governed from each \((\varphi_s, \lambda_s)\) satellite position per considered profile. These values are closely related to the topography of Mars and its impact on the climate model, an aspect which can also be viewed from a detailed description presented in appendix A, and also from figure 3.1 given below.
Examined profiles topographic locations

0001/8664 of 000155700
1374/8664 of 000155700
7600/7952 of 000239506

Figure 3.1. Examined profiles topographic locations. Profiles 0001/8664 of 000155700 (yellow dots), 1374/8664 of 000155700 (cyan dots), and 7600/7952 of 000239506 (white dots) are presented in their respective satellite locations.

In view of figure 3.1, regarding the satellite locations of the three profiles, for 0001/8664 (yellow dots) it is \((45.1^{\circ}, 107.63^{\circ})\), for the second profile 1374/8664 (cyan dots) it is \((-35.0^{\circ}, 300.49^{\circ})\), and for 7600/7952 (white dots) we have \((-4.92^{\circ}, 258.25^{\circ})\).

The first profile is a northern hemisphere mid latitudinal one as is the second for the southern hemisphere, while the third is an equatorial. From figure A.7 of appendix A, a density – contour plot is presented for a pressure level close to the surface, at \(k = 26\), for one MGCM output 000155700, giving the background in both the 0001/8664 and in 1374/8664 performed assimilations. While it is not for \(k = 28\), at the pressure level closest to the surface the pressure values are expected to be greater than those of figure A.7, for all three profiles. It is not in the scope of the current study to track any weather systems of the Martian atmosphere so the pressure levels of figures A.7, A.8, and A.9 of appendix A are
assumed to simply follow the topography of the planet. This is a clarification as to the discrepancies in the range of the horizontal axes of the figures pertaining to the three examined cases. For instance, the topography at the interpolation of 0001/8664 is clearly different from the one for 7600/7952, which explains why in the first case the pressure range goes up to around 800 Pa as opposed to the third which reaches 300 Pa, a fact that can be also viewed from figure 3.1.

With regards to a temporal description of the used profiles, we have that the model specification formats of 000155700 and 000239506 correspond to the Martian model year, either 0001 of 0002, to the sols since perihelion 557 and 395, and to the Martian universal time in hours, 00 and 06. The first two profiles of 0001/000155700 and 1374/000155700 are for the Martian year 24, with a solar longitude $L_s = 180.6^\circ$, and the third one 7600/000239506 for Martian year 25 with $L_s = 97.8^\circ$. The first two profiles with a sol since perihelion equal to 557, seasonally correspond to spring (towards summer), and the third to winter (towards spring). Given the location of the profiles in conjunction with the pertinent Martian timekeeping, the first two profiles are day time, and the third a night time one. From the temperature ranges of figure 3.2, we may also notice that the temperature range (and values) of 7600/000239506 close to the ground is less than the previous two examined cases. An interesting feature of the third profile is also a characteristic ice cloud thermal signature occurring around $p = 1$ Pa well–matched, primarily, with the season.

In every figure of section 3.1 the cyan lines visualize the observations, the black lines the background ensemble mean, the dashed gray lines the background ensemble, and the colored lines the analysis ensemble mean, for each examined case.

In figure 3.2 sub plots (a), (c), (e) we have the graphical representation of the results from the filtering methodology (sections 2.3.1–2.3.2) with observational standard deviation $\sigma_o = 3.0$ K, where the analysis ensemble mean is the orange line. In figure 3.2 sub plots (b), (d), (f) we convey the same information, for $\sigma_o = 5.0$ K, with the analysis ensemble mean being the blue line. These figures correspond to the retrieval global assimilation, described in section 2.3.2. Visually, we distinguish the fact that in the $\sigma_o = 5.0$ K sub plots the analysis ensemble mean is closer to the background in accordance with section 2.3.2.

In figure 3.3, we have the results of the radiance global assimilation, of section 2.4.2 for the full and partial spectral cases. The full spectral cases are depicted in figure 3.3 sub plots (a), (c), (e), where the analysis ensemble mean is the orange line, as well. For the
partial spectral cases, as outlined in section 2.4.1, we have excluded channels for 0001/8664 the first 5 and the last 9, for 1374/8664 the first 8 and the last 43, and for 7600/7952 the first 7 and the last 66. The radiance global assimilation of the partial spectral case is presented in figure 3.3 sub plots (b), (d), (f). With the exception of figure 3.3 sub plots (c) and (d) it is otherwise difficult to graphically discern differences between the full and the partial spectral cases.

In figure 3.4 we have 12 sub plots pertaining to the retrieval local assimilation of sections 2.3.3–2.3.4, $R_o$ modulation included. The first 4 sub plots, figure 3.4 (a), (b), (c), (d) are for 0001/8664 for the cases: (a) $\sigma_o = 3.0$ K with coefficient $c$ from equation (10) equal to $c = 0.015$, (b) $\sigma_o = 3.0$ K with $c = 0.030$, (c) $\sigma_o = 5.0$ K with $c = 0.015$, and (d) $\sigma_o = 5.0$ K with $c = 0.030$. In figure 3.4 sub plots (e), (f), (g), (h) we have the results for profile 1374/8664. Sub plot (e) is for $\sigma_o = 3.0$ K with $c = 0.015$, (f) $\sigma_o = 3.0$ K with $c = 0.030$, (g) $\sigma_o = 5.0$ K with $c = 0.015$, and (h) $\sigma_o = 5.0$ K with $c = 0.030$. Lastly, we have figure 3.4 sub plots (i), (j), (k), (l) for 7600/7952. For sub plot (i) it is $\sigma_o = 3.0$ K with $c = 0.015$, for (j) $\sigma_o = 3.0$ K with $c = 0.030$, for (k) $\sigma_o = 5.0$ K with $c = 0.015$, and for (l) $\sigma_o = 5.0$ K with $c = 0.030$. For each case the analysis ensemble mean is the orange, blue, magenta, and green line respectively.

Following that, we have results for the radiance local per pressure levels assimilation, of section 2.4.4. There are two categories here; figures 3.5, 3.7, and 3.9 present the full spectral case for 0001/8664, 1374/8664, and 7600/7952 respectively. Moreover, figures 3.6, 3.8, and 3.10 correspond to the partial spectral case of the examined profiles given the previous profile order. The analysis ensemble mean is represented as a blue, magenta, green, and light blue line in every one of those figures. Given the order with which the coloring applies, we have for the full and the partial spectral case accounted channels 20, 30, 40, and 60 respectively. The difference lies in whether these channels are extracted from all 143 spectral channels, or from an appropriate partial sub set of those, as explained in section 2.4.1.

There is also a case for 5 used channels either for the full or the partial spectral case, which is not presented in section 3.1, yet it is one additional result covered in the figures of section 3.2. The radiance per spectral channels assimilation is not represented visually in section 3.1 either, largely due to the fact that these pressure versus temperature plots give
limited insight to the differences between each applied technique, information which is mainly conveyed from the results of section 3.2.

In section 3.2 the signed differences between the analysis and background ensemble means for the previous three profile cases, are presented. In this section the vertical axis is as in section 3.1, with the horizontal axis representing those signed differences, $\bar{x}_a - \bar{x}_b$, giving the analysis increments. The difference is taken as such in order to be able to distinguish visually whether there is a warming or a cooling, as a result of the assimilation approaches. For $(\bar{x}_a)_k > (\bar{x}_b)_k$ we have a warming and for $(\bar{x}_a)_k < (\bar{x}_b)_k$ a cooling, since the analysis and background means are temperatures at the model pressure levels.

In figure 3.11 we have the signed differences for the retrieval assimilation, of profile 0001/8664. Sub plot (a) is for the global case, and sub plot (b) for the local one. In sub plot (a) the orange line is for $\sigma_o = 3.0 \text{ K}$ and the blue line for $\sigma_o = 5.0 \text{ K}$. In sub plot (b), from the performed sensitivity analysis we have for the green line $\sigma_o = 3.0 \text{ K}$ with $c = 0.015$, for the blue line $\sigma_o = 3.0 \text{ K}$ with $c = 0.030$, for the magenta line $\sigma_o = 5.0 \text{ K}$ with $c = 0.015$, and for the green line $\sigma_o = 5.0 \text{ K}$ with $c = 0.030$. Figures 3.12 and 3.13 are for the profiles 1374/8664 and 7600/7952 respectively. The corresponding sub plots 3.12 (a), 3.12 (b) and 3.13 (a), 3.13 (b) follow the presentation convention of figure 3.11.

In figure 3.14 we have the radiance global assimilation for 0001/8664. The orange line is for the full and the blue line is for the partial spectral case, where the first 5 and the last 9 channels are excluded, thus leaving the valid observation space with 129 out of 143 channels (from section 2.4.1). Similarly, we have figures 3.16 for profile 1374/8664 and figure 3.18 for 7600/7952. In 1374/8664 the excluded channels are the first 8 and the last 43, and for 7600/7952 the first 7 and the last 66.

Additionally, we have figures 3.15, 3.17, and 3.19 for profiles 0001/8664, 1374/8664, and 7600/7952, for the case of the radiance local per pressure levels assimilation. Sub plots 3.15 (a), 3.17 (a), and 3.19 (a) correspond to the full spectral case, while sub plots 3.15 (b), 3.17 (b), and 3.19 (b) to the partial spectral case. In every case here, the used channels are 5, 20, 30, 40, or 60 following the performed sensitivity analysis of the current study.

The graphical results of the implementation of section 2.4.5 for the radiance local per spectral channels assimilation are presented in figures 3.20, 3.21, and 3.22. Figure 3.20 is for 0001/8664 with sub plot (a) for the full and sub plot (b) for the partial spectral case. In the partial spectral case we neglect the first 5 and the last 9 channels for this profile, similar
to the practice of the radiance global or radiance local per pressure levels assimilation. In figure 3.21, sub plot (a) and sub plot (b) we have the full and partial spectral case for 1374/8664 with neglected channels in the partial spectral case the first 8 and the last 43. Figure 3.22, which concludes the results section, is for 7600/7952. Sub plot (a) and (b) are yet again for the full and the partial spectral case as well, with neglected channels in the partial spectral case the first 7 and the last 66.

Lastly, we have the results of section 3.3 for a graphical representation of the radiance observations (PDS TES observed spectra) \( y_o \), the analysis ensemble mean in observation space \( \mathbf{y}_a \), the background ensemble mean in observation space \( \mathbf{y}_b \), and the background ensemble members in observation space \( \mathbf{y}_b^{(m)} \), for the three examined PDS TES profiles. The results of section 3.3 pertain to one specific performed data assimilation, the radiance local per pressure levels assimilation, for the partial spectral space and for a retained channels plentitude equal to 30, following section 2.4.1. This specific assimilation is regarded as one of the more optimal ones, in the case where we assimilate radiances.

These three figures 3.23, 3.24, and 3.25 are in direct relation to the figures 3.6 (b), 3.8 (b), and 3.10 (b) of section 3.1. In section 3.1 we have graphical representations of the OSS TES observations \( y_o \), the analysis ensemble mean in model space \( \mathbf{x}_a \), the background ensemble mean in model space \( \mathbf{x}_b \), and the background ensemble members in model space \( \mathbf{x}_b^{(m)} \), where the model space is the 28 levels pressure space, and the observation space the reference pressure levels space with levels less than 21.

Figure 3.23 is for the PDS TES profile 0001/8664 of 00015570, as is figure 3.6 (b). Figure 3.24 for the profile 1374/8664 of 000155700 like figure 3.8 (b), and figure 3.25 for 7600/7952 of 000239506 like figure 3.10 (b). In all these figures, the observations whether they are PDS TES observed spectra or OSS TES temperature retrievals, are equally denoted \( y_o \). In pressure space these \( y_o \) are temperatures and in spectral space are spectral radiances. Figures 3.6 (b), 3.8 (b), and 3.10 (b) stem from the implementation of equations (24.a), (24.b), and (24.c) of section 2.4.4, for the assimilation in model (pressure) space. In these three figures 3.6 (b), 3.8 (b), and 3.10 (b) \( \mathbf{x}_a \) is the result of the radiance local per pressure levels assimilation, with \( \mathbf{x}_b \) being known from the climate model interpolations of section 2.3.1 at the satellite location. The individual ensemble members in model space \( \mathbf{x}_b^{(m)} \) are also known from these \( \varphi - \lambda \) interpolations. Given the fact that in the analysis
equations of section 2.4.4 we have the appearance of the term $\mathbf{y}_b$, which is the radiance ensemble mean of each member $\mathbf{y}_b^{(m)}$, these individual members $\mathbf{y}_b^{(m)}$ were evaluated from the application of the OSS forward model operator, which is referenced in section 2.4.1. Conversely, for figures 3.23, 3.24, and 3.25 we already have the states $\mathbf{y}_o$ and $\mathbf{y}_b^{(m)}$, but not $\mathbf{y}_a$ and $\mathbf{y}_b$, since the last two were not a part of the assimilation of section 2.4.4. In order to evaluate those, for the sake of creating these 3.23, 3.24, and 3.25 graphs, we apply the OSS forward model operator on the model space states $\mathbf{x}_a$ and $\mathbf{x}_b$, where first these are mapped from the 28 model space pressure levels to the 21 retrieval observation space levels, given the functionality of the OSS forward model operator (see section 2.4.1).
3.1 Pressure VS Temperature

**Figure 3.2.** Analysis temperature profiles for the retrieval global assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a and b) For profile 0001/8664 of 00155700. (c and d) For profile 1374/8664 of 00155700. (e and f) For profile 7600/7952 of 000239506. Sub plots (a), (c), and (e) are for observational standard deviation \( \sigma_0 = 3.0 \) K, and (b), (d), and (f) for \( \sigma_0 = 5.0 \) K.
Figure 3.3. Analysis temperature profiles for the radiance global assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a and b) For profile 0001/8664 of 00155700. (c and d) For profile 1374/8664 of 00155700. (e and f) For profile 7600/7952 of 000239506. Sub plots (a), (c), and (e) are for the full spectral case while sub plots (b), (d), and (f) for the partial one. For sub plot (b), the excluded channels are the first 5 and the last 9, for (d) the first 8 and the last 43, and for (f) the first 7 and the last 66.
Figure 3.4. Analysis temperature profiles for the retrieval local assimilation, evaluated using the filtering methodology of this study, are plotted against ensemble mean pressure levels. Colored lines (orange, blue, magenta, green) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. (a, b, c, and d) For profile 0001/8664 of 000155700. (e, f, g, and h) For profile 1374/8664 of 000155700. (i, j, k, and l) For profile 7600/7952 of 00239506. Sub plots (a), (e), and (i) correspond to observational standard deviation $\sigma_\omega=3.0$ K with localization coefficient $c = 0.015$. Sub plots (b), (f), and (j) are for $\sigma_\omega=3.0$ K with $c = 0.030$. Sub plots (c), (g), and (k) are for $\sigma_\omega=5.0$ K with $c = 0.015$ and (d), (h), and (l) for $\sigma_\omega=5.0$ K with $c = 0.030$. 

![Figure 3.4](image-url)
**Figure 3.5.** Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 0001/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
Figure 3.6. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 0001/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 129 out of 143. Excluded channels are the first 5 and the last 9. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
**Figure 3.7.** Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 1374/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
Figure 3.8. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 1374/8664 of 000155700. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 92 out of 143. Excluded channels are the first 8 and the last 43. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
Figure 3.9. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 7600/7952 of 000239506. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from all available 143 out of 143. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
Figure 3.10. Analysis temperature profiles for the radiance local per pressure levels assimilation, evaluated using the current filtering methodology, are plotted against ensemble mean pressure levels, for profile 7600/7952 of 000239506. Colored lines (blue, magenta, green, light blue) represent the analysis mean, cyan lines the OSS TES temperature retrievals, black lines the background mean, and dashed lines of reduced opacity the background ensemble members. The used channels are drawn from 70 out of 143. Excluded channels are the first 7 and the last 66. (a) For 20 used channels. (b) For 30 used channels. (c) For 40 used channels. (d) For 60 used channels.
3.2 Signed Differences

Figure 3.11. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both sub plots are for the profile 0001/8664 of 000155700. (a) For the global assimilation; $\sigma_o=3.0$ K (orange line) and $\sigma_o=5.0$ K (blue line). (b) For the local assimilation; $\sigma_o=3.0$ K with $c = 0.015$ (orange line), $\sigma_o=3.0$ K with $c = 0.030$ (blue line), $\sigma_o=5.0$ K with $c = 0.015$ (magenta line), and $\sigma_o=5.0$ K with $c = 0.030$ (green line).
Figure 3.12. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both sub plots are for the profile 1374/8664 of 000155700. (a) For the global assimilation; $\sigma_o=3.0$ K (orange line) and $\sigma_o=5.0$ K (blue line). (b) For the local assimilation; $\sigma_o=3.0$ K with $c = 0.015$ (orange line), $\sigma_o=3.0$ K with $c = 0.030$ (blue line), $\sigma_o=5.0$ K with $c = 0.015$ (magenta line), and $\sigma_o=5.0$ K with $c = 0.030$ (green line).
Figure 3.13. Signed differences between analysis mean and background mean for the retrieval assimilation are plotted against ensemble mean pressure levels. Both sub plots are for the profile 7600/7952 of 000239506. (a) For the global assimilation; $\sigma_0 = 3.0$ K (orange line) and $\sigma_0 = 5.0$ K (blue line). (b) For the local assimilation; $\sigma_0 = 3.0$ K with $c = 0.015$ (orange line), $\sigma_0 = 3.0$ K with $c = 0.030$ (blue line), $\sigma_0 = 5.0$ K with $c = 0.015$ (magenta line), and $\sigma_0 = 5.0$ K with $c = 0.030$ (green line).
Figure 3.14. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 5 and the last 9 channels have been excluded from the analysis, thus rendering the valid channels 129 out of 143.
Figure 3.15. Signed differences between analysis mean and background mean for the radiance local per pressure levels assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from all available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 129 out of 143 channels, excluding the first 5 and the last 9.
Figure 3.16. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 8 and the last 43 channels have been excluded from the analysis, thus rendering the valid channels 92 out of 143.
Figure 3.17. Signed differences between analysis mean and background mean for the radiance local per pressure levels assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from the available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 92 out of 143 channels, excluding the first 8 and the last 43.
Figure 3.18. Signed differences between analysis mean and background mean for the radiance global assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. The orange line is for the full spectral case, where all 143 out of 143 channels are accounted for. The blue line is for the partial spectral case, where the first 7 and the last 66 channels have been excluded from the analysis, thus rendering the valid channels 70 out of 143.
Figure 3.19. Signed differences between analysis mean and background mean for the radiance local per pressure levels assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. (a) For the full spectral case where the 5, 20, 30, 40, and 60 channels are drawn from the available 143 out of 143 channels. (b) For the partial spectral case where the 5, 20, 30, 40, and 60 channels are drawn from 70 out of 143 channels, excluding the first 7 and the last 66.
Figure 3.20. Signed differences between analysis mean and background mean for the radiance local per spectral channels assimilation are plotted against ensemble mean pressure levels, for the profile 0001/8664 of 000155700. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 5 and the last 9 channels from the analysis.
Figure 3.21. Signed differences between analysis mean and background mean for the radiance local per spectral channels assimilation are plotted against ensemble mean pressure levels, for the profile 1374/8664 of 000155700. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 8 and the last 43 channels from the analysis.
Figure 3.22. Signed differences between analysis mean and background mean for the radiance local per spectral channels assimilation are plotted against ensemble mean pressure levels, for the profile 7600/7952 of 000239506. (a) For the full spectral case, using all available 143 out of 143 channels. (b) For the partial spectral case, excluding the first 7 and the last 66 channels from the analysis.
3.3 Radiance Spectral Distributions

Figure 3.23. PDS TES 0001/8664 of 000155700 profile spectral distributions of the observed spectra $y_o$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30.
Figure 3.24. PDS TES 1374/8664 of 000155700 profile spectral distributions of the observed spectra $y_o$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30.

![Radiance, Local, n=30
Used channels 70/143
7600/7952 of 00239506](image)

Figure 3.25. PDS TES 7600/7952 of 000239506 profile spectral distributions of the observed spectra $y_o$, the background ensemble members in spectral space $y_b^{(m)}$, the analysis ensemble mean in spectral space $y_a$, and the background ensemble mean in spectral space $y_b$, for the radiance local per pressure levels assimilation, of the partial spectral space and retained channels plentitude equal to 30.
Chapter 4

4.1 Discussion

In sections 3.1, 3.2, and 3.3 we have the collective results of this study for the three examined profile cases 0001/8664 and 1374/8664 of 000155700, and 7600/7952 of 000239506 of the PDS TES and OSS TES data sets, giving the observed satellite radiances and the OSS retrieved temperatures, as the assimilation observations.

In section 3.1 plots in a space pressure versus temperature are presented. There, we have the results for the retrieval global and local data assimilation performed in this study, implementing the methodology of sections 2.3 – 2.3.4. At the same time we have the results for the radiance global data assimilation applying sections 2.4 – 2.4.2 for the full and the partial spectral spaces. In section 3.1, regarding the radiance local data assimilation, only the results of section 2.4.4 are presented as that relates to the local per pressure levels approach. The results of section 2.4.5 for the radiance local per spectral channels approach are largely indistinguishable from those stemming from the application of section 2.4.4 so that visually there are no discernible differences in this space pressure versus temperature, and due to that fact it is deemed redundant to present both 2.4.4 and 2.4.5 sections graphical results in section 3.1.

In section 3.2 the analysis increments $\mathbf{x}_a - \mathbf{x}_b$ are presented for every applied assimilation implementation, namely for the retrieval global and local, for the radiance global, for the radiance local per pressure levels, and for the radiance local per spectral channels. In the case of the radiance assimilation there is also the distinction between the full and the partial spectral cases considering section 2.4.1. From section 3.2 the discrepancies in the results are more noticeable and in view of that it is from this section that important conclusions of the current study can be drawn.

There also are the results of section 3.3, which present spectral distributions of radiance, similar in nature to the results of section 3.1, only in section 3.3 the space is a portion of the electromagnetic spectrum, $L_{dv}$ versus $v_{cm}^{-1}$. These results pertain to select cases of radiance assimilation and are of an auxiliary nature. As is the case in section 3.1, any differentiations between the applied approaches of sections 2.4.2, 2.4.4, and 2.4.5 are
not evident from the corresponding figures of section 3.3. These 3.3 section figures are also presented in order to highlight the application of the OSS forward model operator. In section 2.4.1, from tables 2.3, 2.4, and 2.5 where we present the input vector to this operator, we notice for instance that certain temperature values at the reference pressure levels are repeated. However, this feature is a part of this OSS operator implementation so that figures 3.23, 3.24, and 3.25 merely point to the calculation of the background in radiance observation space for the analysis mean, the background mean, and the background ensemble state, so that the mappings from temperature to radiance are evaluated correctly.

A general remark to be made when using any Kalman filter method, is that the analysis ensemble mean $\bar{x}_a$ should be in-between the background ensemble mean $\bar{x}_b$ and the observations $y_o$, for those domains where observations are to be found. In general, this behavior is met, at the very least in the retrieval assimilations, global or local, as that can be viewed from figures 3.2 and 3.4, across the corresponding sub plots. In figure 3.2, upon closer examination across all six sub plots (a) – (e), below pressure level 10 Pa this feature is achieved. Similarly, in figure 3.4 all twelve sub plots (a) – (l) exhibit the expected performance below pressure level 10 Pa, in the regime where there are observations.

For the radiance assimilation results, there are those figures pertaining to profile 1374/8664 where we may view this behavior, yet in the other profile cases 0001/8664 and 7600/7952 we cannot visually discern this characteristic from section 3.1 so that we need to resort to the figures of section 3.2. The 1374/8664 graphs that show this feature are figure 3.3 sub plots (c), (d) for the radiance global assimilation and figures 3.8, 3.8 across all four sub plots for each figure, for the radiance local per pressure levels, below 10 Pa. We also notice that in figure 3.3 sub plot (c) there is a deviation from the expected analysis mean behavior, where this inconsistency is attributed to the radiance global approach. The same can be said for the sub plots of figure 3.7, where despite the locality of the radiance assimilation, the approach there is for the full spectral case. From the radiance graphs of section 3.1, for those that depict the separation of $\bar{x}_a$ from $\bar{x}_b$, only figure 3.8 presents results that follow the Kalman filtering stipulation most accurately.

Conclusively, for the results of section 3.1 for pressure levels below 10 Pa across every figure 3.2 – 3.10 we have that the retrieval data assimilation, local or global, adheres to the filtering expected behavior. Conversely, in the radiance data assimilation and for the
cases where discrepancies may be discerned visually, there are differences between the full and the partial spectral cases, primarily viewed from the figures of profile 1374/8664.

The fact that the Kalman filter suggests $\mathbf{x}_a$ should be in-between $\mathbf{x}_b$ and $\mathbf{y}_o$ has a physical meaning; if the OSS TES temperatures $\mathbf{y}_o$ are less than the MGCM outputs leading to $\mathbf{x}_b$, then the analysis ensemble mean $\mathbf{x}_a$ lean towards a cooling. On the other hand if $\mathbf{y}_o$ is greater than $\mathbf{x}_b$, then $\mathbf{x}_a$ should point to a warming. In spite of the fact that the pressure levels of the observations $\mathbf{y}_o$ do not coincide with the pressure levels of $\mathbf{x}_b$ and $\mathbf{x}_a$, still we may infer the in-between values for $\mathbf{y}_o$ and $\mathbf{x}_b$, so that the remark made here can be applied, even qualitatively. From the figures of section 3.1, we have a visual understanding of where the OSS TES observations are in relation to the background ensemble mean and that motivates the introduction of section 3.2, where we may recognize those finer differentiations.

For the graphical representations of section 3.2, the vertical axis is as in section 3.1, with the horizontal axis giving the analysis increments in terms of temperature differences $\mathbf{x}_a - \mathbf{x}_b$, across all 28 model space nodes. In every graph of section 3.2, there exist a zero value on the horizontal axis, so that for values greater than zero we have a warming and for values less than zero a cooling.

The first graph of section 3.2 is figure 3.11 sub plot (a), for the retrieval global assimilation of 0001/8664. For pressure values greater than 10 Pa there appear non zero analysis increments signifying the fact that a data assimilation is performed even for those model space nodes for which no local observations exist nearby. In conjunction with figure 3.2, either sub plot (a) or (b), for $p < 10$ Pa, there are no observations with which an analysis ensemble mean could be associated with. In this respect, first the warming for $p \in [0.035, 1]$ Pa, and then the cooling for $p \in [1, 10]$ Pa cannot be described from the Kalman filter stipulation. For the range $p \in [10, 90]$ Pa there is a cooling, and for $p > 90$ Pa a warming in accordance with the $\mathbf{y}_o$ profile of this case. The orange line of figure 3.11 (a) is for $\sigma_o = 3.0$ K, and the blue line for $\sigma_o = 5.0$ K. In the second case with a greater observational standard deviation the filter trusts more the background, which is theoretically correct and also observed as well, given the fact that this blue line is closer to the zero $\Delta T$ line. So, figure 3.11 (a) gives results that fall in line with the applied theory directives.
Figure 3.11 sub plot (b) is also for profile 0001/8664, for the retrieval local assimilation. Here, it is evident that for \( p < 9 \) Pa there is no performed data assimilation, considering section 2.3.3. Below 9 Pa we have a cooling until \( p \approx 90 \) Pa, and below that a warming, matching the \( y_o \) profile. Comparing figure 3.11 (a) with 3.11 (b), for \( p > 90 \) Pa, we have a similar behavior in the filtering results. The \( \Delta T \) differences are in the same direction (negative or positive), where the assumed \( \sigma_o \) value per case seems to have a more significant impact on the results, that the localization coefficient value, \( c = \{0.015, 0.030\} \) itself. The orange and blue lines of figure 3.11 (b) are closer to the orange line of figure 3.11 (a) for \( \sigma_o = 3.0 \) K, and the same applies to the green and magenta lines of figure 3.11 (b), with those being closer to the blue line of figure 3.11 (a), for \( \sigma_o = 5.0 \) K. The blue and green lines of figure 3.11 (b) for \( c = 0.030 \) are a better match with the orange and blue lines of figure 3.11 (a), which denotes the fact that if in the localized assimilation we consider more local observations, these results will be closer to the global case.

Essentially, the same analysis can be made for figure 3.12 (a), (b) for 1374/8664, as well as for figure 3.13 (a), (b) for 7600/7952. For profile 1374/8664 for \( p \in [10, 200] \) Pa we have a cooling, and below that a slight warming, while for profile 7600/7952 where the inversion takes place for \( p \in [10, 100] \) Pa there is a cooling, then for \( p \in [100, 250] \) Pa a warming, and below that a slight cooling, where in every case the corresponding \( y_o \) profile contributes to this behavior.

A general remark on the retrieval assimilation is that it offers results which conform with what the theory suggests. This points to the fact that the implementation was carried out correctly, and most importantly, we may consider the retrieval assimilation to serve as the template, as the measure with which the radiance assimilation may be compared to.

Figure 3.14 presents the radiance global assimilation analysis increments for 0001/8664. The orange line is for the full spectral case and the blue line is for the partial one. We limit the analysis in the range \( p > 10 \) Pa, where some conclusions may be drawn. In figures 3.11 (a), (b), for \( p \in [10, 90] \) Pa we have a cooling, and for \( p > 90 \) Pa, a warming. In figure 3.14, in the range \( p \in [15, 200] \) Pa we have a cooling in both curves, yet for \( p > 200 \) Pa only the partial spectral space curve points to a warming. The orange
curve, erroneously, continues to point to a cooling and this result insinuates that if we consider all 143 channels the result will be corrupted, yielding a false $\mathbf{X}_a$ profile.

From figure 3.15 we examine the profile 0001/8664 radiance local per pressure levels assimilation. Sub plot 3.15 (a) is for the full spectral space, and 3.15 (b) for the partial spectral space. Comparing these two figures 3.15 (a) and 3.15 (b) with figure 3.11 (b), we notice that only the partial spectral case yields the most similar results to the retrieval local assimilation, in a different $\Delta T$ range no less. Figure 3.15 (a) around $p = 10$ Pa implies a warming if the used spectral channels are 60, presumably too many, which under no circumstances appears in figure 3.2 (a) or (b). In the same sub plot 3.15 (a), if the used spectral channels, namely 5, 20, 30, or 40, are not too many, despite the fact that we use all 143 out of 143 for the local approach, we still have results that point to the correct physical direction of the analysis mean. In opposition to that, in the radiance local assimilation with the partial spectral case, from figure 3.15 sub plot (b), regardless of whether we use few or more channels for the assimilation, we have a very similar behavior pointing to the correct physical direction of $\mathbf{X}_a$. The analysis increments may be less compared to figure 3.11 (b) but at the very least if this $\mathbf{X}_a$ profile were to be used to drive the numerical solver, its contribution would have been the more sensible one. The impact of the plentitude of the used channels in either sub plot 3.15 (a) or 3.15 (b) is also observable.

Proceeding to figure 3.16, we examine 1374/8664 for the radiance global assimilation for the full spectral case (orange line), and the partial one (blue line). We focus our attention to $p > 9$ Pa and upon comparison with figure 3.12 (a) we have that for $p \in [9, 300]$ Pa there ought to be a cooling, and for $p > 300$ Pa a slight warming. In figure 3.16 only the blue line conforms to that. The orange line for $p > 200$ Pa points to a cooling, which is physically incorrect, considering figure 3.2 (c) or 3.2 (d). Again, the full spectral case does not give correct results.

From figure 3.17 we have the radiance local per pressure levels assimilation, for 1374/8664, similarly built to figure 3.15. Sub plot (a) is the full and sub plot (b) for the partial spectral case. We compare figure 3.17 (b) to 3.12 (b) and we find that both plots yield similar results in a different temperature range, where for the retrieval the increments $\mathbf{X}_a - \mathbf{X}_b$ are generally greater that for the radiance assimilations. In figure 3.17 (b), as was the case in figure 3.15 (b), we observe that the plentitude of the used spectral channels in the assimilation does not have a significant impact in the results, either. Whether we use 5,
20, 30, 40, or 60 channels out of the used 92, the results are close to each other. The direction of $\mathbf{x}_a$ is also correct, so that for $p \in [9, 300] \text{ Pa}$ we have a temperature drop, and for $p \in [300, 500] \text{ Pa}$ a slight rise, as in the retrieval results from figure 3.12 (b). On the other hand, if figure 3.17 sub plot (a) where we treat the full spectral case, we observe that the choice of the number of the used channels impacts the results severely. For the pressure range $p \in [300, 500] \text{ Pa}$, if we use many channels, in practice more than 5, we have an erroneous cooling, which should not be the case, judging from the retrieval results of figure 3.12 (b).

The last examined profile is 7600/7952. Figure 3.18 is for the radiance global assimilation, with the orange line for the full and the blue line for the partial spectral case, respectively. This case is quite characteristic of the impact of localization in a radiance data assimilation. The two curves here exhibit pretty much the opposite behavior. Where the blue line suggests a warming the orange line points to a cooling, and vice versa. We compare figure 3.18 with 3.13 (a) of the retrieval global assimilation, which gives physically sensible results, and we observe that in the pressure range $p \in [20, 90] \text{ Pa}$ we ought to have a cooling, for $p \in [90, 250] \text{ Pa}$ a warming, and for $p > 250 \text{ Pa}$ a cooling again. In figure 3.18 the blue line (partial spectral case) follows this direction while the orange line (full spectral case) is in the exact opposite direction. From this comparison in figure 3.18 we conclude that only the partial spectral case gives the correct $\mathbf{x}_a$ profile.

From figure 3.19 (a) we have the radiance local per pressure levels assimilation of 7600/7952 for the full spectral case, and in figure 3.19 (b) for the partial one. We focus our attention in $p > 9 \text{ Pa}$ . From figure 3.19 (b), in the pressure range $p \in [9, 20] \text{ Pa}$ we have a warming, in $p \in [20, 90] \text{ Pa}$ a cooling, then in $p \in [90, 250] \text{ Pa}$ a warming, followed by a cooling for $p > 250 \text{ Pa}$, which is in full conformity with figure 3.13 (a) as well. However, the previous statement applies conditionally for when the used channels are 20 or more, so that here if we use too few, e.g. we have the orange line behavior deviating significantly from the expected. Whether we use 20 or 60 channels in the partial spectral case, has little impact on these results. From figure 3.19 (a), we have a behavior different than what is expected. Even though for 20 or 30 used channels the behavior is consistent with the previous of the partial spectral case, in general the full spectral case, global or local, cannot be trusted to yield physically sensible results.
The next results of section 3.2 are for the case of the radiance local per spectral channels assimilation. Figure 3.20 (a) is the full spectral case of 0001/8664 and figure 3.20 (b) for the partial case. Similarly, figure 3.21 (a) and (b) is for 1374/8664, and figure 3.22 (a) and (b) for 7600/7952. In these figures there is only one curve, the red one, given the nature of this approach (section 2.4.5). Sub plots 3.20 (a), 3.21 (a), and 3.22 (a) may be compared respectively with the orange lines of the figures 3.15 (a), 3.17 (a), and 3.19 (a) where the comparison is between radiance local assimilations.

Specifically, from figures 3.20 (a) and 3.15 (a) similarities are found when we use 30 or 40 channels in the radiance local per pressure levels assimilation of figure 3.15 (a). Between figure 3.21 (a) and 3.17 (a) there are similarities when we use 30, 40, or 60 channels, and between figures 3.22 (a) and 3.19 (a) is apparent that there is a correspondence between the two when we use 60 channels in the per pressure radiance assimilation. In every case, the temperature range of the horizontal axis is roughly the same, meaning that regardless of which approach we would use, the analysis mean would change by the same magnitude.

Furthermore, if we compare figures 3.20 (b) and 3.15 (b) for the localized partial spectral case, we have a similar performance in both approaches, in the same temperature range, and analysis mean changes in the same direction. The only difference is that the per channels assimilation gives a more abrupt profile compared to the per pressure levels one, and at the same time we may wish to consider the computational cost of each approach; in the per pressure levels assimilation, we may get better results by using no more that 20 – 30 channels, whereas in the per channels assimilation we obtain similar results yet here the matrices that appear (some of which require inversions) may be significantly larger, with dimensions as high as 70 – 90. Similar remarks can be made for figures 3.21 (b) and 3.17 (b) for 1374/8664, or for figures 3.22 (b) and 3.19 (b) for 7600/7952. For the partial spectral cases the results are alike, yet the per pressure assimilation seems to be able to track temperature changes in a finer manner.

We perform a scale analysis to examine why the analysis increments in the radiance assimilations are by one order of magnitude less than in the retrieval. This conclusion is drawn from the results of section 3.2, and the presented increments $\mathbf{X}_a - \mathbf{X}_b$ shown there. Supporting data, including tables with representative orders of magnitude of the pertinent Kalman filtering sets are also offered in appendix E.
The analysis increments for both assimilation are equal to either $\bar{x}_a - \bar{x}_b$ or $K\bar{d}$. Given the latter formulation and the analysis of appendix E, we have that the radiance assimilation $K$ and $\bar{d} = y_o - \bar{y}_b$ ordered sets are numerically less than in the retrieval. The same also stands for the set of $Y_p$. We need to keep in mind, however, that in the evaluation of the radiance innovations we apply the OSS forward model operator, as do we for the radiance $Y_p$ set (and its transpose). Matrix $Y_p$ contributes to the evaluation of $K$ following equation (3), so that a $Y_p$ set of a lesser order also leads to a radiance assimilation lesser order $K$ matrix.

In view of the OSS operator functionality, we have that it receives an input vector of several elements, including atmospheric temperature profiles, chemical composition, and radiative properties. In the current study we only dealt with the atmospheric temperature profiles, leaving the rest of the input elements unaltered for every ensemble member, per examined profile. The impact of this choice in the ensemble spread, or otherwise in the evaluation of sets like $Y_p$ (in radiance spectral space) was not recorded herein, and the same applies to the radiance innovations, given how $\bar{y}_b$ is evaluated. The radiance assimilation lesser order for $K$ may be attributed to the current use of this OSS operator.

Another clear distinction between the retrieval and radiance assimilations is in the relative orders of the standard deviations; in the retrieval both $\sigma_b$ and $\sigma_o$ values are numerically close, so that the elements of the retrieval matrices $R_o$ and $R_b$ are of the same order. Therefore, in the retrieval assimilations, there is a balance in the statistical trust between the background and the observations. Conversely, in the radiance assimilation $\sigma_o$ is far greater than $\sigma_b$ (by four orders), so that $R_o$ will correspondingly be greater than $R_b$. This characteristic can be viewed from the perspective of statistical importance, where the radiance background will be the dominant source of information for this assimilation. At the same time, the radiance assimilation $\sigma_o$ is of order $10^0$, as in the retrieval. Between the two assimilations, the factor that tunes the order of $K$ appears to be matrix $Y_p$ solely, with the rest of the sets being in similar range, in both assimilations.

Given the evaluation methodology of the radiance $\sigma_b$ values and thereby of $R_b$, matrix $Y_p$, and vector $\bar{d}$, we note that the temperature to radiance mappings are evenly...
required. It seems that the exact process of these mappings, also via the OSS operator, has an important impact in the analysis results of the radiance data assimilation.

4.2 Summary and Conclusions

In the current study we evaluate certain applications of retrieval and radiance data assimilation approaches by using as observations OSS TES temperature retrievals for the retrieval assimilation, and PDS TES satellite radiance spectra for the radiance assimilation. This study focused on a one–dimensional assimilation problem using the ensemble Kalman filter and a background ensemble generated with the GFDL Martian Global Climate Model (MGCM).

The methods that have been used in the current study are the following; first we applied a retrieval data assimilation where the background and the observations were both temperatures. In like accord, the model and observation spaces were both pressure levels, as described in sections 2.3 – 2.3.4. Two specific implementations pertaining to the retrieval case were a global assimilation (using no vertical localization) and the local assimilation as described in sections 2.3.2 and 2.3.3. The retrieval assimilation was followed by the radiance assimilation. In the radiance assimilation the background and the model space were as in the retrieval case, whereas the observations and the corresponding observation space were spectral distributions of radiance and a portion of the electromagnetic spectrum given in terms of inverse centimeters, respectively. In the radiance assimilation, there was also a separation into a global and a local approach. The global approach, as a method, is presented in section 2.4.2. For the radiance local assimilation, there were two approaches; the per pressure levels and the per spectral channels localization, delineated in sections 2.4.4 and 2.4.5.

A sensitivity analysis was performed for the retrieval and radiance assimilation. In the retrieval case, we used two values of observational standard deviations, namely \( \sigma_o = 3.0 \) K and \( \sigma_o = 5.0 \) K in order to evaluate the response of the filtering process to those assumed observation error metrics. Furthermore, in the retrieval local assimilation we also included two different localization coefficient values \( c = \{0.015, 0.030\} \) (see section 2.3.3) in order to ascertain the impact of these choices to the analysis obtained from the localized retrieval assimilation.
In the radiance assimilation, the observational standard deviation and the localization coefficient values were fixed throughout the study at $1.5 \text{ mW cm}^{-1} \text{ m}^{-2} \text{ sr}^{-1}$ and $0.030$ respectively. In this case, for the radiance global assimilation the distinction in the results only relates to using the full or the partial set of spectral radiances (figures 3.14, 3.16, or 3.18). The sensitivity analysis performed herein (section 3.2, where in figures such as 3.15, 3.17, or 3.19) is primarily focused around the radiance assimilation localized per pressure levels where the number of used channels varied among $5$, $20$, $30$, $40$, or $60$. The last applied approach was for the localized radiance assimilation per spectral channels following section 2.4.5 (figures 3.20, 3.21, 3.22).

The sensitivity analysis offers some insights as to its impact on the evaluated analysis ensemble mean $\bar{x}_a$, per examined case. A general remark on the retrieval global assimilation is that for $\sigma_o = 5.0 \text{ K}$ the analysis ensemble mean is closer to the background, which can be observed from the fact that the blue lines in figures 3.11 (a), 3.12 (a), and 3.13 (a) are always close to the axis of $\Delta T = 0 \text{ K}$. Equivalently, the analysis increments $\bar{x}_a - \bar{x}_b$ will be less, compared to those from the $\sigma_o = 3.0 \text{ K}$ case. This finding offers a means of justification that this simple filtering approach of section 2.2 is operating appropriately.

From the other retrieval local assimilation results, as in figures 3.11 (b), 3.12 (b), and 3.13 (b) we find that the choices of the observational standard deviation and the vertical localization cut off distance may impact the results significantly. For instance, in figures 3.11 (b) and 3.12 (b) there is a clear separation in the four plotted curves, with analysis increments ranging from $-10 \text{ K}$ up to $-4 \text{ K}$, or from $-12 \text{ K}$ up to $-6 \text{ K}$ respectively, whereas in figure 3.13 (b) the four curves appear to be strongly dependent on the choice of the observational standard deviation rather than the localization distance. The value of $c$ (the ad hoc multiplier of the magnitude of the vertical localization distance), which appears in section 2.3.3 and equation (10), is tailored to fit the numerical figures and range of this particular problem. The greater the value of $c$ is, the more local observations from the valid ones will be taken into account in the localized assimilations (both retrieval and radiance), so that for a sufficiently large value of $c$, for the pressure levels closer to the ground, we will incorporate almost every available observation, thus annulling any performed localization. In view of that, for greater $c$ values we would expect to have results closer to the global approach, where no localization is performed. Despite that, in
figure 3.11 (b) for example, we observe that the blue and green lines for \( c = 0.030 \) are separated conspicuously from each other given their different \( \sigma_o \) value. The grouping in this figure and in 3.12 (b), 3.13 (b) follows not the \( c \) but the \( \sigma_o \) value, so that the standard deviation of the observations appears to control the results more, than how many local observations we will use in each assimilation case.

Given the scope of this study, since we do not perform a cycling data assimilation by applying metrics like an RMSE in order to ascertain the data assimilation spin up itself, we are not in the position to elucidate which choices are the optimal. Qualitatively, by comparing the plotted curves of the figures 3.11 (a), 3.12 (a), and 3.13 (a) of the retrieval global approach to those of the retrieval local assimilation 3.11 (b), 3.12 (b), and 3.13 (b), a good match would be to choose \( \sigma_o = 3.0 \) K and a value for \( c \) in the range \( 0.15 - 0.20 \). For further corroboration, one possibility would be to perform an OSSE and by using other applicable metrics like a RMSE or a MAE.

Despite the numerical discrepancies in the retrieval global or local approach, what is consistent throughout is the fact that the direction of the analysis ensemble mean \( \bar{x}_a \) is always the same. That is not to say that in the retrieval assimilation, localization is without merit. Given the rationale behind a localization as in section 2.3.3, as well as computational benefits, the localization is preferable, without suggesting that the global approach will give erroneous results. Given the remarks of section 4.1 and the results of section 3.1 like figure 3.2 (a), (c), (e), with \( \bar{x}_a \) being in-between \( \bar{x}_b \) and \( y_o \), the warming or cooling assimilation driving seems reliable enough.

In the radiance assimilation the results are subject to additional consideration. By using the retrieval assimilation as a way to measure the quality and performance of the radiance assimilation results, we find that in the radiance case, localization and the use of only the partial spectral channel set are paramount in obtaining an analysis ensemble mean that conforms to the correct physical changes, be it warming or cooling.

From figures such as 3.14, 3.16, or 3.18 pertaining to the radiance global assimilation, the full spectral case does not perform correctly. This is attributed to the fact that in the PDS TES observed spectra the first 10–20 and the last 40–60 channels are noisy, with poor information content not indicative of the state of the atmosphere, and their corresponding low signal to noise ratio [6]. The partial spectral case gives analysis ensemble mean results in the correct direction, yet a global approach should be avoided
altogether considering additionally that in the current study observations are known in about only half the model space, so that for pressure levels above 10 Pa the results cannot be evaluated given the absence of such observations.

Even if we apply the radiance local per pressure levels assimilation (figures 3.15 (a), 3.17 (a) and 3.19 (a) pertaining to the full spectral case), we notice that the analysis ensemble mean may conditionally give correct results, but that is strongly dependent on the number of used channels out of all available 143. On the other hand, from figures 3.15 (b), 3.17 (b) and 3.19 (b) we have the radiance local per pressure levels assimilation for the partial spectral case, where those used channels 5, 20, 30, 40, or 60 are drawn from the remaining subset of 143 (see section 2.4.1). For computational reasons, considering that these results as in figures 3.15 (b), 3.17 (b) and 3.19 (b) are similar to each other, the optimal channel number to be used is in the range 20–40. Occasionally, with as few as 5 used channels we may obtain results very similar to a selection of 40 or more channels, but this behavior is not guaranteed, as in figure 3.19 (b). Similar conclusions are drawn from the radiance local per spectral channels assimilation. From figures 3.20, 3.21, and 3.22 the discrepancies between the full and the partial spectral cases are obvious, rendering the full spectral case inoperable.

Comparing figures 3.20 (b) with 3.15 (b), 3.21 (b) with 3.17 (b), and 3.22 (b) with 3.19 (b) for the profiles 0001/8664, 1374/8664, and 7600/7952 respectively, we have a similar performance in both the radiance local per pressure levels and per spectral channels assimilation. The local per pressure levels assimilation is preferable though, since it may be so that in the per spectral channels approach the maximum radiance to temperature sensitivity may occur in the same pressure level for the vast majority of the used channels out of 143. In this regard, once we apply the Kalman filter for pressure levels close to the surface, in the per pressure levels assimilation the matrices that appear may be $20 \times 20$ should we choose 20 channels, while in the per spectral channels assimilation may be $65 \times 65$, for every applicable model space node. The Kalman filter involves matrix inversions, so given the similarities in the results of those two approaches it is preferable to use the one which is more flexible, and that is the radiance local per pressure levels case. Additionally, in the per spectral channels radiance localization, some of the used channels may be window channels or aerosol channels, rather than those being sensitive to the atmospheric temperatures in the CO$_2$ band.
Several studies engaged in Martian reanalyses have been performed, the majority of which utilized PDS TES retrieved temperatures and not OSS TES, like the current one. The PDS TES data sets contained not only the observed spectra but also smoothed temperature retrievals [18], which were published around or after 2001. The OSS TES temperature retrievals and the jacobian matrices used herein were published in 2008 [6]. The broader context of the current work is to be viewed within the scope of those reanalyses, where the hope is that this study will subsidize with additional knowledge the literature pertaining to Martian data assimilations. One additional implication is in relation to not only the Martian case, but also the terrestrial one. In the context of the current work we consider a problem where the only source of information is in the form of satellite spectra. It is to our best interest to examine ways with which more optimal data assimilation applications may come to fruition in cooperation with remote sensing, given that meteorological satellites offer an abundance of observations opposed to spatially fixed radar locations, ground weather stations, or pricey soundings available at the temporally sparse interval of 6 h.

Future work involves the realization of a 3D data assimilation, where every applicable climate model output will be accounted for, including horizontal wind components, dust distributions, the chemical composition of the Martian atmosphere for molecular CO$_2$ and H$_2$O, as well as surface properties at their corresponding geographical locations.
Appendix A

MGCM Resolution and Pressure-Sigma Schemes

In appendix A, relevant information pertaining to the resolution and discretization of the Mars Global Climate Model (MGCM), to the hybrid pressure – sigma coordinate system used in the vertical direction of the climate model, and to the topography of planet Mars, is presented.

Regarding the resolution of the climate model, by construction there exist 28 vertical levels, 36 parallel circles, and 60 meridians, constituting a coordinate system \((p, \phi, \lambda)\). The first coordinate is given in terms of a hybrid pressure – sigma \(p\), the second is the latitude \(\phi\), and the third the longitude \(\lambda\). The physical units for the coordinates are \(Pa\) for pressure, and for the angles \(\phi, \lambda\) either in degrees or decimal. At any \((\phi, \lambda)\) level the grid is structured and orthogonal, whereas in the vertical direction is flow dependent, following the topography of Mars as well as the dynamics of the atmospheric fluid.

In the meridional direction the latitudinal values of the parallel circles are fixed, following table A.1, in degrees North. The first parallel circle is at \(\phi = -88.714^\circ\) and the 36th at \(\phi = 88.714^\circ\), bounding the southern and northern polar caps, respectively. In view of that, the polar caps are excluded from simulations performed by the climate model and therefore these spatial domains of the Martian surface and atmosphere are not considered in any form of analysis. It can also be seen from table A.1 that the equatorial line is not represented in the discretization of the climate model either, since there is no \(\phi = 0^\circ\) parallel circle.

| -88.714 | -84.857 | -79.714 | -74.571 | -69.429 | -64.286 |
| -59.143 | -54.000 | -48.857 | -43.714 | -38.571 | -33.429 |
| 2.571  | 7.714  | 12.857  | 18.000  | 23.143  | 28.286 |
| 33.429 | 38.571 | 43.714  | 48.857  | 54.000  | 59.143 |
| 64.286 | 69.429 | 74.571  | 79.714  | 84.857  | 88.714 |

Table A.1. Latitudinal MGCM discretization values, defining the parallel circles locations, in degrees North. The data are to read per row, from left to right, in ascending order.
The latitudinal discretization of the climate model is structured, yet the parallel circles are not equally spaced. Conversely, in the zonal direction the longitudinal discretization is structured with the meridians being equally spaced, in degrees East. The first meridian is at $\lambda = 3^\circ$ and the 60th at $\lambda = 357^\circ$ with a constant longitudinal step $\Delta \lambda = 6^\circ$, so that assuming we use an index $i$ for the enumeration of the meridians in the range $i = \{1, 2, \ldots, 60\}$, the $i$-th meridian is given $\lambda(i) = \lambda(1) + (i - 1) \Delta \lambda$. Following that, the prime meridian at $\lambda = 0^\circ$ is not represented either. An interesting point to be made in conjunction with appendix B, as that relates to the $\varphi - \lambda$ interpolation conducted in the retrieval data assimilation (see section 2.3.1) is that close to the prime meridian the horizontal grid of the climate model exhibits periodicity, an aspect that entails computational implications treated in appendix B.

In the vertical direction the used coordinate is a hybrid pressure – sigma denoted simply as $p$. The values of this coordinate are not fixed; they are flow dependent and are related to the state of the atmosphere although the topography has a strong impact as well. Vertically there are 28 levels yet the climate model does not compute directly pressure values at the levels, rather pressure differences at interfaces, which bound the levels. The pressures at the levels are considered the spatial average of the pressures at the interfaces bounding those levels.

For the mathematical description of this pressure – sigma coordinate scheme, a corresponding index nomenclature is introduced as follows; given the coordinate system $(p, \varphi, \lambda)$, despite the fact that it is not the geographical one $(\lambda, \varphi, r)$ for which a typical index notation would include the use of $i$ for the zonal, $j$ for the meridional, and $k$ for the vertical direction, regardless we may use these indices for here as well. According to that, one discrete value for the longitude may be posed $\lambda(i) \equiv \lambda_i$, for the latitude $\varphi(j) \equiv \varphi_j$, and for the pressure $p(k, j, i; n) \equiv p_{k,j,i}^n$, where $k$ enumerates vertical levels and index $n$ (in the current context of appendix A) time frames.

Like stated, there are interfaces bounding the 28 levels. The interfaces are in total 29 and one level is bounded between two consecutive interfaces, those nearest to that level. By construction, the range of index $k$ for the levels is $k = \{1, 2, \ldots, 28\}$ and for the interfaces $k = \{1, 2, \ldots, 29\}$, where the enumeration starts from a low pressure level (close to the upper boundary of the atmosphere) until just above the surface for the levels, and at the
surface for the interfaces. In this regard, at $k = 29$ we have the interface which coincides with the topography. The relation between the $k$–th interface and level is that the $k$–th level is bounded between interface $k$ and $k + 1$.

For notational simplicity, we drop index $n$ from the following structures, while we retain only the spatial dependence for the pressure values. The pressure – sigma scheme is defined from the following two equations:

$$
\tilde{p}_{k, i, j} = b_k (p_{sfc})_{j,i} + a_k, \quad (A.1)
$$

$$
\bar{p}_{k, i, j} = \frac{\tilde{p}_{k+1, i, j} - \tilde{p}_{k, i, j}}{\ln(\frac{\tilde{p}_{k+1, i, j}}{\tilde{p}_{k, i, j}})}.
\quad (A.2)
$$

Equation (A.1) defines pressure $\tilde{p}_{k, i, j}$ at interface $k$, and equation (A.2) defines pressure $\bar{p}_{k, i, j}$ at level $k$. The tilde and overbar are simply used to differentiate the notations and are not related to any statistical considerations. The $a_k$, $b_k$ coefficients appearing in equation (A.1) further quantify this scheme. Their fixed values are given in table A.2, where $a_k$ is in Pa and $b_k$ dimensionless. These $a_k$, $b_k$ coefficients are time and horizontal ($\varphi_i$, $\lambda_i$) location independent. In equation (A.1) we also have a surface pressure $(p_{sfc})_{j,i}$. Given table A.2 and equation (A.1), it follows $(p_{sfc})_{j,i} \equiv \tilde{p}_{29, i, j}$, at any $(\varphi_i, \lambda_i)$ location. The impact of the topography is observed through equation (A.1) and table A.2; closer to or at the surface, the pressures at the interfaces $\tilde{p}_{k, i, j}$ for index values $k > 20$ are closely related to the value $(p_{sfc})_{j,i}$, and via equation (A.2) this dependence also impacts the pressures at the levels $\bar{p}_{k, i, j}$. The higher we ascend in altitude (or pressure levels), the topographical dependence wanes and for $k \leq 5$ has no further connection with either $\tilde{p}_{k, i, j}$ or $\bar{p}_{k, i, j}$.

Given the fact that the surface or the interfaces are not a part of the grid of the climate model, the following procedure is implemented in order to reach to those required $p_{k, i, j}$ pressure values. Like previously stated, the relevant climate model pressure outputs are pressure differences at the interfaces. These may be denoted $(\Delta p)_{k, i, j} \equiv \tilde{p}_{k+1, i, j} - \tilde{p}_{k, i, j}$.
These numerical figures \((\Delta p)_{k,j,i}\) are directly known from the climate model so that the surface pressure may be evaluated following

\[
\sum_{k=1}^{28} (\Delta p)_{k,j,i} = (\tilde{p}_{2,j,i} - \tilde{p}_{1,j,i}) + \ldots + (\tilde{p}_{29,j,i} - \tilde{p}_{28,j,i}) = \tilde{p}_{29,j,i} - \tilde{p}_{1,j,i},
\]

(A.3)

which in turn is combined with \(\tilde{p}_{29,j,i} = (p_{sfc})_{j,i}\) and \(\tilde{p}_{1,j,i} = a_1\), in order to yield

\[
(p_{sfc})_{j,i} = a_1 + \sum_{k=1}^{28} (\Delta p)_{k,j,i}.
\]

(A.4)

The total number of the MGCM nodes are \(28 \times 36 \times 60 = 60480\). Consequently, a total number of \(60480\) \((\Delta p)_{k,j,i}\) values are known, from which at each \((j,i)\) location, the application of equation (A.4) is performed in order to yield a total number of \(36 \times 60 = 2160\) values for one profile of the surface pressure \((p_{sfc})_{j,i}\), implicitly for one time frame \(n\).

It then follows from equation (A.1) that the pressures \(\tilde{p}_{k,j,i}\) at the interfaces are directly computable. After the evaluation of one \(\tilde{p}_{k,j,i}\) profile we implement equation (A.2) for the required profile of the pressures at the levels, \(\tilde{p}_{k,j,i}\). Specifically, in the range \(k = \{1, 2, \ldots, 27\}\) we apply equation (A.2) as is, and for \(k = 28\) the following

\[
\tilde{p}_{28,j,i} = \frac{(p_{sfc})_{j,i} - \tilde{p}_{28,j,i}}{\ln((p_{sfc})_{j,i})}.
\]

(A.5)

Thus, from the original MGCM pressure related outputs \((\Delta p)_{k,j,i}\) (for the any given time frame \(n\)) we reach to the required information regarding the profiles \(\tilde{p}_{k,j,i}\).

Having calculated the pressures at the levels, the final step involves the evaluation of its ensemble mean, given the fact that in the current study we have an ensemble of \(M = 16\) members, where \(M\) is the ensemble size. For any ensemble approach in the context of a Kalman filtering method one applies the numerical solver, for here the MGCM, as many times as the ensemble size, in order to acquire as many trajectories for every related dynamical and thermodynamical variable involved in the problem at hand. Essentially, the
previous analysis is performed $M$ times, for the evaluation of each $p_{k,j,i}^{(m)}$ profile, where index $m$ enumerates those ensemble members. The ensemble mean then follows

$$p_{k,j,i} = \frac{1}{M} \sum_{m=1}^{M} p_{k,j,i}^{(m)}$$  \hspace{1cm} (A.6)

In equation (A.6), the ensemble mean of the pressures at the levels is denoted $p_{k,j,i}$. In this notation no overbar is used. It is retained exclusively for the representation of this ensemble mean and is used in the methodology presented in chapter 2, in sections like 2.3.1 or 2.4.1. This profile $p_{k,j,i}$ is used in both the retrieval and radiance data assimilation performed in this study for the establishment of the model space, which is common in both assimilations. In any event, in equations (A.1) – (A.5) implicitly we assume an index $n$ for the time frames and an index $m$ for the ensemble members as superscripts, yet for notational simplicity alone, these indices are obviated.
Table A.2. Definition of the coefficients $a$ and $b$ for the hybrid pressure – sigma MGCM coordinate system, in the vertical direction.

<table>
<thead>
<tr>
<th>Interface</th>
<th>$a$ coefficient (Pa)</th>
<th>$b$ coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.02</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.057381273</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>0.19583981</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>0.5922958</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>1.5660228</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>2.4454965</td>
<td>0.0019366394</td>
</tr>
<tr>
<td>7</td>
<td>2.7683755</td>
<td>0.0074419133</td>
</tr>
<tr>
<td>8</td>
<td>2.8851692</td>
<td>0.016227267</td>
</tr>
<tr>
<td>9</td>
<td>2.9172228</td>
<td>0.027075192</td>
</tr>
<tr>
<td>10</td>
<td>2.9087039</td>
<td>0.043641</td>
</tr>
<tr>
<td>11</td>
<td>2.8598939</td>
<td>0.068106804</td>
</tr>
<tr>
<td>12</td>
<td>2.7687652</td>
<td>0.1028024</td>
</tr>
<tr>
<td>13</td>
<td>2.6327054</td>
<td>0.14971954</td>
</tr>
<tr>
<td>14</td>
<td>2.4509219</td>
<td>0.20987133</td>
</tr>
<tr>
<td>15</td>
<td>2.2266811</td>
<td>0.28270233</td>
</tr>
<tr>
<td>16</td>
<td>1.9684681</td>
<td>0.3658161</td>
</tr>
<tr>
<td>17</td>
<td>1.6894832</td>
<td>0.4552023</td>
</tr>
<tr>
<td>18</td>
<td>1.4055812</td>
<td>0.54593599</td>
</tr>
<tr>
<td>19</td>
<td>1.1324258</td>
<td>0.6331097</td>
</tr>
<tr>
<td>20</td>
<td>0.88289177</td>
<td>0.71267629</td>
</tr>
<tr>
<td>21</td>
<td>0.66548467</td>
<td>0.78196151</td>
</tr>
<tr>
<td>22</td>
<td>0.4840102</td>
<td>0.8397753</td>
</tr>
<tr>
<td>23</td>
<td>0.33824119</td>
<td>0.88620345</td>
</tr>
<tr>
<td>24</td>
<td>0.22510704</td>
<td>0.92223168</td>
</tr>
<tr>
<td>25</td>
<td>0.13995719</td>
<td>0.94934533</td>
</tr>
<tr>
<td>26</td>
<td>0.077611554</td>
<td>0.96919618</td>
</tr>
<tr>
<td>27</td>
<td>0.033085503</td>
<td>0.98337259</td>
</tr>
<tr>
<td>28</td>
<td>0.002</td>
<td>0.99326941</td>
</tr>
<tr>
<td>29</td>
<td>0.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

In table A.2 we have these $a_k$ and $b_k$ coefficients used in the hybrid pressure – sigma coordinate scheme. Close to the surface the topography of Mars has a significant impact in the evaluated ensemble mean pressures $p_{k,j,i}$, as that can be seen from the application of the previous equations (A.1) – (A.6). This impact is also reflected in the results of sections 3.1 and 3.2. In these two sections, certain profiles that have been used in this study are differentiated from each other in time and satellite location ($\phi_s, \lambda_s$), following the analysis of section 2.3.1. One feature of the results in sections 3.1 and 3.2 is that in one profile case, the ensemble mean pressure may be in the range $p \in [0.02, 800] \text{ Pa}$, while in another in...
the range $p \in [0.02, 300]$ Pa, where this symbol "p" used here is for the horizontally interpolated ensemble mean pressure at the satellite location (see section 2.3.1 in conjunction with appendix B). In light of that, pressure values at the level $k = 28$ (just above the surface) can vary, typically in the range $p \in [250, 950]$ Pa. It is worthwhile to explore the impact of the topography on the pressures that are used in the current study and in the next part of appendix A additional figures illustrating this impact are presented.

The subsequent figures A.1, A.2, and A.3 were created by using one additional data set included in the climate model and used by it. The inception of the MGCM occurred during the 90's and the embedded topography used in the model originates from that era. Higher resolution topographical data sets exist, yet are not considered herein due to the fact that are not used by the climate model. In the performed calculations only what is pertinent to the evaluation of the model outputs, with regards to its resolution, is accounted for.

Figures A.1, A.2, and A.3 portray the Martian topography and were plotted by applying the two dimensional interpolation scheme of appendix B on this topographical data set which contains $36 \times 60$ altitudinal values, for a total of 2160 known altitudes. The applied longitudinal – latitudinal interpolation of the current context is the same as the one used in section 2.3.1 only instead of pressures and temperatures here we interpolate altitudes. The level of zero altitude is assumed, arbitrarily, at the lowest altitude of the topographical data set.

The next figures A.4, A.5, and A.6 show examples of horizontally interpolated pressure profiles for an MGCM output at 000155700, following the interpolation technique of appendix B, as well. From this MGCM output, initially we have $M = 16$ ensemble members. Equations (A.1) – (A.5) are applied 16 times on that MGCM output, and then equation (A.6). From the resulting pressure profile $p_{k,i,i}$, across its 28 levels, here we plot three levels, for $k = 26$, $k = 13$, and $k = 8$ corresponding to figures A.4, A.5, and A.6. The dots appearing in these three figures are the values $p_{k,i,i}$ of equation (A.6), for those three levels. The smoothness of the surfaces is attributed to a custom resolution, following the used longitudinal – latitudinal interpolation scheme of appendix B.

A comparison between figure A.3 and figures A.4, A.5, and A.6 shows an explicit dependence of the climate model pressure outputs on the considered topography. The topography continues to have the same impact on pressure profiles until level $k = 6$, where
past that point is diminished and the profiles flatten out, in view of table A.2 and equations (A.1) – (A.6).

Lastly, figures A.7, A.8, and A.9 are density–contour plots pertaining, respectively, to figures A.4, A.5, and A.6, in order to demonstrate from a top view those pressure variations per \((\phi, \lambda)\) location.

---

**Figure A.1.** The Martian topography from a top view. The geographic coordinates, longitude \(\lambda\) and latitude \(\phi\) are in degrees. The Southern and Northern polar caps are not included in the analysis.
Figure A.2. Surface plot of the Martian topography from a front right view point.

Figure A.3. Surface plot of the Martian topography from a top left view point.
Figure A.4. Surface plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 26$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution.

Figure A.5. Surface plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 13$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution.
Figure A.6. Surface plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 8$. The dots represent solely the MGCM outputs for this model level, whereas the surface is produced from interpolation with a custom resolution.

Figure A.7. Density – contour plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 26$. 
Figure A.8. Density – contour plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 13$.

Figure A.9. Density – contour plot of the $\varphi - \lambda$ horizontally interpolated ensemble mean MGCM pressure, for model level $k = 8$. 
Appendix B

Longitudinal – Latitudinal Interpolation

Appendix B describes a mathematical analysis pertaining to a two dimensional interpolation, which is used in the retrieval data assimilation [8]. The notation used herein is for the needs of appendix B alone and under no circumstances should be confused with the notation used in the main body of the text, for example of sections like 2.3.1.

The fact that the satellite position \((\varphi_s, \lambda_s)\) does not coincide with any horizontal \((\varphi_j, \lambda_i)\) MGCM location, necessitates such an interpolation in order to estimate climate model pressures and temperatures at \((\varphi_s, \lambda_s)\). Evidently, there is no unique method to perform an interpolation. However, the spatial distribution of the known points and the domain these points exist in, play a pivotal role in the selection of the interpolation scheme, and thereby the used interpoland function. In the current case, at any horizontal level, there is a structured (orthogonal) grid given from the intersections of the meridians and the parallel circles, as that relates to the discretization of the MGCM. Strictly speaking, since the third coordinate is a hybrid pressure sigma and not the altitude, the domain of interpolation is curvilinear but not of a spherical symmetry, especially closer to the ground, where the pressure levels follow strongly the topography of Mars (see appendix A). In this regard the coordinate curves horizontally, are not exactly meridians and parallel circles. Despite the fact that the domain of interpolation at any model level \(k\) is curvilinear and not affine, in the following we assume a local regime of interpolation so that the curvature may be obviated and in turn the used interpoland assumes its structure from an affine manifold.

The simplest case is to apply a bilinear interpolation using the four MGCM grid closest neighbors to any \((\varphi_s, \lambda_s)\) point of the continuous space, and as an extension to that, a local neighborhood may be defined by more than four points in order to increase the estimation accuracy without violating significantly the affine manifold condition. The analysis continues with the examination of the Lagrange interpoland for one dimension and is followed by a generalization of the two dimensional case.
Since the manifold is assumed affine, the geodesic is a line segment. Speaking generally, we assume points existing on a line segment like \( \{x_1, x_2, \ldots, x_n\} \), or \( D_X = \{x_j\}_{j=1}^n \), where \( D_X \) is the template set, which by construction increases monotonically so that it is \( x_j < x_{j+1}, \forall j \). On those \( x_j \) locations, we assume known images abutting on as \( D_Y = \{y_j\}_{j=1}^n \), where \( D_Y \) is the known images set. Theoretically, there exists possibly an unknown mapping \( y = f(x) \), or \( D_Y = \hat{f} \circ D_X \), where "\( \circ \)" is the function composition notation. The goal of the interpolation is to approximate this mapping \( f(x) \), by another one, the interpoland function, derived through the applied interpolation scheme. The simplest mathematical structure is the polynomial, which for here will be denoted \( P(x) \). The Lagrange interpoland in one dimension, is given

\[
P_{n-1}(x) = \sum_{j=1}^{n} y_j L_j(x), \tag{B.1}
\]

for the case in which we consider \( n \) elements of \( D_X \) and \( D_Y \). In \( P_{n-1}(x) \), \( n-1 \) is the grade of the polynomial, \( y_j \) the known images, and \( L_j(x) \) the Lagrange coefficients. By definition it is \( P_{n-1}(x_j) \equiv y_j \), so that the interpoland passes through every element of \( D_Y \), or \( L_j(x_k) = \delta_{jk} \), where \( \delta_{jk} \) is Kronecker's delta. Structure (B.1) stems from the general form of a polynomial

\[
P_{n-1}(x) = \sum_{q=0}^{n-1} c_q x^q, \tag{B.2}
\]

where \( c_q \) is the \( q \)–th coefficient of \( P_{n-1}(x) \). By solving an algebraic system for

\[
y_j = \sum_{q=0}^{n-1} c_q x_j^q,
\]

and by proper factorization, we obtain the left hand side of (B.1), with

\[
L_j(x; \{x_j\}_{j=1}^n) = \frac{\prod_{m=1}^{n} (x - x_m)}{\prod_{m=1}^{n} (x_j - x_m)}, \tag{B.3}
\]
where \( m \) is the product dummy index. The notation \( L_j(x;\{x_j\}_{j=1}^n) = L_j(x;D_X) \) denotes the fact that the Lagrange coefficients are polynomials of the any given argument \( x \), for which it is \( x_1 < x < x_n, x \notin D_X \), and of the corresponding regime of interpolation \( D_X \).

At a technical level, typically we do not consider every element of \( D_X \), rather only a few points \( x_j \), those closest to argument \( x \), and we interpolate locally. The form of (B.1) does not require the distances \( x_{j+1} - x_j \) to be equal, which stands in the two dimensional case as well, yet in two dimensions we need to have a structured grid and not scattered points, which is the case in the horizontal discretization of the MGCM.

The two dimensional interpolation with the Lagrange coefficient structures is a direct extension of the one dimensional case, with two requirements; the template set needs to be structured (not scattered points), and the domain of interpolation an affine manifold. For the template set we consider the Cartesian product \( D_X \times D_Y \), where \( D_X = \{x_i\}_{i=1}^I \), for \( i = \{1, 2, \ldots, I\} \), and \( D_Y = \{y_j\}_{j=1}^J \), for \( j = \{1, 2, \ldots, J\} \), as well as the known images set \( D_Z \) given by \( D_Z = \{z_n\}_{n=1}^N \), for \( n = \{1, 2, \ldots, N\} \), where \( N = I \times J \). Additionally, \( D_Z = \hat{w} (D_X \times D_Y) \) or \( z_n = w(x_i,y_j) = w_{i,j} \), with an appropriate index mapping, e.g. \( n = I (j-1) + i \), and \( \hat{w} \) an unknown operator (if extant in the first place) that the interpoland will approximate. The sets \( D_X \) and \( D_Y \), like in the one dimensional case need to increase monotonically \( x_i < x_{i+1}, \forall i \) and \( y_j < y_{j+1}, \forall j \), by construction.

Due to the fact that the grid is also orthogonal, first we may interpolate per fixed \( y \) level and apply the one dimensional case. Specifically, if we interpolate for \( y_q = \text{const} \), for the entire \( D_X \) set, we have a structure

\[
P_y(x;D_X,q) = \sum_{p=1}^1 L_p(x;D_X)w_{p,q}. \tag{B.4}
\]

The subscript "\( y \)" in the notation \( P_y(x;D_X,q) \) denotes the direction of the one dimensional interpolation, for constant \( y \) and across the \( x \) regime, and the value of index \( q \) denotes the appropriate fixed \( y_q \) level. The values of \( w_{p,q} \) are considered known, and apart from that, the other symbols are as previously stated. The next step of the process is to
consider an interpolation across the \( y \) regime, where in the interpoland we have not the values of \( \omega_{p,q} \), but the previous form of (B.4). Accordingly, the two dimensional polyonomic interpoland is given

\[
P(x, y; D_X, D_Y) = \sum_{q=1}^{J} L_q(y; D_Y) P_y(x; D_X, q). \tag{B.5}
\]

As is the case in one dimension, here it also is \( P(x = x_p, y = y_q; D_X, D_Y) \equiv \omega_{p,q} \), so that the two dimensional interpoland passes through every point of the images set \( D_Z \). The Lagrange coefficients in two dimensions are given from the following two equations:

\[
L_p(x; D_X) = \frac{\prod_{m=1}^{J} (x - x_m)}{\prod_{m=1, m\neq p}^{J} (x_p - x_m)}, \tag{B.6.a}
\]

\[
L_q(y; D_Y) = \frac{\prod_{r=1}^{J} (y - y_r)}{\prod_{r=1, r\neq q}^{J} (y_q - y_r)}. \tag{B.6.b}
\]

Structures (B.6.a) and (B.6.b) can be posed as numerators and denominators like

\[
\mathcal{N}_{x,p}(x) = \prod_{m=1, m\neq p}^{J} (x - x_m), \tag{B.7.a}
\]

\[
\mathcal{N}_{y,q}(y) = \prod_{r=1, r\neq q}^{J} (y - y_r). \tag{B.7.b}
\]

and

\[
\mathcal{D}_{x,p} = \prod_{m=1, m\neq p}^{J} (x_p - x_m), \tag{B.7.c}
\]
\[ \mathbb{D}_{y,q} = \prod_{r=1 \atop r \neq q}^{J} (y_q - y_r). \]  
(B.7.d)

The denominators \( \mathbb{D}_{x,p}, \mathbb{D}_{y,q} \) are real numbers and the numerators functions of \( x \) and \( y \).

By combining equations (B.4), (B.5), and (B.7.a) – (B.7.d), we obtain the interpoland function in the form of

\[ P(x, y; D_x, D_y) = \sum_{q=1}^{J} \sum_{p=1}^{I} \frac{N_{y,q}(y) N_{x,p}(x)}{\mathbb{D}_{y,q} \mathbb{D}_{x,p}} w_{p,q}. \]  
(B.8)

The point we wish to make here can best be illustrated by a rather practical example. Consider, for instance, a regime of interpolation defined as \( D_x = \{x_1, x_2, x_3, x_4, x_5\} \) and \( D_y = \{y_1, y_2, y_3\} \). Conceptually, we may see figure B.1:

**Figure B.1.** Conceptual draft outlining the scripting approach for a two dimensional known images set, locally.

By construction, we introduce matrix \( \mathbf{W} \), with dimensions \( I \times J \), e.g. \( 5 \times 3 \). It will be \( \mathbf{W} = w_{k,l} \hat{e}_k \otimes \hat{e}_l \), where "\( \otimes \)" is the dyadic product operator. The summation convention is used, where every column of \( \mathbf{W} \) will have the known images \( w_{k,l} \) in ascending \( x \) order, starting from \( y_1 = \text{const} \), etc until \( y_J = \text{const} \). In this example, we have:
We then introduce one additional matrix pertaining to the Lagrange coefficient structures, as
\[ L = l_{p,q} \mathbf{e}_p \otimes \mathbf{e}_q = L_{x,p} L_{y,q} \mathbf{e}_p \otimes \mathbf{e}_q, \]
where \( L_{x,p} \) is given from (B.6.a) and \( L_{y,q} \) from (B.6.b). Matrices \( \mathbf{W} \) and \( L \) are of equal dimensions. By using the structures of (B.7.a) – (B.7.d), for \( L \) in this example it is:

\[ L = \begin{pmatrix}
N_{x,1}(x) & N_{y,1}(y) & N_{x,1}(x) & N_{y,2}(y) & N_{x,1}(x) & N_{y,3}(y) \\
\mathbb{D}_{x,1} & \mathbb{D}_{y,1} & \mathbb{D}_{x,1} & \mathbb{D}_{y,2} & \mathbb{D}_{x,1} & \mathbb{D}_{y,3} \\
N_{x,2}(x) & N_{y,1}(y) & N_{x,2}(x) & N_{y,2}(y) & N_{x,2}(x) & N_{y,3}(y) \\
\mathbb{D}_{x,2} & \mathbb{D}_{y,1} & \mathbb{D}_{x,2} & \mathbb{D}_{y,2} & \mathbb{D}_{x,2} & \mathbb{D}_{y,3} \\
N_{x,3}(x) & N_{y,1}(y) & N_{x,3}(x) & N_{y,2}(y) & N_{x,3}(x) & N_{y,3}(y) \\
\mathbb{D}_{x,3} & \mathbb{D}_{y,1} & \mathbb{D}_{x,3} & \mathbb{D}_{y,2} & \mathbb{D}_{x,3} & \mathbb{D}_{y,3} \\
N_{x,4}(x) & N_{y,1}(y) & N_{x,4}(x) & N_{y,2}(y) & N_{x,4}(x) & N_{y,3}(y) \\
\mathbb{D}_{x,4} & \mathbb{D}_{y,1} & \mathbb{D}_{x,4} & \mathbb{D}_{y,2} & \mathbb{D}_{x,4} & \mathbb{D}_{y,3} \\
N_{x,5}(x) & N_{y,1}(y) & N_{x,5}(x) & N_{y,2}(y) & N_{x,5}(x) & N_{y,3}(y) \\
\mathbb{D}_{x,5} & \mathbb{D}_{y,1} & \mathbb{D}_{x,5} & \mathbb{D}_{y,2} & \mathbb{D}_{x,5} & \mathbb{D}_{y,3}
\end{pmatrix}. \quad (B.10)

From the affine manifold approximation, the elements of \( L \) can also be brought to the form of:

\[ l_{p,q} = L_{x,p} L_{y,q} = \frac{N_{x,p}(x) N_{y,q}(y)}{\mathbb{D}_{x,p} \mathbb{D}_{y,q}} = \prod_{m=1}^{I} \int_{x_m}^{x_p} \prod_{r=1}^{J} \int_{y_r}^{y_q} dy, \quad (B.11)\]

by incorporating integral structures, which can be generalized appropriately for the case of the actual \( \varphi - \lambda \) interpolation.

It can be seen that the interpoland function, given previously from (B.8) as a double summation, can also be posed
\[ P(x, y; D_x, D_y) = S(L \circ W), \]  \hspace{2cm} \text{(B.12)}

where in this notation "\( \circ \)" is the Schur product operator, and "\( S \)" an operator returning a scalar as the sum of the matrix elements of \( L \circ W \), its argument. Essentially, by calculating \( S(L \circ W) \), we evaluate one unknown value \( P(x, y; D_x, D_y) \), given as the point \((x, y)\) in the continuous space, for which it is \( x_1 < x < x_1 \) and \( y_1 < y < y_j \), with \( x \not\in D_x \), \( y \not\in D_y \).

The previous structures pertain to a global regime of interpolation. However, in the applied interpolation, due to the curvature limitation of the domain, we interpolate locally. Therefore, we will now consider an interpolation in a local subset of the template set \( D_x \times D_y \). In the \( x \) direction the global template set is \( D_x = \{x_1, x_2, \ldots, x_I\} \). The argument in the continuous space is a point \((x, y)\), for which it is \( x_{k-1} < x < x_k \), where \( k \) is a parameter, one of the values of \( i = \{1, 2, \ldots, I\} \). To put it visually, we have the figure B.2:

![Figure B.2. Conceptual draft outlining an one dimensional local regime of interpolation.](image)

According to the previous statements, initially we have \( y_j = \text{const} \). The number of elements of the global set \( D_x \) that will be taken into account is of our own choice, at the very least two. Assume that we wish to consider only four elements of \( D_x \), namely the closest neighbors of the argument \( x \). The local regime of interpolation in the \( x \) direction can be posed \( D_x^{(L)} = \{x_{k-2}, x_{k-1}, x_k, x_{k+1}\} \). The Lagrange coefficient \( L_p(x; D_x) \) pertains to the global set \( D_x \) so in order to conform the structures and describe the corresponding coefficient for the local regime, we have
L_p(x; D^{(L)}_X) = \prod_{m=p_1, m\neq p}^{p_2} \frac{(x - x_m)}{x_p - x_m}, \quad \text{(B.13.a)}

N_{x,p}(x) = \prod_{m=p_1, m\neq p}^{p_2} \frac{(x - x_m)}{x_p - x_m}, \quad \text{(B.13.b)}

D_{x,p} = \prod_{m=p_1, m\neq p}^{p_2} \frac{(x_p - x_m)}{x_p - x_m}, \quad \text{(B.13.c)}

where p_1 = k - 2, and p_2 = k + 1, with p as the dummy summation index in the structure of the interpoland function, taking values in the range p = \{k - 2, k - 1, k, k + 1\}. Similarly, we may apply the above notions in the y direction as well, and speak of the local regime of interpolation D^{(L)}_Y = \{y_{\ell-2}, y_{\ell-1}, y_{\ell}, y_{\ell+1}\}, assuming that we consider four local neighbors of y, for which it will be \(y_{\ell-1} < y < y_{\ell}\). In general, the number of elements in \(D^{(L)}_X\), \(D^{(L)}_Y\) needs not be equal. In this case we will have for the dummy summation index q values in the range q = \{\ell - 2, \ell - 1, \ell, \ell + 1\}, with q_1 = \ell - 2, q_2 = \ell + 1. The symbols p_1, p_2, q_1, and q_2 are compound where in this context the subscripts "1" and "2" denote the first and last value of each given local regime of interpolation. The corresponding Lagrange coefficients will be written

L_q(y; D^{(L)}_Y) = \prod_{r=q_1, r\neq q}^{q_2} \frac{(y - y_r)}{y_q - y_r}, \quad \text{(B.14.a)}

N_{y,q}(y) = \prod_{r=q_1, r\neq q}^{q_2} (y - y_r), \quad \text{(B.14.b)}
Thus, the interpoland can be posed

\[ P(x, y; D_X^{(L)}, D_Y^{(L)}) = \sum_{q=0}^{q_2} \sum_{p=0}^{p_2} \frac{N_{y,q}(y)}{D_{y,q}} \frac{N_{x,p}(x)}{D_{x,p}} w_{p,q}, \]

or through the form of \( S(L \circ W) \), where the values for the indices \( p, q \) giving position in the discretized domain will have their appropriate values. In practice, this is accomplished by introducing mappings that evaluate the closest neighbors of the argument \((x, y)\), and by doing so establishing the proper local neighborhood of the interpolation for the any given \((x, y)\) case.

In order to apply the previous structures, like (B.12) or (B.15), for a two dimensional interpolation, we need to have the sets \( D_X, D_Y \) (locally or globally) be in ascending order. However, it is possible that in at least one direction, either in \( x \) or \( y \), there may be periodicity, a fact that needs to be taken into account so that we do not violate the ascending order condition of the template sets. In the actual implementation that we are considering, we have periodicity in the \( x \) direction alone (close to the prime meridian), where \( x \) becomes \( \lambda \) and \( y \) becomes \( \phi \). According to that, we are interested to clarify the crucial aspects of this case.

This consideration can be illustrated with an example as well. If we have periodicity in the \( x \) direction, then algebraically it will be \( x_2 - x_1 > 0 \), \( x_1 - x_{1-1} > 0 \), but \( x_1 - x_{1} < 0 \). Assume that the argument \( x \) in the continuous space is close to the bound of the \( x \) direction, either \( x < x_{1} \), or \( x_{1} < x \), and that we wish to interpolate locally in

\[ D_X^{(L)} = \{x_{1-1}, x_1, x_1, x_2\} \]. Then this set needs to be rewritten as follows: we introduce the differences \((\Delta x)_i = x_{i+1} - x_i\), we get \( x_1 - x_1 = (\Delta x)_1 \), and \( x_1 - x_{1-1} = (\Delta x)_{1-1} \), where \((\Delta x)_1 \) is the actual distance between \( x_1 \) and \( x_1 \). The local regime of interpolation is then written like \( D_X^{(L)} = \{x_1 - (\Delta x)_1 + (\Delta x)_{1-1}, x_1 - (\Delta x)_1, x_1, x_2\} \), following figure B.3:
According to this conversion, we will then acquire $D_X^{(L)}$ with elements in ascending order so that the previous forms may be implemented.

In the context of the MGCM, the coordinates used are $(p, \varphi, \lambda)$, that is in the horizontal direction we have the geographical coordinates $(\lambda, \varphi)$, and in the vertical a hybrid pressure–sigma $p$. This coordinate system is not natural in all three directions, but it is so in the horizontal direction that we are interested in.

A generalization that works well with structured and orthogonal grids, locally, for the case of the approximation of the curvilinear manifold with an affine one, can be put in terms of:

$$f_{p,q} = L_{u^1,p} L_{u^2,q} = \frac{N_{u^1,p} (u^1) N_{u^2,q} (u^2)}{\mathcal{D}_{u^1,p} \mathcal{D}_{u^2,q}} = \prod_{m=1}^{I} \int (dl)_{u^1_m} \prod_{r=1}^{J} \int (dl)_{u^2_r} = \prod_{m=1}^{I} \int (dl)_{u^1_m} \prod_{r \neq q}^{J} \int (dl)_{u^2_r} \prod_{r \neq q}^{J} \int (dl)_{u^2_r}. \quad (B.16)$$

The coordinates $(u^1, u^2)$ are the contravariant of a curvilinear coordinate system that we may consider. For this case, in the horizontal direction of the MGCM lattice, we have $(u^1, u^2) = (\lambda, \varphi)$. Essentially, we have a natural coordinate system in two dimensions in which the covariant and contravariant systems coincide, yet we follow the above notation in the following.

The terms $(dl)_{u^1}$, $(dl)_{u^2}$ are the components of the linear element $dl$ per direction, $(dl)_{u^1} = dl \cdot \hat{e}_1$ and $(dl)_{u^2} = dl \cdot \hat{e}_2$. For this case, it is $(dl)_\lambda = dl \cdot \hat{e}_\lambda = r \cos \varphi \, d\lambda$, and $(dl)_\varphi = dl \cdot \hat{e}_\varphi = r \, d\varphi$, where $r$ is for a constant altitude level, assuming in general
the system of the geographic coordinates \((\lambda, \phi, r)\). The fact that even locally, we proceed from the system \((p, \phi, \lambda)\) to \((\lambda, \phi, r)\) is of course an approximation with minimal impact.

The covariant basis and the linear element in the geographical coordinates are:

\[
\begin{align*}
\hat{e}_\lambda & = -\sin \lambda \hat{i} + \cos \lambda \hat{j}, \\
\hat{e}_\phi & = -\cos \lambda \sin \phi \hat{i} - \sin \lambda \sin \phi \hat{j} + \cos \phi \hat{k}, \\
\text{d}l & = r \cos \phi \, d\lambda \hat{e}_\lambda + r \, d\phi \hat{e}_\phi + \text{d}r \hat{e}_r,
\end{align*}
\]

where \(\{\hat{i}, \hat{j}, \hat{k}\}\) is the natural basis of vectors in the Cartesian (rectangular) system. The four integrals of interest then yield

\[
\begin{align*}
\int_{u^1}^{u^2} (\text{d}l)_{u_1} & = \int_{\lambda_m}^{\lambda_p} r \cos \phi \, d\lambda = r \cos \phi_q (\lambda - \lambda_m), \\
\int_{u^1}^{u^2} (\text{d}l)_{u_2} & = \int_{\phi_r}^{\phi_q} r \, d\phi = r (\phi - \phi_r), \\
\int_{u^1}^{u^2} (\text{d}l)_{u_3} & = \int_{\phi_r}^{\phi_q} r \, d\phi = r (\phi_q - \phi_r).
\end{align*}
\]

A constant latitudinal level is given at \(\phi_q\), as was the case for a constant \(y\) level. For the elements of \(L\), we then have

\[
\ell_{p,q} = \prod_{m=1}^{I} \int_{\lambda_m}^{\lambda_p} r \cos \phi_q \, d\lambda \prod_{r=1}^{J} \int_{\phi_q}^{\phi_r} r \, d\phi = \frac{\prod_{m=1}^{I} (\lambda - \lambda_m) \prod_{r=1}^{J} (\phi_q - \phi_r)}{\prod_{m=1}^{I} r \cos \phi_q \, d\lambda \prod_{r=1}^{J} r \, d\phi} \quad (B.19)
\]

This structure (B.19) is a good approximation in a local regime of interpolation on a sphere, with \(r = \text{const}\), where the curvature of the manifold is neglected. In practice we consider...
domains $D^{(L)}_{\lambda}$, $D^{(L)}_{\phi}$, in the local neighborhood of each argument $(\varphi_s, \lambda_s)$, and since in the Cartesian case the values of $x$, $y$ are decimal, so is the case here for $\lambda$, $\varphi$ respectively.
Appendix C

Retrieval Forward Model Operator

In the context of the retrieval data assimilation, both the observations \( \mathbf{y}_o \), and the background in observation space \( \mathbf{y}_b^{(m)} \), per ensemble member \( m \), are temperatures in \( \mathbf{K} \), as is the case for the background ensemble state \( \mathbf{x}_b^{(m)} \).

The observations \( \mathbf{y}_o \) abut on the reference pressure space, or equivalently the observation space given though coordinate \( \zeta_r \), from equation (7.b). The values of the reference pressures are given in table 2.1 section 2.3, from which the observation space \( \mathbb{D}_\zeta = \{\zeta_r\}_{r=1}^R \) is obtained, as that is described in section 2.3.1. The total number of observations is always 21, which is a given fact from the PDS TES data set. The discrepancy between the total 21 values and those valid ones that are actually used, as \( R \leq 21 \), stems from the fact that some pressure levels may actually be greater than the skin pressure, or greater than the greatest possible horizontally interpolated MGCM ensemble mean pressure, at vertical model level \( k_{max} = K = 28 \). In this regard, due to either physical reasoning or lack of background information below model level \( k_{max} \), some of the observations are neglected. On the other hand, we assume the model space \( \mathbb{D}_{\xi} = \{\xi_k\}_{k=1}^K \), in terms of the coordinate \( \xi_k \), defined from equation (7.a), as the natural logarithm of the horizontally interpolated MGCM pressure ensemble mean at each time frame of interest.

In order to carry out the data assimilation scheme, the innovations vector (or observation increment) \( \mathbf{d} \) is required. Regardless of the approach, namely whether we use the formulation \( \mathbf{d}^{(m)} = \mathbf{y}_o - \mathbf{y}_b^{(m)} \), or \( \mathbf{d} = \mathbf{y}_o - \mathbf{y}_b \) (of the background ensemble mean in observation space \( \overline{\mathbf{y}}_b \)), the background in observation space is to be evaluated from

\[
\hat{f}(\mathbf{x}_b^{(m)}) = \mathbf{y}_b^{(m)}, \tag{C.1}
\]

or
\[ h(\mathbf{x}_b) = \mathbf{y}_b, \quad (C.2) \]

with \( h \) the retrieval forward model operator. Computationally, whether we apply (C.1) individually on each background ensemble member \( \mathbf{x}^{(m)}_b \), in order to obtain \( \mathbf{y}^{(m)}_b \), and then evaluate the background ensemble mean in observation space \( \mathbf{y}_b \), or first evaluate the background ensemble mean \( \mathbf{x}_b \), and from that directly \( \mathbf{y}_b \), is equivalent.

The key point here is that \( [\xi] = [\zeta] \), where the brackets denote physical units. Both model and valid observation spaces are in \( \ln(\text{Pa}) \), and in cases such as this, where these two spaces are of the same dimensions, the mapping from model to observation space, through operator \( \hat{h} \), is achieved from an interpolation, in this case one dimensional.

From appendix B, the general mathematical consideration for interpolating in linear manifolds, applied in this study, is presented. In the current context of appendix C, we assume the template set as \( \mathcal{D}_\xi \), the known images set \( \mathcal{D}^{(m)}_{\mathbf{x}_b} = \{ (\mathbf{x}^{(m)}_b)_k \}_{k=1}^K \), \( \forall \ m \), and the values of the continuous space to be used as arguments in the interpoland function will be \( \mathcal{D}_\zeta \). The regime of interpolation is a line segment itself, thus affine, at the vertical direction of the satellite position \((\lambda_s, \phi_s)\). In addition, \( \mathcal{D}_\xi \) increases monotonically, \( \xi_k < \xi_{k+1} \), \( \forall \ k \), as does \( \mathcal{D}_\zeta \), \( \zeta_r < \zeta_{r+1} \), \( \forall \ r \), which in turn renders the structures of Appendix B valid for this case, as well. A visual representation of the current consideration can be illustrated as below:

![Conceptual draft](image)

**Figure C.1.** Conceptual draft showing 9 model space values \( \xi_k \), for \( k = \{1, 2, \ldots, 9\} \), and 6 observation space values \( \zeta_r \), for \( r = \{1, 2, \ldots, 6\} \). This draft is to be viewed vertically.

We wish to derive an expression as \( H \mathbf{x}^{(m)}_b \), starting from \( h(\mathbf{x}^{(m)}_b) = \mathbf{y}^{(m)}_b \), where \( H \) is an \( R \times K \) matrix form of \( \hat{h} \). From the one dimensional interpolation scheme we have equation (B.1). In the current context, instead of \( \mathbf{x} \) we have the \( \zeta_r \) values. Then, instead of
If we assume, for instance, \( \xi_{q-1} < \zeta_r < \xi_q \), and \( D_{\xi}^{(L)} = \{\xi_{q-2}, \xi_{q-1}, \xi_q, \xi_{q+1}\} \) for an interpolation with four local points, it will also be \( s_1 = q - 2 \), and \( s_2 = q + 1 \). In an application such as this, per row \( r \) in matrix \( H \), the non zero columns will be those for
\{q - 2, q - 1, q, q + 1\}, where the simplest possible interpolation is the linear one by considering only two local points, for each row \(r\), as \(\{q - 1, q\}\).
Appendix D

TES Spectra Inversion

In the introduction of the current study, we mention that from the various observational networks we obtain observations, which are considered a given quantity, subject only to the technical specifications of the instruments used in their procurement, e.g. standard deviation of measurements. Like stated, in remote sensing in the context of satellite measurements, the observations (spectral radiances) are not directly usable in a model evolving *prognostic* equations, since radiance is not one such variable that appears in those equations. From the prognostic equations we have variables like velocity, pressure, density, temperature, and a measure of humidity, but not radiance. Inversion algorithms are then implemented in order to retrieve prognostic variables (e.g. temperature) from the observed radiances. However, these inversions are not unique, therefore we have to consider not only the accuracy of the direct measurements, but additional factors related to the inversion method itself. The inversion methods do not give the same estimations.

Appendix D per se, is not related explicitly to the current study, yet delineates the process of the OSS TES temperature retrievals, from the PDS TES radiances [6]. A general treatment of inversion algorithms can also be found in [16]. Nevertheless, it is included to offer an insight to one particular inversion process, and at the same time it also highlights the appearance, applicability, and role of the jacobian matrices also treated in section 2.4.3.

The notation used in appendix D is retained exclusively for the analysis that appears herein, and *should not be associated with symbols used in sections 2.2 – 2.4.5*. With respect to the used notation hereafter, we have $x_b$ a subjective prior of the *inverse methodology*, $y_o$ the observations, and $h(x)$ the background in observation space. Currently, $x_b$ refers to temperature and $y_o$, $h(x)$ to spectral radiance.

Due to the fact that the inverse methodology involves an iterative algorithm, we also have the appearance of symbols like $x_i$ and $y_i = h(x_i)$, where index $i$ is an iteration counter. The difference between $x_b$ and $x_i$ is that the former symbol pertains to a first guess (an unaltered prior) while the latter to a profile (temperatures) that constantly
changes. This $\mathbf{x}_i$ temperature profile is an input to the OSS forward model operator $\hat{h}$ [15], so that at the $i$–th iteration spectral radiances $\mathbf{y}_i$ are produced. A regression test takes place incorporating $\mathbf{x}_b$ and $\mathbf{y}_o$ with $\mathbf{x}_i$ and $\mathbf{y}_i$, and upon convergence of $\mathbf{y}_o - \mathbf{y}_i$ to a certain accuracy threshold, the iteration concludes. The inversion algorithm used in this study uses a prior $\mathbf{x}_b$ of temperatures at the 21 reference pressure levels (table 2.1), not related to the MGCM discretization (section 2.1.1 and appendix A).

For the procurement of the background radiances in spectral space $(L_b^{(m)})_n, \forall m$ (see section 2.4.1) we have the application of the OSS forward model operator $\hat{h}(\mathbf{x}_b^{(m)})$, where in appendix D, $\mathbf{x}_b^{(m)}$ corresponds to the 21 reference pressure levels background temperatures in pressure space. In other words, the retrieval forward model operator (appendix C), which takes input profiles $(T_b^{(m)})_k$, produces $\mathbf{y}_b^{(m)}$, following the nomenclature of section 2.3.1. In appendix D, this section 2.3.1 symbol $\mathbf{y}_b^{(m)}$ becomes $\mathbf{x}_b^{(m)}$, so that the prior in the inverse methodology coincides with the background in observation space of the retrieval data assimilation of sections 2.3 – 2.3.4. Then, these $\mathbf{x}_b^{(m)}$ 21 reference pressure levels retrieval temperature profiles, per ensemble member $m$, are then inserted individually as inputs to the OSS forward model operator [15], which in turn returns the background radiances in spectral space $(L_b^{(m)})_n$.

The process of the inverse methodology involves the minimization of a cost function $\varphi(\mathbf{x})$ in a mathematical approach similar to the maximization of the cot function in the variational data assimilation approaches.

A statistical assumption that the variables $\mathbf{x}$, $\mathbf{y}_o$, and $\hat{h}(\mathbf{x})$ follow Gaussian distributions is made. From Bayes' theorem it is

$$\text{pdf}(\mathbf{x} | \mathbf{y}_o \land \mathbf{x}_b) = \frac{\text{pdf}(\mathbf{y}_o \land \mathbf{x}_b | \mathbf{x}) \cdot \text{pdf}(\mathbf{x})}{\text{pdf}(\mathbf{y}_o \land \mathbf{x}_b)},$$ (D.1)

where $\text{pdf}(\mathbf{x} | \mathbf{y}_o \land \mathbf{x}_b)$ is the probability density function (pdf) for the system state being $\mathbf{x}$ under the constraint of observations $\mathbf{y}_o$ and a background estimation $\mathbf{x}_b$, $\text{pdf}(\mathbf{y}_o \land \mathbf{x}_b)$ is the system prior pdf, $\text{pdf}(\mathbf{y}_o \land \mathbf{x}_b | \mathbf{x})$ is the likelihood function of the
eventuality \( y_o \land x_b \) given a background state \( x \), and \( \text{pdf}(x) \) the corresponding pdf of the system being at state \( x \). The symbol \( \land \) is for the logical intersection.

The prior density \( \text{pdf}(y_o \land x_b) \) does not depend on the state \( x \) and \( \text{pdf}(x) \) may be set equal to a uniform pdf due to the fact that a priori every value of \( x \) is equally likely. From the previous relation, we then have

\[
\text{pdf}(x \mid y_o \land x_b) \propto \text{pdf}(y_o \land x_b \mid x). \tag{D.2}
\]

Assuming that there are no statistical correlations between the errors in model space (reference pressure levels) and observation (spectral) space, it is

\[
\text{pdf}(y_o \land x_b \mid x) = \text{pdf}(y_o \mid x) \text{pdf}(x_b \mid x). \tag{D.3}
\]

From the statistical assumptions, it also is

\[
\text{pdf}(y_o \mid x) \propto \frac{1}{\sqrt{|R_o|}} \exp \left[ -\frac{1}{2} d^\text{tr} R_o^{-1} d \right], \tag{D.4}
\]

\[
\text{pdf}(x_b \mid x) \propto \frac{1}{\sqrt{|P_b|}} \exp \left[ -\frac{1}{2} \Delta x^\text{tr} P_b^{-1} \Delta x \right], \tag{D.5}
\]

where \( x - x_b \equiv \Delta x \), and \( y_o - \hat{f}(x) \equiv d \). This vector \( d \) represents an innovation in the context of the inverse methodology. Matrix \( R_o \) represents the observation and \( P_b \) the model error covariances respectively. The dimensions of these sets are \( N \times N \) for \( R_o \), with \( N = 143 \), and \( Q \times Q \) for \( P_b \), with \( Q = 21 \) (as in section 2.3.1 for both matrix dimension cases). Similarly, \( \Delta x \) is represented as an \( Q \times 1 \) and \( d \) as an \( N \times 1 \) column vector.

The cost function \( \phi(x) \) we seek to minimize is defined from

\[
\ln(\text{pdf}(y_o \land x_b \mid x)) + \text{const} \equiv \phi(x). \tag{D.6}
\]

By setting the constant to be opposite of the sum of the natural logarithms of the normalization factors of the previous two pdf's, we obtain

\[
\phi(x) = \frac{1}{2} d^\text{tr} R_o^{-1} d + \frac{1}{2} \Delta x^\text{tr} P_b^{-1} \Delta x. \tag{D.7}
\]
The minimization is performed from \( \nabla_x \varphi(x) = 0 \), where \( \nabla_x \) is the gradient operator with respect to \( x \). In the current it is \( \varphi(x) \in \mathbb{E}^1 \), \( h(x) \in \mathbb{E}^N \), so that \( \varphi(x) \) is a scalar function and \( h(x) \) a vector one. The vector space is considered the Cartesian Rectangular System (CRS), denoted hereafter simply as rectangular. The basis vectors in the rectangular system are denoted \( \hat{e}_j \in \mathbb{E}^D \), where \( \hat{e}_j \) is the ordered set with elements everywhere zero except its \( j \)–th, and \( D \) the corresponding dimension of the Euclidian vector space \( \mathbb{E}^D \). Thus, the basis of vectors is \( \{ \hat{e}_j \}_{j=1}^D \), assumed constant.

The gradient (from the left) of a scalar function \( \varphi(x) \), for the rectangular system, is given

\[
\text{grad} (\varphi(x)) \equiv \nabla_x \varphi(x) = \left( \frac{\partial}{\partial x_j} \hat{e}_j \right) \varphi(x) = \frac{\partial \varphi(x)}{\partial x_j} \hat{e}_j. \tag{D.8}
\]

The gradient (from the left) of a vector function \( h(x) = \hat{h}_j \hat{e}_j \), is

\[
\text{grad} (h(x)) \equiv \nabla_x \otimes h(x) = \left( \frac{\partial}{\partial x_k} \hat{e}_k \right) \otimes \left( \hat{h}_j \hat{e}_j \right) = \frac{\partial \hat{h}_j}{\partial x_k} \hat{e}_k \otimes \hat{e}_j, \tag{D.9}
\]

where in the previous formalisms \( j, k \) are generic dummy summation indices, not to be confused with other notations used elsewhere. We introduce the jacobian matrix \( \mathbf{J} \), where by definition it is for the rectangular system

\[
\mathbf{J} \equiv \frac{\text{d} \hat{h}(x)}{\text{d} x} = \frac{\partial \hat{h}_j}{\partial x_k} \hat{e}_j \otimes \hat{e}_k. \tag{D.10}
\]

We also denote the gradient (from the left) of a vector function \( \text{grad} (h(x)) \equiv \mathbf{G} \), so that it is \( \mathbf{G}^{\text{tr}} = \mathbf{J} \).

To make a connection with section 2.3.1, the summation indices that will be used henceforth are \( q \) for the prior in the context of the inverse methodology, and \( n \) for the observations. It follows from 2.3.1 that it is \( q = \{1, 2, \ldots, 21\} \) and \( n = \{1, 2, \ldots, 143\} \), so that the jacobian matrices currently are posed

\[
\mathbf{J} = \frac{\partial \hat{h}_n}{\partial x_q} \hat{e}_n \otimes \hat{e}_q \tag{D.11}
\]
These $J$ matrices are $N \times Q = 143 \times 21$, describing the radiance to temperature sensitivity at each spectral channel and reference pressure level (also from section 2.4.3).

Regarding the minimization of $\varphi(x)$, it follows from $\nabla_x \varphi(x) = 0$, $\in E^Q$:

$$-(\nabla_x \otimes \hat{h}(x)) R_o^{-1} d + P_b^{-1} \Delta x = 0 \quad \text{(D.12.a)}$$

$$\Rightarrow -GR_o^{-1} d + P_b^{-1} \Delta x = 0 \quad \text{(D.12.b)}$$

$$\Leftrightarrow -J^{tr} R_o^{-1} d + P_b^{-1} \Delta x = 0 \quad \text{(D.12.c)}$$

$$\Leftrightarrow -J^{tr} R_o^{-1} (y_o - \hat{h}(x)) + P_b^{-1} \Delta x = 0. \quad \text{(D.12.d)}$$

A linearization of $\hat{h}(x)$ is performed, about the state of $x_b$, by retaining only first order terms

$$\hat{h}(x) \approx \hat{h}(x_b) + \frac{d\hat{h}(x)}{dx} \bigg|_{x_b} \Delta x = \hat{h}(x_b) + J \Delta x. \quad \text{(D.13)}$$

The background in observation space is posed $\hat{h}(x_b) \equiv y_b$. From equations (D.12.d) and (D.13) it follows

$$-J^{tr} R_o^{-1} (y_o - y_b - J \Delta x) + P_b^{-1} \Delta x = 0 \quad \text{(D.14.a)}$$

$$\Leftrightarrow J^{tr} R_o^{-1} (-y_o + y_b) + J^{tr} R_o^{-1} J \Delta x + P_b^{-1} \Delta x = 0 \quad \text{(D.14.b)}$$

$$\Leftrightarrow J^{tr} R_o^{-1} (-y_o + y_b) = -(J^{tr} R_o^{-1} J + P_b^{-1}) \Delta x \quad \text{(D.14.c)}$$

$$\Leftrightarrow J^{tr} R_o^{-1} (y_o - y_b) = (J^{tr} R_o^{-1} J + P_b^{-1}) \Delta x. \quad \text{(D.14.d)}$$

Equation (D.14.d) is brought to the form

$$\Delta x = (J^{tr} R_o^{-1} J + P_b^{-1})^{-1} J^{tr} R_o^{-1} (y_o - \hat{h}(x_b)). \quad \text{(D.15)}$$

At the $i - \text{th}$ iteration, it is $\Delta x = x_{i+1} - x_b$. One additional linearization is performed on the background in observation space $\hat{h}(x_b)$ about a state of $x_i$:

$$\hat{h}(x_b) \approx \hat{h}(x_i) + \frac{d\hat{h}(x)}{dx} \bigg|_{x_i} (x_b - x_i) = y_i + J_i (x_b - x_i), \quad \text{(D.16)}$$
where \( \hat{h}(x_i) \equiv y_i \) is the background in observation space at the \( i \)-th iteration. The iterative scheme is then given from

\[
x_{i+1} = x_b + (J_i^{\text{tr}} R_o^{-1} J_i + P_b^{-1})^{-1} J_i^{\text{tr}} R_o^{-1} (y_o - y_i - J_i (x_b - x_i)).
\]  

(D.17)

Matrix \( P_b \) is not full rank, thus not invertible. An eigen decomposition of \( P_b \) is performed. Covariance matrices are positive definite so the eigen values are positive numbers. For \( P_b \), the majority of its eigen values are expected to be the same, but not all of them. The eigen vectors of \( P_b \) in the current context are called empirical orthogonal functions (EOFs). Diagonalizing \( P_b \) yields \( \Lambda = U^{\text{tr}} P_b U \), or \( P_b = U \Lambda U^{\text{tr}} \). Matrix \( \Lambda \) is diagonal containing the corresponding eigen values and \( U \) an orthogonal matrix containing the eigen vectors, column-wise. The dimensions of \( P_b \), \( \Lambda \), and \( U \) are all \( Q \times Q \). For the reduction of the dimensionality of the problem, the most distinct eigen values with their corresponding eigen vectors are selected. For instance, with \( Q = 21 \), it may be so that only \( 3 - 6 \) eigen values and vectors are to be taken into account. We denote this reduced dimension as \( Q' \) and we introduce a \( Q' \times Q' \) matrix \( \Lambda' \) and an \( Q \times Q' \) matrix \( U' \) containing these most distinct eigen values and vectors, as a subset of \( \Lambda \) and \( U \). The column-wise tabulation applies to \( U' \) as well.

Equation (D.17) will be transformed appropriately, in order to yield sensible results. In order to bypass the presence of the term \( P_b^{-1} \), we have the following transformations; matrix \( P_b \) is set \( \Lambda' = U' \Lambda U^{\text{tr}} \). Then, for \( P_b^{-1} \) it is \( \Lambda'^{-1} = U'^{\text{tr}} \Lambda' U' \). For a projection of the jacobian \( J_i \) onto the space of the EOFs we have \( \tilde{J}_i \equiv J_i U' \), where \( \tilde{J}_i \) will now be \( N \times Q' \). Similarly for \( \Delta x_{i+1} = U'^{\text{tr}} \Delta x_{i+1} \) and \( \Delta x_i = U'^{\text{tr}} \Delta x_i \), where these vectors are now \( Q' \times 1 \).

Equation (D.17) is first brought to the form

\[
\Delta x_{i+1} = (J_i^{\text{tr}} R_o^{-1} J_i + P_b^{-1})^{-1} J_i^{\text{tr}} R_o^{-1} (y_o - y_i + J_i \Delta x_i),
\]

(D.18)

with \( \Delta x_{i+1} = x_{i+1} - x_b \), and \( \Delta x_i = x_i - x_b \). The term of the inversion within the parenthesis is written

\[
J_i^{\text{tr}} R_o^{-1} J_i + U' \Lambda'^{-1} U^{\text{tr}}
\]

(D.19.a)
\[
\begin{align*}
\mathbf{U}^{\top} \mathbf{R}_0 \mathbf{J}_i \mathbf{U}^{\top} & = \mathbf{U}^{\top} \mathbf{J}_i \mathbf{U}^{\top} \mathbf{R}_0^{-1} \\
& = \mathbf{U}^{\top} (\mathbf{J}_i \mathbf{U}^{\top}) \mathbf{R}_0^{-1} (\mathbf{J}_i \mathbf{U}^{\top}) \mathbf{U}^{\top} + \mathbf{U}^{\top} \Lambda^{-1} \mathbf{U}^{\top} \\
& = \mathbf{U}^{\top} \mathbf{J}_i \mathbf{U}^{\top} \mathbf{R}_0^{-1} \mathbf{J}_i \mathbf{U}^{\top} + \mathbf{U}^{\top} \Lambda^{-1} \mathbf{U}^{\top} \\
& = \mathbf{U}^{\top} (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1}) \mathbf{U}^{\top}. \quad \text{(D.19.b)}
\end{align*}
\]

For the inversion of term (D.19.e), it is
\[
\begin{align*}
(\mathbf{U}^{\top} \mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1}) \mathbf{U}^{\top} & = (\mathbf{U}^{\top})^{-1} (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1})^{-1} \mathbf{U}^{\top} \\
& = \mathbf{U}^{\top} \mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1} \mathbf{U}^{\top} \\
& = \mathbf{U}^{\top} (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1})^{-1} \mathbf{U}^{\top}. \quad \text{(D.20.a)}
\end{align*}
\]

Then, equation (D.18) becomes
\[
\Delta \mathbf{x}_{i+1} = \mathbf{U}^{\top} \mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1} \mathbf{U}^{\top} \mathbf{R}_0^{-1} (\mathbf{y}_0 - \mathbf{y}_i + \mathbf{J}_i \Delta \mathbf{x}_i) \\
\mathbf{U}^{\top} \Delta \mathbf{x}_{i+1} = (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1})^{-1} (\mathbf{J}_i \mathbf{U}^{\top}) \mathbf{R}_0^{-1} (\mathbf{y}_0 - \mathbf{y}_i + \mathbf{J}_i \mathbf{U}^{\top} \Delta \mathbf{x}_i) \\
\Delta \tilde{\mathbf{x}}_{i+1} = (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1})^{-1} \mathbf{J}_i \mathbf{R}_0^{-1} (\mathbf{y}_0 - \mathbf{y}_i + \mathbf{J}_i \Delta \tilde{\mathbf{x}}_i) \\
\tilde{\mathbf{x}}_{i+1} = \tilde{\mathbf{x}}_b + (\mathbf{J}_i \mathbf{R}_0^{-1} \mathbf{J}_i + \Lambda^{-1})^{-1} \mathbf{J}_i \mathbf{R}_0^{-1} (\mathbf{y}_0 - \mathbf{y}_i + \mathbf{J}_i (\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_b)).
\]

From the previous analysis it can be seen that originally we have 21 temperatures, as in equation (D.17), whereas in equation (D.21.d) due to the projection onto the EOFs subspace, we will have 3 – 6. Additional statistical analyses are performed in order to estimate more accurately and at the same time assess the retrieved temperatures, which represent only coarse features of the actual atmospheric state. Nevertheless, reasonable temperature profiles for all 21 reference pressure levels can be obtained as such.
Appendix E

Scale Analysis

In the current study the analysis increments $\bar{x}_a - \bar{x}_b$ in the retrieval assimilation appear to be of one order of magnitude greater than their radiance assimilation counterparts. Since the background ensemble mean $\bar{x}_b$ is common in both assimilations this means that in the radiance assimilation the second term of the analysis equation $K(y_o - \bar{y}_b)$ yields lesser numerical figures than in the retrieval. In appendix E we present orders of magnitude of relevant ordered sets to the analysis equation (1), namely the innovations $\bar{d} = y_o - \bar{y}_b$ and $X_p$, $Y_p^{lr}$, $R_o$, and $R_b$ that lead to the evaluation of Kalman gain $K$ via equation (3).

In the following, pertinent numerical figures to the profile 7600/7952 of 000239506 are presented. The other two examined cases 0001/8664 and 1374/8664 of 000155700 exhibit a very similar behavior so that the inclusion of supplementary data does not contribute any additional insights to the analysis. For the profile 7600/7952 we consider the global assimilations, retrieval and radiance; in the retrieval we have the $\sigma_o = 3.0$ K case, and in the radiance the partial spectral space case with 70 accounted channels (neglected channels are the first 7 and the last 66).

Since the interest is not on the numerical figures per se, rather on the representative orders of magnitude that appear in these sets, we only present partial matrices also accounting for the dimensionality of the current problem, per performed assimilation. In both assimilations we have a model space with 28 levels. The ensemble size is equally 16, yet the valid observation space in the retrieval has 14 out of 21 elements (reference pressure levels, as in table 2.1) while in the radiance 70 out of 143 (spectral channels, as in table 2.2). The dimensions of the ordered sets for this case (7600/7952) are in the retrieval assimilation $28 \times 16$ for $X_p$, $16 \times 14$ for $Y_p^{lr}$, $14 \times 14$ for both $R_o$ and $R_b$, leading to a $28 \times 14$ $K$ following equation (3), while in the radiance assimilation the dimension of 14 becomes 70, with $X_p$ remaining the same. The matrices appearing hereafter offer
information for some ensemble members (5 out of 16), and for some valid observation space elements (5 out of 14 for the retrieval and 5 out of 70 for the radiance), yet the other matrix elements that are not presented have orders of magnitudes in the same range as those included below.

**Table E.1.** Analysis increments $\mathbf{x}_a - \mathbf{x}_b$ for a performed data assimilation on profile 7600/7952 of 000239506. Column 1 pertains to the model space levels. Column 2 is for the case of retrieval global assimilation with $\sigma_o = 3.0 \text{ K}$ and column 3 for the radiance global assimilation of the partial spectral space with used channels 70/143, where the neglected channels are the first 7 and the last 66.

<table>
<thead>
<tr>
<th>Background Level</th>
<th>$\overline{\mathbf{x}_a} - \overline{\mathbf{x}_b}$ (K) Retrieval</th>
<th>$\overline{\mathbf{x}_a} - \overline{\mathbf{x}_b}$ (K) Radiance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.896</td>
<td>0.206</td>
</tr>
<tr>
<td>2</td>
<td>3.949</td>
<td>0.603</td>
</tr>
<tr>
<td>3</td>
<td>2.972</td>
<td>0.552</td>
</tr>
<tr>
<td>4</td>
<td>-4.322</td>
<td>-0.506</td>
</tr>
<tr>
<td>5</td>
<td>-2.890</td>
<td>-0.626</td>
</tr>
<tr>
<td>6</td>
<td>-1.746</td>
<td>-0.402</td>
</tr>
<tr>
<td>7</td>
<td>0.670</td>
<td>0.008</td>
</tr>
<tr>
<td>8</td>
<td>2.019</td>
<td>0.297</td>
</tr>
<tr>
<td>9</td>
<td>0.811</td>
<td>0.147</td>
</tr>
<tr>
<td>10</td>
<td>-1.696</td>
<td>-0.178</td>
</tr>
<tr>
<td>11</td>
<td>-2.089</td>
<td>-0.176</td>
</tr>
<tr>
<td>12</td>
<td>-1.437</td>
<td>-0.038</td>
</tr>
<tr>
<td>13</td>
<td>-1.966</td>
<td>-0.071</td>
</tr>
<tr>
<td>14</td>
<td>-1.740</td>
<td>-0.090</td>
</tr>
<tr>
<td>15</td>
<td>1.509</td>
<td>0.243</td>
</tr>
<tr>
<td>16</td>
<td>4.357</td>
<td>0.579</td>
</tr>
<tr>
<td>17</td>
<td>5.391</td>
<td>0.763</td>
</tr>
<tr>
<td>18</td>
<td>4.545</td>
<td>0.671</td>
</tr>
<tr>
<td>19</td>
<td>2.548</td>
<td>0.399</td>
</tr>
<tr>
<td>20</td>
<td>0.733</td>
<td>0.196</td>
</tr>
<tr>
<td>21</td>
<td>-0.743</td>
<td>-0.015</td>
</tr>
<tr>
<td>22</td>
<td>-1.117</td>
<td>-0.083</td>
</tr>
<tr>
<td>23</td>
<td>-1.337</td>
<td>-0.070</td>
</tr>
<tr>
<td>24</td>
<td>-0.938</td>
<td>-0.090</td>
</tr>
<tr>
<td>25</td>
<td>-0.651</td>
<td>-0.053</td>
</tr>
<tr>
<td>26</td>
<td>-2.921</td>
<td>-0.325</td>
</tr>
<tr>
<td>27</td>
<td>-3.297</td>
<td>-0.379</td>
</tr>
<tr>
<td>28</td>
<td>-3.510</td>
<td>-0.415</td>
</tr>
</tbody>
</table>
Speaking in terms of orders of magnitude, we notice from table E.1 that the analysis increments in the retrieval assimilation are about $10^0 \text{K}$ while in the radiance $10^{-1} \text{K}$, a characteristic also encountered throughout the results of section 3.2. Figures such as 3.13 (a) and 3.18 are based respectively on columns 2 and 3 of table E.1. For the retrieval assimilation of figure 3.13 (a) we refer to the orange curve given $\sigma_o = 3.0 \text{K}$, and for the radiance assimilation of figure 3.18 to the blue curve, for the partial spectral space.

For the retrieval assimilation innovations per valid reference pressure level and the background standard deviations in observation space $\sigma_b$, we have the following table E.2.

**Table E.2.** Retrieval global assimilation of profile 7600/7952 of 000239506 with $\sigma_o = 3.0 \text{K}$ relevant numerical figures. Column 1 is for the enumeration of the valid reference pressure levels. Column 2 is for the numerical values of those levels. Column 3 presents the innovations, and column 4 the background standard deviation in observation space.

<table>
<thead>
<tr>
<th>Reference pressure level</th>
<th>(p) (Pa)</th>
<th>((y_o)_r - (y_b)_r) (K)</th>
<th>(\sigma_b) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11.173</td>
<td>5.484</td>
<td>1.261</td>
</tr>
<tr>
<td>2</td>
<td>14.346</td>
<td>2.033</td>
<td>1.240</td>
</tr>
<tr>
<td>3</td>
<td>18.420</td>
<td>-0.151</td>
<td>1.362</td>
</tr>
<tr>
<td>4</td>
<td>23.652</td>
<td>-0.924</td>
<td>1.399</td>
</tr>
<tr>
<td>5</td>
<td>30.370</td>
<td>-1.963</td>
<td>1.197</td>
</tr>
<tr>
<td>6</td>
<td>38.996</td>
<td>-2.941</td>
<td>0.974</td>
</tr>
<tr>
<td>7</td>
<td>50.072</td>
<td>-2.623</td>
<td>1.166</td>
</tr>
<tr>
<td>8</td>
<td>64.294</td>
<td>-0.775</td>
<td>1.717</td>
</tr>
<tr>
<td>9</td>
<td>82.554</td>
<td>4.871</td>
<td>1.235</td>
</tr>
<tr>
<td>10</td>
<td>106.002</td>
<td>11.19</td>
<td>1.179</td>
</tr>
<tr>
<td>11</td>
<td>136.109</td>
<td>11.13</td>
<td>2.713</td>
</tr>
<tr>
<td>12</td>
<td>174.768</td>
<td>7.447</td>
<td>2.384</td>
</tr>
<tr>
<td>13</td>
<td>224.407</td>
<td>3.632</td>
<td>0.683</td>
</tr>
<tr>
<td>14</td>
<td>288.144</td>
<td>10.19</td>
<td>0.947</td>
</tr>
</tbody>
</table>

The column 4 numerical figures of table E.2, given the corresponding \(R_b\), are evaluated by first extracting the main diagonal elements of this matrix and then calculating their square roots, thereby obtaining the background standard deviations in observation space $\sigma_b$. The observational standard deviations $\sigma_o$ are by construction set to $3.0 \text{K}$, so that this $\sigma_o$ figure and the $\sigma_b$ values from matrix $R_b$ can then be directly compared.

Tables E.3 and E.4 offer pertinent information for the radiance global assimilation, across the used 70/143 spectral channels.
Table E.3. Radiance global assimilation of the partial spectral space innovations data set for profile 7600/7952 of 000239506. The data are to be read per row, from left to right, for a total number of elements equal to 70, excluding the first 7 and the last 66 spectral channels. Physical units in mW (cm\(^{-1}\))\(^{-1}\) m\(^{-2}\) sr\(^{-1}\), for included channels 8 to 77 out of 143.

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.135</td>
<td>1.396</td>
<td>1.315</td>
<td>1.579</td>
<td>1.609</td>
<td>1.377</td>
</tr>
<tr>
<td>1.113</td>
<td>0.802</td>
<td>-0.274</td>
<td>-0.667</td>
<td>-0.966</td>
<td>0.377</td>
</tr>
<tr>
<td>0.324</td>
<td>0.338</td>
<td>0.195</td>
<td>0.326</td>
<td>0.202</td>
<td>0.262</td>
</tr>
<tr>
<td>0.199</td>
<td>0.198</td>
<td>0.193</td>
<td>0.085</td>
<td>0.184</td>
<td>0.051</td>
</tr>
<tr>
<td>0.022</td>
<td>0.158</td>
<td>0.022</td>
<td>0.362</td>
<td>-0.170</td>
<td>0.011</td>
</tr>
<tr>
<td>0.408</td>
<td>0.389</td>
<td>0.545</td>
<td>0.652</td>
<td>0.384</td>
<td>0.812</td>
</tr>
<tr>
<td>0.897</td>
<td>1.298</td>
<td>1.110</td>
<td>1.311</td>
<td>1.343</td>
<td>1.476</td>
</tr>
<tr>
<td>0.493</td>
<td>1.239</td>
<td>0.942</td>
<td>0.779</td>
<td>0.662</td>
<td>0.873</td>
</tr>
<tr>
<td>0.508</td>
<td>0.559</td>
<td>0.014</td>
<td>0.504</td>
<td>0.380</td>
<td>0.241</td>
</tr>
<tr>
<td>0.028</td>
<td>0.363</td>
<td>0.320</td>
<td>0.269</td>
<td>0.070</td>
<td>0.199</td>
</tr>
<tr>
<td>-0.020</td>
<td>0.148</td>
<td>-0.079</td>
<td>0.079</td>
<td>-0.010</td>
<td>0.127</td>
</tr>
<tr>
<td>-0.215</td>
<td>-0.089</td>
<td>-0.432</td>
<td>-0.327</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table E.4. Radiance global assimilation of the partial spectral space background standard deviations in observation space for profile 7600/7952 of 000239506. The data are to be read per row, from left to right, for a total number of elements equal to 70, excluding the first 7 and the last 66 spectral channels. Physical units in mW (cm\(^{-1}\))\(^{-1}\) m\(^{-2}\) sr\(^{-1}\), for included channels 8 to 77 out of 143.

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.034</td>
<td>0.017</td>
<td>0.013</td>
<td>0.027</td>
<td>0.011</td>
<td>0.018</td>
</tr>
<tr>
<td>0.014</td>
<td>0.011</td>
<td>0.010</td>
<td>0.010</td>
<td>0.010</td>
<td>0.012</td>
</tr>
<tr>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
<td>0.014</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>0.015</td>
<td>0.017</td>
<td>0.017</td>
<td>0.017</td>
<td>0.019</td>
<td>0.019</td>
</tr>
<tr>
<td>0.020</td>
<td>0.019</td>
<td>0.019</td>
<td>0.019</td>
<td>0.019</td>
<td>0.020</td>
</tr>
<tr>
<td>0.020</td>
<td>0.020</td>
<td>0.019</td>
<td>0.024</td>
<td>0.035</td>
<td>0.058</td>
</tr>
<tr>
<td>0.079</td>
<td>0.089</td>
<td>0.122</td>
<td>0.165</td>
<td>0.114</td>
<td>0.185</td>
</tr>
<tr>
<td>0.223</td>
<td>0.167</td>
<td>0.113</td>
<td>0.148</td>
<td>0.096</td>
<td>0.064</td>
</tr>
<tr>
<td>0.052</td>
<td>0.039</td>
<td>0.021</td>
<td>0.013</td>
<td>0.010</td>
<td>0.010</td>
</tr>
<tr>
<td>0.010</td>
<td>0.007</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>0.006</td>
<td>0.007</td>
<td>0.007</td>
<td>0.007</td>
<td>0.007</td>
<td>0.007</td>
</tr>
<tr>
<td>0.007</td>
<td>0.008</td>
<td>0.008</td>
<td>0.008</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table E.4 presents the radiance assimilation background standard deviations in observation space \(\sigma_b\), as was the case for the retrieval. Its 70 elements follow the dimensions of the associated \(\mathbf{R}_b\), being a 70\(\times\)70 matrix, for the partial spectral case of profile 7600/7952. Table E.4 is then directly comparable with the radiance assimilation \(\sigma_o = 1.5\) mW(cm\(^{-1}\))\(^{-1}\) m\(^{-2}\) sr\(^{-1}\).
Tables E.5 and E.6 highlight representative numerical figures of matrix $\mathbf{Y}_{p}^{ir}$, for each assimilation case. Table E.5 is for the retrieval and table E.6 for the radiance assimilation.

In the retrieval the dimensions of $\mathbf{Y}_{p}^{ir}$ are $16 \times 14$ and in the radiance $16 \times 70$. In tables E.5 and E.6 the included information pertains to select ensemble members. With regards to the included elements of each applicable valid observation space, for the retrieval we have reference pressure levels 1, 4, 8, 12, 14, and for the radiance spectral channels 10, 25, 45, 55, 70. The rest of the data that are not presented are of the same order of magnitude as those shown in these two tables E.5 and E.6. Table E.7 presents data of the background perturbation matrix $\mathbf{X}_{p}$ for both retrieval and radiance assimilations. The rows correspond to model space pressure levels and the columns to select cases of ensemble members, given the dimensionality $K \times M = 28 \times 16$. Elements that do not appear are in the same numerical range of those elements presented below in table E.7. The two remaining tables to be shown in appendix E relate to the representative orders of magnitude of the numerical figures appearing in the two Kalman gain matrices for this examined case (7600/7952). Table E.8 is for the retrieval global assimilation and table E.9 for the radiance global assimilation of the partial spectral space. The full dimensions of $\mathbf{K}$ are $28 \times 14$ for the retrieval and $28 \times 70$ for the radiance case. Tables E.8 and E.9 are structured so that the rows refer to select model space levels and the columns to select cases of valid observation space elements. Like in tables E.5 and E.6, in tables E.8 and E.9 we include the reference pressure levels of 1, 4, 8, 12, 14 and the spectral channels of 10, 25, 45, 55, 70, with the remaining data being in the same range as those that are actually shown.

**Table E.5.** Transpose of the background perturbation matrix in observation space of the retrieval global assimilation (7600/7952 of 000239506). The rows pertain to select ensemble members and the columns to select cases of valid reference pressure levels. Physical units in K.

<table>
<thead>
<tr>
<th>m/r</th>
<th>1</th>
<th>4</th>
<th>8</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.63x10^{-1}</td>
<td>-1.54x10^{-1}</td>
<td>-1.10x10^{-1}</td>
<td>3.16x10^{-1}</td>
<td>-5.95x10^{-2}</td>
</tr>
<tr>
<td>3</td>
<td>6.01x10^{-1}</td>
<td>-9.49x10^{-1}</td>
<td>2.01x10^{-1}</td>
<td>-1.56x10^{-1}</td>
<td>1.38x10^{-1}</td>
</tr>
<tr>
<td>5</td>
<td>-4.31x10^{-1}</td>
<td>-2.14x10^{-1}</td>
<td>9.52x10^{-1}</td>
<td>-5.76x10^{-1}</td>
<td>8.43x10^{-1}</td>
</tr>
<tr>
<td>7</td>
<td>-2.53x10^{-1}</td>
<td>-1.84x10^{-1}</td>
<td>-1.16x10^{-1}</td>
<td>2.81x10^{-1}</td>
<td>-4.07x10^{-1}</td>
</tr>
<tr>
<td>9</td>
<td>3.64x10^{-1}</td>
<td>1.61x10^{-1}</td>
<td>1.70x10^{-1}</td>
<td>-2.68x10^{-1}</td>
<td>3.82x10^{-1}</td>
</tr>
<tr>
<td>11</td>
<td>-1.59x10^{-1}</td>
<td>3.57x10^{-1}</td>
<td>1.48x10^{-1}</td>
<td>-1.52x10^{-1}</td>
<td>-2.91x10^{-1}</td>
</tr>
<tr>
<td>13</td>
<td>-3.35x10^{-1}</td>
<td>-5.29x10^{-1}</td>
<td>-2.41x10^{-1}</td>
<td>2.29x10^{-1}</td>
<td>-9.99x10^{-2}</td>
</tr>
<tr>
<td>15</td>
<td>8.04x10^{-1}</td>
<td>1.84x10^{-1}</td>
<td>6.07x10^{-1}</td>
<td>-3.37x10^{-1}</td>
<td>6.36x10^{-2}</td>
</tr>
</tbody>
</table>
Table E.6. Transpose of the background perturbation matrix in observation space of the radiance global and partial spectral space assimilation (7600/7952 of 000239506). The rows pertain to select ensemble members and the columns to select cases of valid spectral channels. Physical units in mW (cm$^{-1}$)$^{-1}$ m$^{-2}$ sr$^{-1}$.

<table>
<thead>
<tr>
<th>m/n</th>
<th>10</th>
<th>25</th>
<th>45</th>
<th>55</th>
<th>70</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.56×10$^{-2}$</td>
<td>3.03×10$^{-2}$</td>
<td>1.59×10$^{-2}$</td>
<td>1.47×10$^{-2}$</td>
<td>1.28×10$^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>-3.87×10$^{-2}$</td>
<td>-6.56×10$^{-2}$</td>
<td>6.88×10$^{-2}$</td>
<td>2.64×10$^{-2}$</td>
<td>2.00×10$^{-2}$</td>
</tr>
<tr>
<td>5</td>
<td>-3.48×10$^{-2}$</td>
<td>-6.55×10$^{-2}$</td>
<td>-8.60×10$^{-2}$</td>
<td>-2.71×10$^{-2}$</td>
<td>-2.28×10$^{-2}$</td>
</tr>
<tr>
<td>7</td>
<td>1.10×10$^{-2}$</td>
<td>2.16×10$^{-2}$</td>
<td>6.40×10$^{-2}$</td>
<td>1.07×10$^{-2}$</td>
<td>9.31×10$^{-2}$</td>
</tr>
<tr>
<td>9</td>
<td>-1.12×10$^{-2}$</td>
<td>-2.19×10$^{-2}$</td>
<td>-5.71×10$^{-2}$</td>
<td>-1.03×10$^{-2}$</td>
<td>-9.06×10$^{-2}$</td>
</tr>
<tr>
<td>11</td>
<td>-6.18×10$^{-2}$</td>
<td>-1.20×10$^{-2}$</td>
<td>-5.46×10$^{-2}$</td>
<td>-5.87×10$^{-2}$</td>
<td>-5.18×10$^{-2}$</td>
</tr>
<tr>
<td>13</td>
<td>6.71×10$^{-2}$</td>
<td>1.31×10$^{-2}$</td>
<td>1.80×10$^{-2}$</td>
<td>6.24×10$^{-2}$</td>
<td>5.51×10$^{-2}$</td>
</tr>
<tr>
<td>15</td>
<td>-1.89×10$^{-2}$</td>
<td>-3.70×10$^{-2}$</td>
<td>-1.83×10$^{-2}$</td>
<td>-1.85×10$^{-2}$</td>
<td>-1.58×10$^{-2}$</td>
</tr>
</tbody>
</table>

Table E.7. Background perturbation matrix of the retrieval global and radiance global of the partial spectral space assimilations (7600/7952 of 000239506). The rows pertain to select model space levels and the columns to select ensemble members. Physical units in K.

<table>
<thead>
<tr>
<th>k/m</th>
<th>1</th>
<th>3</th>
<th>7</th>
<th>13</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.48×10$^{-1}$</td>
<td>-1.59×10$^{-1}$</td>
<td>2.14×10$^{-1}$</td>
<td>1.00×10$^{-1}$</td>
<td>1.37×10$^{-1}$</td>
</tr>
<tr>
<td>5</td>
<td>-3.00×10$^{-1}$</td>
<td>2.60×10$^{-1}$</td>
<td>-5.63×10$^{-1}$</td>
<td>-2.37×10$^{-1}$</td>
<td>-1.15×10$^{-1}$</td>
</tr>
<tr>
<td>10</td>
<td>-1.11×10$^{-1}$</td>
<td>1.13×10$^{-1}$</td>
<td>-2.05×10$^{-1}$</td>
<td>-4.27×10$^{-1}$</td>
<td>-1.15×10$^{-1}$</td>
</tr>
<tr>
<td>15</td>
<td>5.33×10$^{-1}$</td>
<td>1.04×10$^{-1}$</td>
<td>6.21×10$^{-1}$</td>
<td>2.73×10$^{-1}$</td>
<td>9.28×10$^{-1}$</td>
</tr>
<tr>
<td>20</td>
<td>6.07×10$^{-1}$</td>
<td>1.25×10$^{-1}$</td>
<td>1.83×10$^{-1}$</td>
<td>-3.30×10$^{-1}$</td>
<td>-5.48×10$^{-1}$</td>
</tr>
<tr>
<td>25</td>
<td>-8.78×10$^{-1}$</td>
<td>1.53×10$^{-1}$</td>
<td>-4.15×10$^{-1}$</td>
<td>-1.06×10$^{-1}$</td>
<td>-1.88×10$^{-1}$</td>
</tr>
<tr>
<td>28</td>
<td>-3.34×10$^{-1}$</td>
<td>2.92×10$^{-1}$</td>
<td>-1.31×10$^{-1}$</td>
<td>-2.17×10$^{-1}$</td>
<td>-2.91×10$^{-1}$</td>
</tr>
</tbody>
</table>

Table E.8. Kalman gain (dimensionless) for the retrieval global assimilation of 7600/7952 of 000239506, with $\sigma_o = 3.0$ K. The rows pertain to select model space levels and the columns to select cases of valid reference pressure levels.

<table>
<thead>
<tr>
<th>k/r</th>
<th>1</th>
<th>4</th>
<th>8</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-2.04×10$^{-2}$</td>
<td>-3.97×10$^{-2}$</td>
<td>-4.96×10$^{-2}$</td>
<td>8.25×10$^{-2}$</td>
<td>-1.81×10$^{-2}$</td>
</tr>
<tr>
<td>5</td>
<td>-8.51×10$^{-2}$</td>
<td>-4.62×10$^{-2}$</td>
<td>4.68×10$^{-2}$</td>
<td>-8.45×10$^{-2}$</td>
<td>3.86×10$^{-2}$</td>
</tr>
<tr>
<td>10</td>
<td>4.10×10$^{-2}$</td>
<td>9.34×10$^{-2}$</td>
<td>1.13×10$^{-1}$</td>
<td>-8.75×10$^{-2}$</td>
<td>3.29×10$^{-2}$</td>
</tr>
<tr>
<td>15</td>
<td>1.17×10$^{-1}$</td>
<td>-1.44×10$^{-1}$</td>
<td>-1.90×10$^{-1}$</td>
<td>4.69×10$^{-1}$</td>
<td>4.48×10$^{-1}$</td>
</tr>
<tr>
<td>20</td>
<td>9.49×10$^{-3}$</td>
<td>-3.49×10$^{-3}$</td>
<td>3.36×10$^{-3}$</td>
<td>2.40×10$^{-3}$</td>
<td>2.66×10$^{-3}$</td>
</tr>
<tr>
<td>25</td>
<td>1.28×10$^{-2}$</td>
<td>3.47×10$^{-2}$</td>
<td>5.52×10$^{-2}$</td>
<td>-4.50×10$^{-2}$</td>
<td>5.52×10$^{-2}$</td>
</tr>
<tr>
<td>28</td>
<td>4.72×10$^{-2}$</td>
<td>5.67×10$^{-2}$</td>
<td>1.00×10$^{-1}$</td>
<td>-1.48×10$^{-1}$</td>
<td>6.32×10$^{-2}$</td>
</tr>
</tbody>
</table>
Table E.9. Kalman gain (K (mW (cm\(^{-1}\))\(^{-1}\) m\(^{-2}\) sr\(^{-1}\))\(^{-1}\)) for the radiance global assimilation of the partial spectral space of 7600/7952 of 000239506 (70/143 used channels). The rows pertain to select model space levels and the columns to select cases of valid spectral channels.

<table>
<thead>
<tr>
<th>k/n</th>
<th>10</th>
<th>25</th>
<th>45</th>
<th>55</th>
<th>70</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.02\times10^{-3}</td>
<td>7.85\times10^{-3}</td>
<td>1.93\times10^{-2}</td>
<td>3.81\times10^{-3}</td>
<td>3.31\times10^{-3}</td>
</tr>
<tr>
<td>5</td>
<td>-4.22\times10^{-3}</td>
<td>-8.02\times10^{-3}</td>
<td>-6.00\times10^{-3}</td>
<td>-3.50\times10^{-2}</td>
<td>-3.05\times10^{-2}</td>
</tr>
<tr>
<td>10</td>
<td>-4.19\times10^{-3}</td>
<td>-8.28\times10^{-3}</td>
<td>-1.48\times10^{-2}</td>
<td>-4.22\times10^{-3}</td>
<td>-3.64\times10^{-3}</td>
</tr>
<tr>
<td>15</td>
<td>2.49\times10^{-1}</td>
<td>4.83\times10^{-1}</td>
<td>2.22\times10^{-1}</td>
<td>2.30\times10^{-2}</td>
<td>1.99\times10^{-3}</td>
</tr>
<tr>
<td>20</td>
<td>1.18\times10^{-1}</td>
<td>2.34\times10^{-1}</td>
<td>1.55\times10^{-1}</td>
<td>1.24\times10^{-2}</td>
<td>1.05\times10^{-3}</td>
</tr>
<tr>
<td>25</td>
<td>-2.23\times10^{-1}</td>
<td>-4.34\times10^{-1}</td>
<td>-6.88\times10^{-1}</td>
<td>-2.03\times10^{-2}</td>
<td>-1.78\times10^{-3}</td>
</tr>
<tr>
<td>28</td>
<td>-7.44\times10^{-1}</td>
<td>-1.45\times10^{-1}</td>
<td>-3.95\times10^{-2}</td>
<td>-6.97\times10^{-3}</td>
<td>-6.06\times10^{-3}</td>
</tr>
</tbody>
</table>

The previous tables offer an insight regarding representative orders of magnitude of those quantities appearing in the analysis equation (1) and the Kalman gain evaluation equation (3), of section 2.2.

For the retrieval assimilation of 7600/7952, from table E.2, column 3, the range of the orders of magnitude for the retrieval innovations is given, being \(10^{-1} - 10^{+1}\). From table E.5, for \(Y_p^\text{tr}\), the corresponding range is \(10^{-1} - 10^{0}\), while from table E.7 for \(X_p\), it is \(10^{-1} - 10^{0}\). The retrieval background standard deviations in observation space are given in table E.2, column 4. A typical magnitude for \(\sigma_b\) is around \(10^{0}\), while the retrieval observational standard deviations are fixed at \(\sigma_o = 3.0\, \text{K}\). Therefore, both retrieval assimilation standard deviations, are scaled equally, around \(10^{0}\). In turn, both error covariance matrices \(R_o\) and \(R_b\) will be of order \(10^{0}\), following rough formulations \(\sigma_o^2\) and \(\sigma_b^2\), for the main diagonal elements. Then, the term \((R_o + R_b)^{-1}\), which is related to an algebraic reciprocal, will also be of order \(10^{0}\).

In view of equation (3), \(K = (M - 1)^{-1} X_p Y_p^\text{tr} (R_o + R_b)^{-1}\), for the retrieval assimilation the order of Kalman gain is derived from a scale analysis following a term like \(10^\alpha \times 10^\beta \times 10^0\). Coefficient \(\alpha\) is the magnitude of \(X_p\), \(\beta\) the magnitude of \(Y_p^\text{tr}\), and 0 the magnitude of \((R_o + R_b)^{-1}\). In view of \(\alpha, \beta \in \mathbb{Z}\), with \(\alpha = \{-1, 0\}\) and \(\beta = \{-1, 0\}\), we have for \((\alpha, \beta) = (-1, -1)\) a result as \(10^{-1} \times 10^{-1} \times 10^0 = 10^{-2}\), while for
(α, β) = (0, 0) it will be $10^0 \times 10^0 \times 10^0 = 10^0$. Table E.8 gives several elements of the retrieval assimilation Kalman gain, with most of them being of order $10^{-2}$, a fact that conforms with the previous rationale.

From the analysis equation (1), $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y}_o - \mathbf{y}_b)$, the second term of the right hand side is then equal to the analysis increment $\mathbf{x}_a - \mathbf{x}_b$, the orders of which are given in column 2 of table E.1, for the retrieval case. These terms are of order $10^{-1} - 10^0$, and so this must be the case also for the term $\mathbf{K}(\mathbf{y}_o - \mathbf{y}_b)$. The innovations order is $10^{-1} - 10^1$, which is then multiplied by a typical $\mathbf{K}$ order $10^{-2}$ (possibly greater), to yield the retrieval assimilation analysis increments order, around $10^0$.

For the radiance assimilation, we have a similar reasoning, following typical orders of magnitude of tables E.7 for $\mathbf{X}_p$, table E.6 for $\mathbf{Y}_p^{\text{tr}}$, table E.3 for the innovations, table E.4 for the $\sigma_b$ values, and table E.9 which gives the order of the corresponding $\mathbf{K}$. The term $\mathbf{X}_p$ is as in the retrieval assimilation, of order $10^{-1} - 10^0$. Matrix $\mathbf{Y}_p^{\text{tr}}$ has a typical order of $10^{-3} - 10^{-1}$, where a brief comparison between tables E.5 and E.6 shows a clear differentiation in the typical orders of the retrieval and radiance $\mathbf{Y}_p$ (or their transposes). For the order of $\mathbf{R}_b$, we square the elements of table E.4, to reach to an exponent range $10^{-5} - 10^{-4}$. For the order of $\mathbf{R}_o$, with fixed $\sigma_o = 1.5 \text{ mW} (\text{cm}^{-1})^{-1} \text{ m}^{-2} \text{ sr}^{-1}$, it follows a magnitude of $10^0$. Consequently, the term $\mathbf{R}_o + \mathbf{R}_b$ in the radiance assimilations is roughly equal to $\mathbf{R}_o$, so that the filtering will trust more the background (from the application of the OSS operator, see section 2.4.1). In any case, the reciprocal here will equally be of order $10^0$.

For Kalman gain, a representative order follows the scheme $10^a \times 10^b \times 10^c$, with coefficient values $\alpha = \{-1, 0\}$ and $\beta = \{-3, -2, -1\}$. From table E.9 we infer a $\mathbf{K}$ order around $-2$, so that typically both $\alpha, \beta$ will be negative. From table E.1, column 3, the radiance analysis increments are of order around $10^{-1} - 10^0$. Assuming a $\mathbf{K}$ order of $10^{-2}$, and a $\mathbf{d}$ order around $10^{-0.5}$ (table E.3), the order of the term $\mathbf{Kd} = \mathbf{K}(\mathbf{y}_o - \mathbf{y}_b)$ will then be around $10^{-1}$. 
The previous analysis may be rather qualitatively, yet it is quite clear that in the radiance assimilation, both orders for $K$ and $\bar{d}$ are quite less than in the retrieval assimilation. Then, the order of the product $K\bar{d}$ equally outlines the order of the analysis increments, per performed assimilation, retrieval and radiance. Appendix E supplements relevant conclusions offered in the discussion section 4.1.
References


