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Influence of Vertical Resolution on the Validation of Atmospheric Chemistry Instruments

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Abstract

A large number of validation campaigns for atmospheric chemistry instruments are being carried out and more such studies will be performed in the future. The aims of validation are to confirm the accuracy and precision of the measurement of a new instrument. There are many factors that may deteriorate the validation results and one of them is the vertical resolution of instruments when using the profiles intercomparison approach. The influence from the vertical resolution can be eliminated by using the averaging kernel method but it is necessary to find the conditions for using the method. This study simulated the influence of vertical resolution for a certain curvature. The results show that both the curvature of a profile and the difference of vertical resolution between two instruments have positive correlation with the differences between their measurements. The quantitative estimations of influence for some practical vertical resolutions were obtained. The combined error of two instruments was defined as the criteria to judge the significance of influence. A case study based on the simulated results was demonstrated to show when the influence from the vertical resolution should be considered and when such influence can be omitted in order to avoid some unnecessary works in validation.

Keywords: Simulation, Validation, Vertical Resolution, Atmospheric Chemistry Instrument

1. Introduction

Limb-scanning remote-sounding atmospheric chemistry instruments onboard satellites are widely used to measure atmospheric parameters like the density of gases, temperature and pressure at different altitudes, thus forming profiles of parameters. For the validation of a new remote sounder, it is necessary to compare its measurements with the observations of other proved instruments at the same time and location. There are many factors that can deteriorate the validation results, for example, measuring different air masses because of atmospheric fluidity, the chemical reaction in the atmosphere, the different characteristics of instruments like the vertical and horizontal resolution, *etc.* [1,2]. The vertical resolution should be especially concerned during the validation for limb-scan remote sounders which usually present their output data with profile form of atmospheric parameters. **Figure 1** shows an intercomparison of temperature profiles during the validation for MIPAS/ENVISAT, Michelson Interferometer for Passive Atmospheric Sounding aboard the Environmental Satellite of European Space Agency [3,4] (this instrument is named MIPAS-E hereafter) by using the data from MIPAS-B — a remote sounder that is similar to MIPAS-E but aboard a large Balloon [5-7]. Both instruments adopted limb-sounding geometry and can measure tens of atmospheric parameters profiles like pressure and temperature profiles, mixing volume ratio profiles of O_3, H_2O, HNO_3, N_2O, CH_4 and NO_2 *etc.* within a short period of time. In the figure, the right panel gives the temperature profile of MIPAS-E with vertical resolution 3 km, the profile of the same parameter from MIPAS-B but with vertical resolution 1 km which is the nominal resolution of the instrument. An additional retrieved temperature profile from MIPAS-B with vertical resolution 3 km was also presented. The left panel gives the differences of profiles between MIPAS-E and MIPAS-B with vertical resolution 3 km, 1 km and its smoothed profile (details in section 3.3), respectively. The agreements between the MIPAS-E and MIPAS-B profiles are generally good in the whole altitude range of comparison. However, in the range of 169 - 126 hPa (11 - 15 km), the differences are obviously larger when using the MIPAS-B profile with vertical resolution 1 km than the differences when using another MIPAS-B profile with verti-

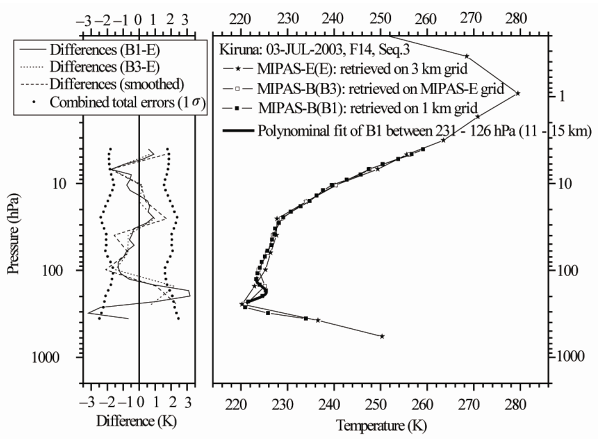

Figure 1. Intercomparison of temperature profiles between MIPAS/ENVISAT (MIPAS-E) and MIPAS-B [13] (Zhang, 2006).

cal resolution 3 km. This indicates that if the vertical resolution of an instrument used for validation is different from that of the instrument to be validated, the validation results may be incorrect. Therefore, the vertical resolution of all instruments that involved in validation should be equal in principle. However, because of the limitation of characteristics of each instrument, this requirement will not be always satisfied. In this case, for eliminating the influence due to vertical resolution, the method using averageing kernel matrix to smooth the profile with fine vertical resolution may be performed [8,9]. However, sometimes this step will not be carried out if the influence can be ignored based on empirical knowledge of validation [10-12]. However, this kind of empirical judgment is not always correct. Hence, it is worth to evaluate the condition that what difference of vertical resolution between the instruments involved in validation is acceptable or unacceptable since it is beneficial to scientist for reducing the computational burden, financial cost and saving time in validation.

2. Reasons of Vertical Resolution Influencing Validation

In general, the atmospheric parameters like temperature and density of gases are variables with respect to altitude. As a result, the profiles of atmospheric parameters are smoothly continuous curves which have different curvature at different level of altitude. However, instruments can only measure atmospheric parameters at certain altitude levels. Then the measured profiles form the broken lines as the temperature profiles shown in **Figure 1**. Vertical resolutions may be tens of meters (in situ measurement), several kilometers (limb-viewing remote sensing), and more than ten kilometers (nadir remote sensing).

In the validation when using a method of profiles intercomparison, the first step should be to interpolate all the profiles onto a defined vertical grid (represented by altitude levels or pressure levels) by using logarithm, or linear, or spline algorithms. The interpolation algorithm may introduce extra errors to the intercomparison and the errors have positive correlation to the difference of vertical resolution among the profiles. This is because that the profile which has rough vertical resolution can not resolve the fine structure of atmospheric parameter field. Obviously, if the profiles are straight lines, the extra errors disappear and the vertical resolution has no influence on intercomparisons. Therefore, in order to evaluate the errors introduced by the vertical grid, two factors should be considered simultaneously the vertical resolution and the curvature of profile.

3. Simulation and Results Analysis

3.1. Curvature in a Profile

In general, there are many different values of curvature for a profile of atmospheric parameters. See **Figure 1**, for the MIPAS-B measured temperature profile at 1 km vertical grid, between the height region 126 - 231 hPa, the profile has relative large curvatures, *i.e.* small radii of curvature comparing with the segments which are nearly straight lines in regions of 360 - 268 hPa, 109 - 28.6 hPa and 25 - 4 hPa. For performing simulation and assuming a segment of a profile, which represents the true values of an atmospheric parameter at different altitude levels, has a radius of curvature *r*. The arbitrary unit of atmospheric parameter is used without incur any wrong conclusion. Small *r* represents that the profile has fine structure. Further, it is assumed that all instruments that adopt different vertical grid measure the true value of atmospheric parameters. Some of atmospheric chemistry instruments used to adopt one of the following vertical resolutions [0.5, 1, 2, 3, 4, 5, 6] km. The choosed curvature radius of the profile for simulation should not be less than 1 km in order to ensure that at least two points can be extracted from the profile. In order to ensure that the simulation can be carried out for all the vertical resolutions just mentioned above, we choose a curve with a curvature radius 4 km to represent the true profile of an atmospheric parameter.

3.2. The Profile Number for Intercomparison

For validation of instruments, a definite conclusion should depend on statistical results of intercomparisons. **Figure 2** gives the simulation results for the influence of the number of profiles involved in intercomparison to the

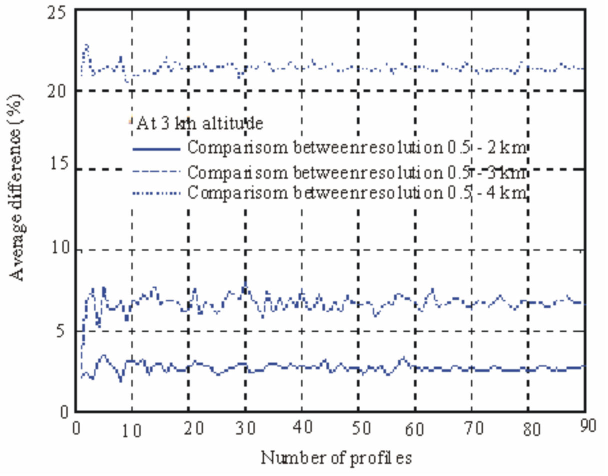

Figure 2. Influence of the profile number to the comparison between profiles with different vertical resolution.

comparison results, *i.e.* the measurement difference of a proved instrument and an unproved one. It is clear that the differences vary with the number of profiles especially when the number is less than 20. However, the differences approach a constant with the increasing of profile number. This actually indicates the changing trend of the standard error of comparison with the number of intercomparisons. Here, 70 simulated profiles will be used during the simulation comparisons.

3.3. Simulation Comparison

The simulation procedure includes the following steps. Firstly, let the curve $x = \sqrt{r^2 - (h-r)^2}$ ($0 \le h \le 2r$) represents the true profile of an atmospheric parameter. Here, h is the altitude, and r is the curvature radius. Parameter x has an arbitrary unit. Secondly, for each vertical grid given above, 70 profiles were produced by extracting a point from the true profile at each level of altitude. These 70 simulated profiles represent the measured profiles of an instrument without any errors. Thirdly, for each comparison, the values of the parameter at each level of altitude were calculated by interpolating all the profiles linearly into the vertical grid with the vertical resolution 0.5 km. Finally, the calculations for the average difference at each level of altitude in the comparison for the two kinds of profile were carried out. For eliminating the influence of the absolute value of parameter to conclusions, the average difference in percentage was used. The standard deviations of each average were also calculated to denote the dispersing extent of average difference.

There are many different combinations of intercomparison according to the given vertical resolutions. Here, the vertical resolutions which are frequently appeared during practical validation activities were considered. **Figure 3** shows the simulation results for the comparisons between vertical resolutions of 0.5 - 1 km, 0.5 - 2 km, 0.5 - 3 km, 0.5 - 4 km, 0.5 - 5 km, 0.5 - 6 km, and 1 - 3 km. The results clearly shows that the vertical resolution of instruments has influence on intercomparison, *i.e.* the differences of comparisons have positive correlation with the difference of vertical resolution between two kinds of profiles even if both instruments measured the true value of atmospheric parameters. The averaged standard deviation bars indicate that with increasing of difference of vertical resolution the precision of comparison decreases. This may lead to an underestimation of precision of an instrument. Even if the difference of vertical resolution is equal for each comparison (**Figure 4**), the influence to comparison is not the same. This is because the influence of vertical resolution is related with the curvature of the true profile. For a fixed curvature, the larger vertical resolution of instruments incurs larger differences between their measurements.

In fact, the true profile of any atmospheric parameter is unavailable. Fortunately, for most of the cases of validation, the profiles from those proved instruments have finer vertical resolution than the profiles from the instruments which need to be validated. Thus, these profiles with fine vertical resolution can be regarded as true profiles. The curvature of a profile can be deduced from the fitted curve of the profile. Generally, the curvature varies with point of the fitted curve. Therefore, the curvature of the curve (or a segment of curve) needs to be determined? For estimating the influence of vertical resolution, the averaged curvature of the curve (or a segment of a curve) can be regarded as the curvature of the whole curve. In **Figure 1**, the fitted curve of MIPAS-B temperature profile in the range of 11 - 15 km is a polynomial curve. And the averaged curvature radius of the curve around the peak point is about 1 km.

The criteria whether the influence of vertical resolution can be omitted depend on the measurement errors of two instruments which are involved in intercomparison. Assuming two instruments have measurement errors σ_1, σ_2, respectively, the combined error is

$$\sigma = \sqrt{\sigma_1^{\,2} + \sigma_2^{\,2}} \,. \tag{1}$$

If the differences of simulated comparison are larger than the combined errors, then the influence of vertical resolution to validation should not be neglected. **Figure 3** shows that the differences between profiles of vertical resolution 1 km and 3 km are 2 - 16% when the curvature radius is 4 km. This is just the case in terms of vertical resolution for the validation of MIPAS-E by using MIPAS-B data. In the range of 11 - 15 km, the maximum of the combined error of temperature differences between MIPAS-E and MIPAS-B is 1.7%. Since the curvature radius around the peak point of the fitted curve is about 1 km, the simulation can not be carried out because the interpolation algorithm is invalid for the MPAS-E profile which has a vertical resolution of 3 km (> 1 km). However, it is clear that the simulated differences in this case will be larger than 2 - 16% because the curvature radius 1 km is less than 4 km and it is definitely larger than the maximum of the combined error 1.7%. Therefore, in the range of 11 - 15 km, the results of direct comparison between the measurements of MIPAS-E and MIPAS-B（**Figure 1**） doesn't give the true differences of the measurements between the two instruments, *i.e.* the differences of comparison in 11 - 15 km may include significant contribution from the influence of vertical resolution. Therefore, for this case the influence of vertical resolution should be considered. For the segments of temperature profiles above 15 km and below 11 km, since their curvatures are very small, the influence of vertical resolution can be omitted.

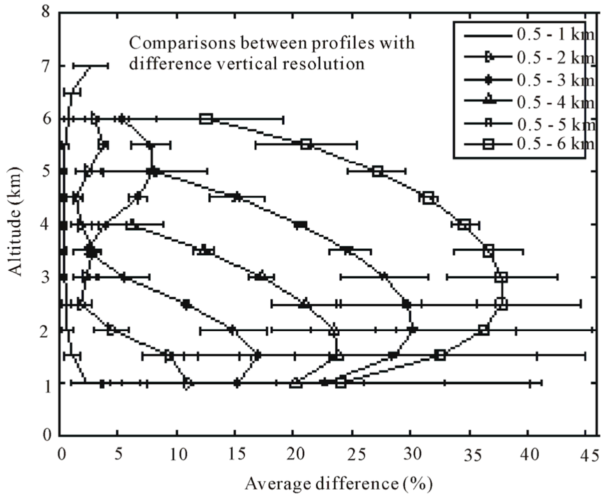

Figure 3. Simulated comparisons between two profiles with different vertical resolution.

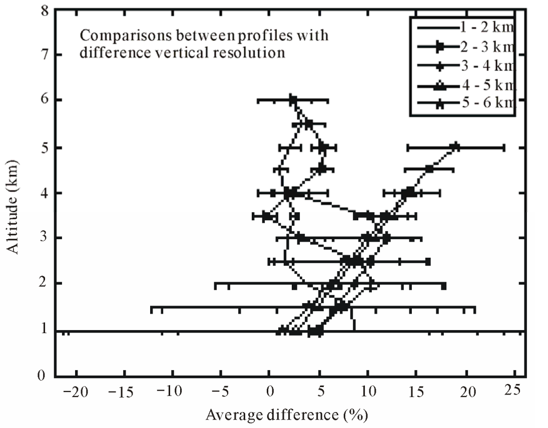

Figure 4. Simulated comparisons between two profiles with different vertical resolution where the difference of vertical resolution is equal for each comparison.

If the influence of vertical resolution can not be omitted and therefore direct comparison is unacceptable, the following two approaches for improving validation can be adopted. One is to retrieve the profiles of atmospheric parameter with the same vertical resolution for both instruments. As an example, the result from this kind of approach is shown in **Figure 1**. This approach, however, is often limited by the characteristics of instrument, retrieval algorithm, *etc.*, and not always feasible. The second approach is the method to use the averaging kernel. This approach was described by Rodgers and Connor [14]. Before performing the comparison, the profiles with higher vertical resolution need to be smoothed. If disregarding noise, the retrieved profile X_{re} is a weighted average of the "*true*" profile X_{true} and the a priori profile X_a in the form of

$$X_{re} = AX_{true} + (I - A)X_a, \tag{2}$$

where A is the averaging kernel matrix and I denotes the identity matrix. The higher-resolved profiles X_B of instrument B are smoothed by applying the averaging kernel matrix of the low-resolved profiles X_E of instrument E. And the profile smoothing is done by

$$\tilde{X}_B = A_E X_B + (I - A_E) X_{Ea}, \tag{4}$$

where X_{Ea} denotes the a priori profile of instrument E. Comparing equation (3) with equation (2), it is clear that $\tilde{X}_B$ is the result derived from the instrument E inverse mode, if X_B is assumed to be the true profile. Thus, in the difference of $\tilde{X}_B$ - X_E the contributions originating from different vertical resolution are reduced. **Figure 1** also presents the difference profile between smoothed MIPAS-B temperature and MIPAS-E measurements (for clarity, the smoothed MIPAS-B temperature profile was not plotted). Above 15 km and below 11 km, the difference profile is very close to the one of direct comparison. This indicates that the vertical resolution influences on the validation are very small and consistent with the simulation results mentioned here. However, the improvement of comparison between altitudes 11 - 15 km is obvious. It indicates that after adopting the averaging kernel approach to smoothing the higher-resolved MIPAS-B profile, the influence of vertical resolution to the comparisons was reduced.

4. Conclusions and Outlook

For the validation of an atmospheric chemistry instrument by comparison with the profiles from proved instruments, vertical resolution of profiles can deteriorate the validation results. The quantitative simulation results show the extent of deterioration due to the difference of vertical resolution between the profiles for comparison for a certain curvature of profile. The results also show that when the difference of vertical resolution is equal for each pair of comparison, the larger vertical resolutions have more influence on comparison for a given curvature. The influence of vertical resolution on a validation has to be considered if its caused difference is beyond the combined errors of two instruments. In general, this kind of influence can be eliminated or reduced by using the averaging kernel of profile with rough vertical resolution to smooth the profile with fine vertical resolution.

Since the number of validation activities will increase in the future, it is useful to simulate the influence of vertical resolution on validation for different combinations of vertical resolution and different curvatures of profile. Our next aim is to establish a database based on the complete simulation results. The database will be freely accessible for all scientists engaging in validation.

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