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Pixel Maps in the FMI Inversion Method
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1. Introduction

In September 2002 an unprecedented event took place over the Antarctic: the stratospheric polar vortex split in two leading to a corresponding split in the ozone hole. The split was caused by sudden stratospheric warming which has never been observed before in the southern hemisphere and is unusual even in the northern hemisphere. OSIRIS on board Odin is one of the satellite instruments that can help to clarify the course of events that led to the split. Moreover, the OSIRIS measurements can be used in a global mapping of the ozone concentration profiles throughout the stratosphere and mesosphere. One of Odin's scientific goals is also to provide the world with detailed data relating to the extent and the mechanisms responsible for ozone depletion [1].

The Odin satellite (figure 1) was launched in February 2001 carrying two instruments: OSIRIS (the Optical Spectrograph and Infrared Imaging System) and SMR (the Sub-Millimetre Radiometer). Odin is a sun-synchronous satellite following a circular orbit at an altitude of 600 km. For aeronomy measurements the spacecraft scans the Earth's atmosphere up and down from 15 to 120 km at a rate of up to 60 scans per orbit and 15 orbits per day. Odin is a Swedish-led satellite project funded jointly by Sweden (SNSB), Canada (CSA), Finland (Tekes) and France (CNES). [2]

The optical part of OSIRIS consists of a UV-visible spectrograph designed to measure scattered sunlight in the atmosphere. The OSIRIS measurements are processed at the Finnish Meteorological Institute by using an inversion algorithm. The goal of the inversion is to retrieve the vertical density profiles of the neutral atmosphere, aerosols, and atmospheric trace gases (O₃, NO₂, OClO, and BrO). However, when I began this work at the end of May 2003 the results obtained from the inversion were not quite accurate according to different sources of validation data. One of the ways in which we hoped to improve the results was finding the right wavelengths for the inversion.

![Figure 1. Odin satellite. Picture from SSC (Swedish Space Corporation).](image-url)
2. Objectives

In brief, the main objective of my work was to study how the FMI processing could be improved by using different pixel maps i.e. wavelengths in the inversion. This paper describes several approaches which were based on some physical fact or procedures used elsewhere for the processing of the OSIRIS measurements. The chief aspiration was to ameliorate the density profiles obtained from the inversion (and ozone profiles in particular) in comparison with validation data. The secondary and a closely related objective was to check the corrections of data handling i.e. the numbering of the data pixels in the algorithms.

3. The OSIRIS data

OSIRIS is a spectrograph designed measure the amount of scattered sunlight along the line of sight (LOS). The optical part of OSIRIS consists of a grating spectrometer covering the spectral range between approximately 280 nm and 800 nm with the resolution of 1 nm. OSIRIS also has three IR channels near 1260, 1270 and 1560 nm. This paper concentrates on the measurements done in the UV-visible wavelengths. OSIRIS is a limb-scanning instrument which means that it looks through the atmosphere into the space. The lowest point OSIRIS sees in the atmosphere is called the tangent point. The Odin satellite physically scans the limb enabling OSIRIS to take scans of limb-scattered sunlight spectra for tangent heights between about 80 km and 10 km. The main purpose of this atmospheric mission is to measure minor stratospheric constituents (O₃, NO₂, OCIO, and BrO) and stratospheric aerosol extinction. OSIRIS is one of the first limb-viewing instruments that can measure stratospheric chemistry with a good vertical resolution: the pointing accuracy in the aeronomy mode is 1.2 arc min, which is equivalent to one kilometer's uncertainty in the tangent height. [2, 3]

The OSIRIS level 2 data processing is carried out at the FMI’s Arctic Research Centre in Sodankylä after the radiance data has been obtained from the level 1 processing performed in Saskatoon, Canada. The level 2 processing includes the data inversion which converts the radiance measurements into, among other things, ozone profiles. The greatest problem with the original inversion results were the divergent ozone profiles. In these profiles the number density values started to increase rapidly below 30 km and grew much higher than $8 \times 10^{12}$ $1/cm^3$, which is the physically feasible limit. On the other hand, the profiles of some scans had systematically smaller density values than the corresponding validation data. An example of a divergent ozone profile (scan number 8744008) is seen in appendix A and a correct profile (scan number 8744048) in appendix B.

OSIRIS data processing is also carried out independently at the York University in Canada where the processing is done by using the so-called Flittner method. The results obtained by using the Flittner method are fairly accurate below 40 km and can consequently be used as a standard of comparison for the FMI inversion results. However, above this altitude the Flittner profiles become unreliable. The neutral density profiles can be verified by comparing them with profiles obtained from meteorological analysis and more specifically from the European Centre for Medium-Range Weather Forecasts (ECMWF).
The results of this work are based on the measurement data of the satellite's orbit number 8744 or 2228 in hexadecimal form (figure 2). These measurements were made on 1st October 2002 starting at about 15:00 UTC. This orbit had 65 scans in total and 61 of them filled the requirements necessary for the inversion (the solar zenith angle was less than 90°). The version number of the inversion code was 2.2. The constituents to be retrieved in the first peeling were ozone, neutral density, and aerosols but in the second peeling we also tried to retrieve NO₂. BrO and OCIO have been excluded from the second peeling because their inclusion often caused a strong fluctuation in the residuals. The neutral density shift has not been used.

Our main attempt was to retrieve ozone and therefore the different test results are largely represented in the form of ozone profiles. When the ozone profiles were correct, the air profiles were usually accurate as well. The maximum and minimum altitudes used in the data inversion are 70 km and 12 km and because the radiance measurements are not necessarily accurate at the lowest altitude (e.g. as a result of cloudiness), the ozone values at this altitude have generally been disregarded. The inversion results can also be assessed by looking at the residual spectra (the difference between the measured and the modeled radiances) and the values of $\chi^2$ at each tangent altitude.
Figure 2. The measured radiance spectra of scan number 8744008. Each line represents a measurement at a different tangent altitude and the higher the altitude, the smaller the measured radiance. The wavelength gap from approximately 480 nm to 530 nm relates to the instrument's measurement properties.

4. The FMI inversion method

4.1. Principles of the inversion

The basic data needed in the inversion are the measured radiances \( I^\text{meas}(\lambda, h_j) \) from one scan (\( h_j \) denotes the tangent altitude and \( \lambda \) the wavelengths). To obtain self-calibration, the radiances are not used directly but instead we use the following radiance ratios:

\[
F(\lambda, h_j) = \frac{I^\text{meas}(\lambda, h_j)}{I^\text{meas}_\text{ref}(\lambda, h_{\text{ref}})}.
\]  

(1)

\( F(\lambda, h_j) \) is called the transfer spectrum. The reference spectrum \( I^\text{meas}_\text{ref}(\lambda, h_{\text{ref}}) \) is a measurement at a high tangent altitude \( h_{\text{ref}} \), which is called the reference altitude. The reference altitude has been chosen to be the highest layer between 50 km and 45 km.
The transfer spectrum is used in order to diminish the effects due to e.g. the Earth’s surface albedo and clouds.

The modeled transfer spectrum (figure 3) is

\[ M(\lambda, h_j, \rho) = \frac{I_{\text{model}}^{\text{model}}(\lambda, h_j, \rho)}{I_{\text{ref}}^{\text{model}}(\lambda, h_{\text{ref}}, \rho_{\text{ref}})}, \tag{2} \]

where \( I_{\text{model}}^{\text{model}}(\lambda, h_j, \rho) \) is the modeled radiance and \( I_{\text{ref}}^{\text{model}}(\lambda, h_{\text{ref}}, \rho_{\text{ref}}) \) the modeled radiance spectrum at the reference altitude. Parameter \( \rho \) stands for the unknown constituent densities we are trying to retrieve. Since it is difficult and time-consuming to model the measured spectra of scattered sunlight in the atmosphere, the process has been simplified by

1. calculating the ratios of multiple and single scattering beforehand for different solar angles and background atmospheres using the LIMBTRAN program [4]

2. using these tabled ratios and the values obtained for multiple scattering in the inversion so that only the single scattering element \( M_{ss}(\lambda, h_j, \rho) \) needs to be determined.

The modeled transfer spectrum can now be calculated by using the formula

\[ M(\lambda, h_j, \rho) = \frac{M_{ss}(\lambda, h_j, \rho) R(\lambda, h_j, \bar{\rho})}{M_{\text{ref}}(\lambda, h_{\text{ref}}, \bar{\rho}_{\text{ref}})}, \tag{3} \]

where \( M_{\text{ref}}(\lambda, h_{\text{ref}}, \bar{\rho}_{\text{ref}}) \) is the tabled value for multiple scattering at the reference altitude and \( R(\lambda, h_j, \bar{\rho}) \) the tabled ratio of multiple and single scattering

\[ R(\lambda, h_j, \bar{\rho}) = \frac{M(\lambda, h_j, \bar{\rho})}{M_{ss}(\lambda, h_j, \bar{\rho})}. \tag{4} \]

\( \bar{\rho} \) denotes the constituent densities based on a priori knowledge whereas \( \rho \) represents the densities fitted in the inversion. The required a priori data of neutral density profiles is attained by comparing the density profile obtained from the ECMWF to three different background atmospheres (arctic, midlatitude and tropical) and selecting the closest. More information on the radiative transfer model can be found in LIMBTRAN: A pseudo three-dimensional radiative transfer model for the limb-viewing imager OSIRIS on the Odin satellite [4].
The data inversion uses the so-called Modified Onion Peeling Method [5]. This method assumes that the atmosphere consists of layers and that in each layer lays the tangent point of one measurement. Therefore the number of layers is the same as the number of measurements. The densities of different constituents are assumed to remain constant in each layer and the measurement is assumed to depend only on constituent densities in and above the current layer. In the first peeling of the inversion we only retrieve the profiles of $O_3$, neutral density and aerosols but in the second peeling $NO_2$, OCIO and BrO can be retrieved as well.

The onion peeling method is used in an iterative manner. First the constituent densities for the uppermost layer are solved by using a non-linear, least-squares fitting method and initial guesses for the density values. The densities of the next layers are then solved by using the densities of the previous layer as starting values or, after the first iteration, the starting values are the densities fitted in the previous iteration. The objective is to achieve a new and better approximation for the density values in every iteration of the peeling process.

The inverse problem in each layer is solved by minimizing the sum of squared residuals $\chi^2(j)$

\[ \chi^2(j) = \sum (\text{model} - \text{measurement})^2 \]
\[ \chi^2(j) = [M(\lambda, h_j, \rho) - F(\lambda, h_j)]C^{-1}[M(\lambda, h_j, \rho) - F(\lambda, h_j)], \]  

(5)

where \( F(\lambda, h_j) \) is the transfer spectrum in layer \( j \), \( M(\lambda, h_j, \rho) \) the modeled transfer spectrum at different wavelengths and constituent densities in the same layer and \( C' \) the inverse of the covariance matrix of the measurement error. The solution is found by using the Levenberg-Marquardt method, a combination of the inverse-Hessian method and the steepest descent method. Besides the fitted densities, the Levenberg-Marquardt method also returns error estimates.

### 4.2. The inversion algorithm

The inversion method can be summarized by the following algorithm:

1. Initialize the first guess of the ratio spectra (formula 4) and simulate the reference spectrum by using \( a \text{ priori} \) values.

2. Repeat the peeling two times. At the first time fit only ozone, aerosols and neutral density; at the second time it is also possible to fit minor absorbers. In each peeling:
   - First select the constituents to retrieve.
   - Working from top to down for every tangent height \( h \), solve the non-linear least-squares problem (formula 5) using the Levenberg-Marquardt method and adjusting only the densities \( \rho \) in each layer \( j \).

3. After the first peeling it is also possible to use the neutral density shift:
   - Compare the retrieved neutral density profile with the corresponding ECMWF profile and, if necessary, adjust the reference spectrum by scaling with a constant factor. The ratio spectrum does not need to be scaled.
   - We now have an adjusted reference spectrum for the neutral density. Proceed to the second peeling (repeat step 2).

The inversion method has been described in greater detail by Auvinen et al. [5].

### 5. Pixel number checking

The OSIRIS instrument covers the spectral range between approximately 280 nm and 800 nm. The resolution of the instrument is 1350 pixels, each pixel representing a wavelength. Originally 956 pixels were chosen for the inversion and these pixels have been used in the official OSIRIS Level 2 processing. The original pixel map only covers the wavelength range between approximately 280 nm and 675 nm. In the following figures this pixel map will be denoted by mod3 and plotted with a solid blue line. The original pixel map was the standard point of comparison and the basis of most other pixel maps subsequently used in the inversion. These latter pixel maps will be plotted with a solid green line and the wavelengths they include can be seen in appendix C.

Besides the inversion pixels, there is also a separate pixel map for the radiative transfer model (RTM). The pixels used in the inversion must be included both in the
list of RTM pixels and in the inversion pixel map. The radiative transfer model only uses 410 pixels and therefore the maximum number of pixels that can be used in the inversion is in fact 410. The pixels used in the radiative transfer model have been chosen in order to avoid the absorption and emission wavelengths of gases not included in the inversion, e.g. O$_2$, H$_2$O and [O$_3$] [6]. The absorption and emission lines can be seen in the measured radiance spectra (figure 2). Some troublesome pixels can also be determined by scrutinizing the residual spectra. Unsuitable absorption and emission wavelengths had for the most part been removed from the radiative transfer model pixels or from the original inversion pixel map. However, if the reference altitude is changed, new residual spikes may emerge and the inversion pixel map needs to be reinspected.

The attempt to remove the remaining absorption and emission wavelengths of O$_2$, H$_2$O and [O$_3$] gave the initiative to inspect the residual and transfer spectra. Some minor remaining spikes could still be found but, strangely, the exact corresponding wavelengths were not included in the inversion pixel map. Later it was discovered that there was a numbering error in the inversion code: the numbering of the pixels in the inversion module had been started from zero whereas in the input files (including the pixel maps) it began from one. When this slip was fixed the remaining spikes vanished as can be seen in figure 4. Nevertheless, this did not improve the ozone profiles.

Figure 4. The transfer and residual spectra of scan number 8744008 while using the original inversion pixel map (mod3) after the pixel numbering error had been corrected.
6. Choosing wavelengths for the inversion

6.1. Enlarging the wavelength range

The original pixel map had been limited to pixels whose wavelengths were shorter than 675 nm perhaps because in the longer wavelengths the transfer and residual spectra become more fluctuational. However, when longer wavelengths up to 760 nm were included in the inversion pixel map (denoted by mod4), the ozone profiles of divergent scans improved and even lost some of their divergent quality (figure 5), though the residuals increased over the longer wavelengths (appendix A). The inversion results of scans that were originally fairly accurate stayed mostly the same or somewhat improved. Out of 60 scans (8744004-8744063), only in seven cases the results worsened slightly compared with the Flittner profile (figure 6). At wavelengths shorter than 300 nm the measured transfer spectra contain some fluctuations that are not present in the modeled transfer spectra; thus these wavelengths were omitted from the enlarged pixel map, although this does not significantly alter the results.

![Graph](image)

**Figure 5.** The ozone profile and the relative difference (e.g. 100 (mod4-Flittner)/Flittner) for scan 8744008 using the enlarged pixel map (mod4).
Figure 6. The ozone profile and the relative difference for scan 8744048 using the enlarged pixel map (mod4). The ozone hole can be observed clearly below 22 kilometer's altitude. The measurements were made over the Antarctic.

Wavelengths 760-770 nm had been removed from the radiative transfer model pixels because of an O$_2$ absorption line and therefore 760 nm seemed like a suitable wavelength limit. However, when the entire wavelength range from 280 or 300 nm to 800 nm was employed in the inversion, the outcome was very similar compared with the previous results (figure 7). Again only in seven cases out of 60 (scans 8744004-8744063) the results worsened compared to the Flittner result and the changes were not very significant. The residuals increased again in comparison with the original results (appendix A). The pixel map ranging from 300 nm to 800 nm is denoted by mod5.
On the whole, although enlarging the wavelength range generally improved the ozone profiles it also had some unwanted side effects: the residuals increased over the longer wavelengths and in some cases the density values of NO$_2$ augmented as well. Especially if the density values of NO$_2$ had originally been feasible despite the uncorrect ozone profiles, the improvement of the ozone and air profiles often resulted in a clear deterioration of the NO$_2$ profiles. An example of this phenomenon is seen in appendix A.

### 6.2. Using more than one pixel map

In the FMI inversion method it is also possible to use different pixel maps at different altitudes. However, there is one limitation: in order to calculate the transfer spectrum, all the selected wavelengths must be used at the reference altitude. The altitude range used in the inversion is from 70 km to 12 km. Since the visible region becomes more pronounced at lower altitudes, it seemed reasonable to try using two different pixel maps. At high altitudes the used inversion pixels encompassed the entire wavelength range and at lower altitudes only (a part of) the visible region. However, there proved to be a problem in this approach: the change of pixels maps often resulted in a jump or an angle in the ozone profile (and in the other profiles as well). This angle is pointed out in figure 10. Changing the altitude limit separating the two different pixel maps (e.g. from 20 or 30 km to 40 or 50 km) did not help but only changed the place of the problem.
The experiment was carried out with three different pixel maps below the selected altitude limit, containing the wavelengths longer than 400, 500 or 600 nm. Using the wavelength limit of 400 nm (figure 8) often resulted in better ozone profiles than the other limits. Compared with the original results, using only the visible wavelengths below a selected altitude limit helped to ameliorate the profiles of some divergent cases, as did using only the enlarged pixel map. When the wavelength limit was altered from 400 nm to 500 or 600 nm (figure 9), the ozone profiles often deteriorated: the number density values increased below 30 km. The density profiles of NO₂ and aerosols also degenerated.

Figure 8. The ozone profile and the relative difference while using the enlarged pixel map mod4 above 35 km and only the wavelengths longer than 400 nm below this altitude.
6.3. Using the ozone absorption bands

There are three major ozone absorption bands: the Hartley, Huggins and Chappuis bands. The Chappuis absorption band contains the wavelengths of light absorbed by ozone in the visible region, approximately from 450 nm to 800 nm. The Hartley and Huggins bands are responsible for absorbing and filtering the solar ultraviolet radiation. The Hartley band spans approximately from 240 nm to 300 nm and the Huggins band from 300 nm to 360 nm. Because the main aspiration was to retrieve ozone profiles, these ozone absorption bands would probably contain wavelengths useful in the inversion. [7]

At first the effects of each absorption band were tested separately. For the Chappuis and Hartley bands the results were of a completely wrong order of magnitude. For the Huggins band the profiles were somewhat better but the ozone density values deteriorated (i.e. increased or exploded) below 20 km.

Since using only small ranges of wavelengths had previously proved to be ineffective, the next step was to apply the following three combinations of the Chappuis and Huggins bands: 1. both the Chappuis and Huggins wavelengths, 2. at high altitudes both the Huggins and Chappuis bands and below the altitude limit (35 km) only the Chappuis band, and 3. at first only the Huggins wavelengths, between 50 and 26 km both the Huggins and Chappuis wavelengths and below 26 km the Chappuis
wavelengths (figure 10). Why these particular altitude limits were employed in the latter case becomes clearer in the next chapter. In total, this covered the spectral range 300 nm to 360 nm and 450 nm to 800 nm. But once again, the results were not promising: the ozone profiles did not improve at low altitudes compared with the results obtained from using an enlarged pixel map. Also the change of pixel maps resulted again in an angle in the ozone profile.

**Figure 10.** The ozone profile and the relative difference while using only the Huggins wavelengths above 50 km, both the Huggins and Chappuis wavelengths between 50 and 26 km, and the Chappuis wavelengths below 26 km. The second change of pixel maps resulted in a clear angle in the ozone profile.

### 6.4. Using the Flittner method wavelengths

We also followed the example set by the Canadian team whose method only uses a few pixels from the Chappuis and Huggins bands. In the Flittner algorithm, data over the range 10 km to 50 km is used for Chappuis retrievals and from 26 km to 66 km for Huggins retrievals. For Chappuis retrievals the method only uses pixels numbered 652, 826 and 998, corresponding to wavelengths approximately 532.2, 601.9 and 671.3 nm. In addition, three pixels around these centre pixels are averaged to reduce the noise. For Huggins retrievals the used pixels are 81, 107 and 206, corresponding to wavelengths 306.1, 316.2 and 355.0 nm (no averaging is used in this case). In this method, the reference altitude is the uppermost layer. [8]

Although in theory the minimum amount of pixels necessary for the inversion is the same as the number of retrieved gases, in reality the pixels used in the Flittner...
algorithm are not enough for the FMI inversion method. For instance, the order of magnitude of the inversion results for ozone was $10^{27}$ when it should be $10^{12}$. Therefore we tried using pixels from a range of 10 nm around the Flittner pixels (excluding the absorption and emission wavelengths of O$_2$, H$_2$O and [O$_2$]). However, this proved to be insufficient. For some scans the inversion results were again completely of the scale. There were also scans for which the results were sufficient but the density profiles did not improve or even worsened compared with the results obtained from employing the entire absorption bands.

The altitude limits that were used for the different pixel maps were the same as in the Flittner method: from 70 km to 50 km we employed the Huggins wavelengths, from 50 km to 26 both the Chappuis and Huggins wavelengths, and from 26 km to 12 km the Chappuis wavelengths. The maximum and minimum altitudes (75 km and 12 km) differ from those of the Flittner method (60 km and 10 km). While testing the Flittner method wavelengths, NO$_2$ was omitted from the list of species to be retrieved in the second peeling. Besides ozone air and aerosols must be retrieved in the FMI inversion method and so this was the closed we could get to imitating the Flittner method which only retrieves ozone profiles. [8]

7. Conclusions

When searching for suitable inversion wavelengths, the different approaches included removing the absorption and emission wavelengths of O$_2$, H$_2$O and [O$_2$]; enlarging the wavelength range; using different pixel maps at different altitudes; testing the wavelengths used in the Flittner method; and exploring the possibility of using the ozone absorption bands. The results of these experiments were somewhat disappointing: although enlarging the wavelength range helped to control some of the divergent ozone profiles, the maximum values of these profiles were still too high. The other approaches proved even less helpful. Although using only the visible region below a selected altitude limit helped to reduce divergence, the ozone profiles still deteriorated below 20 km. The change of pixel maps also usually resulted in an angle in the ozone profile. Using the Flittner method wavelengths or the entire ozone absorption bands did not help to decrease the maximum values of ozone.

Besides ozone profiles, NO$_2$ profiles also reveal that all is not as it should be: the order of magnitude of these profiles is often about $10^{10}$, which is ten times more than it should be according to climatology. The residuals and the $\chi^2$ values confirm that something is amiss. And although it was possible to reduce the $\chi^2$ values and the residuals by omitting more wavelengths, the (ozone) profiles did not show corresponding improvements. In fact, the ozone profiles often seemed to decline even further when the number of inversion wavelengths was reduced. Finding the suitable wavelengths for the inversion should, theoretically at least, result in correct density profiles and in very small residual and $\chi^2$ values. Contrary to the Flittner algorithm, the FMI inversion method requires a large number of wavelengths; and generally using a large amount of pixels yields the best results as opposed to using only small wavelength ranges or few scattered pixels.
As to what is the "right" pixel map for the inversion, there are no clear recommendations to make. If the ozone profiles were the only concern, the obvious suggestion would be to use an enlarged version of the original pixel map. The wavelength range could be from 280 or 300 nm to 760 nm or even up to 800 nm. But as it is, it is slightly doubtful whether the improvement in the ozone profiles is sufficient to compensate for the deterioration in the NO₂ profiles. All in all, we have come to the conclusion that it is not possible to solve the problems of the inversion results simply by finding the right inversion wavelengths. The fundamental problem lies elsewhere, possibly somewhere in the inversion code, in the radiative transfer model or perhaps in the Levenberg-Marquardt algorithm. When this work was completed in August, the problem with the inversion results still remained unresolved.
References


Appendix A

Results for scan number 8744008

The original inversion results for scan number 8744008.
The inversion results for scan number 8744008 when using the enlarged pixel map (mod4) ranging from approximately 300 nm to 760 nm.
The inversion results for scan number 8744008 when using the enlarged pixel map (mod5) ranging from approximately 300 nm to 800 nm.
The inversion results for scan number 8744008 when using

1. the entire enlarged pixel map (mod4) above 35 km
2. only the wavelengths longer than 400 nm below 35 km
The inversion results for scan number 8744008 when using

1. the entire enlarged pixel map (mod4) above 35 km
2. only the wavelengths longer than 600 nm below 35 km
The inversion results for scan number 8744008 when using

1. the Huggins wavelengths (300-360 nm) above 50 km
2. both the Huggins and Chappuis wavelengths from 50 km to 26 km
3. the Chappuis wavelengths (450-800 nm) below 26 km
Appendix B

Results for scan number 8744048

The original inversion results for scan number 8744048.
The radiative transfer model pixels and the various pixel maps used in the inversion.