Interactive comment on "TomoSim: a tomographic simulator for DOAS" by Rui Valente de Almeida et al.

Anonymous Referee #1

The manuscript describes the development and some tests of evaluation software for a drone-based absorption spectroscopic (DOAS) instrument for the mapping of trace gas concentration fields on an area of about a square kilometre. The instrument is presently under design and construction, thus only model results are presented. The manuscript can be called a progress report. Since it contains a number of non-trivial pieces of information and interesting considerations it could be considered for publication in AMT.

However, there are many points in the manuscript which are extremely poorly explained and justified. In particular the geometric approach of the scattered-sunlight DOAS measurements is not clearly described. As this reviewer understands it the measurements are done in pairs with one spectrum taken at a point of a circle around the AOI serves as the measurement spectrum, while a second spectrum taken a point approximately

at the opposite side of the circle can serve as reference spectrum. From the ratio of both spectra the column density between both positions can be calculated, which would amount to a projection. Unfortunately this is not spelled out clearly in the manuscript and details of the observation geometry (pointing of the telescope at different positions around the circle) are lacking. There are no data on how long a series of measurements for a single sinogram would take to acquire and what kind of detection limits for trace gas concentrations could be expected. Therefore it is impossible to judge from the information given in the manuscript whether the approach is actually viable.

Regarding tomographic determination of atmospheric trace gas distributions there are a number of relevant publications which are not referenced in the manuscript. These include: Todd and Bhattacharyya, Appl. Opt. 36 (30), 7678 – 7688, 1997. Hashmonay et al., Atmos. Environ. 33, 267 – 274, 1998. Hartl et al., Atmos. Chem. Phys. 6, 847–861, 2006.

In addition, the input data of the model calculations are only vaguely described, also the assumed errors of the DOAS measurements are not given. In the plots describing the results (Figures 6 – 10) there are no coordinates and shading scales given. So the uncertainty of the reconstruction can not be judged.

Further points not discussed are: How many projections are actually required in order to produce a reconstruction with a given spatial resolution? A further problem in tomography are ambiguities, i.e. different distributions of absorbers can give the same set of projections, how is the situation here?

From the manuscript in its present form it is hardly possible to understand in detail what the authors actually studied and what the results are. In addition there are many inaccuracies and open questions in the manuscript, see numbered list below.

In summary: In view of the numerous problems with the manuscript I can not recommend publication.

1) Page 1, 'Introduction': The manuscript is lacking some introductory sentences placing the tomographic technique into context. After all, if drones are used anyway they could as well carry in-situ instrumentation directly measuring the concentration field. The authors should add a statement explaining what the advantages of their approach might be.

2) Page 1, lines 15, 16: What is FCT NOVA and why is it important that it is the 'oldest IT group in Portugal'?

3) In Fig. 2 the projection angles and the definition of variable t is missing.

4) Page 2, lines 1,2: what is the meaning of 'circular trajectories' and 'fan beam arrays'? This becomes only (somewhat) clear later in the manuscript, so these terms (and their meaning) should be explained here.

5) Page 2, line 9: The term 'tomographic phantom' should be explained here.

6) Page 2, line 11: what is the meaning of 'cost effective' in this context?

7) Page 2, lines 11-15: This text gives results and is not understandable at this point, it rather belongs into the results section.

8) Page 3, line 2: Probably the authors mean 'absorption cross section' here.

9) Page 3, line 5 (and several other occurrences throughout the manuscript): Platt and Stutz 2007 should read 'Platt and Stutz 2008'.

10) Page 3, line 7: Which quantity shows 'little variability'?

11) Page 3, lines 11, 12: The statement that 'DOAS measures the difference in absorption at two different wavelengths' is not correct (see also different explanation on page 4, lines 17-18). DOAS rather measures the amplitude of absorption structures, which are measured at many different wavelengths.

12) Page 3, lines 18-19 and 24: The statement about the 'light path not known' needs

to be made only once.

13) Page 3, Eq. (3): The boundaries of the integration need to be given.

14) Page 4, line 1: It is stated that 'A(...) denotes the fraction of light that gets scattered into the detector'. This is unclear and probably incorrect. Which fraction is referred to? Fraction of total amount of radiation reaching Earth? Is A(...) not rather a normalizing factor?

15) Page 4, Eq. (5): Bounds of integration are missing.

16) Page 4, lines 15, 16: Grammar of the sentence is wrong.

17) Page 4, Eq. (6): What are Iref and Aref?.

18) Page 4, lines 21-26: The polynomial (or generally high-pass filtering) is also a feature of DOAS. The determination of the polynomial coefficients requires a linear least squares fit (a polynomial is a linear function of its coefficients), which can be determined analytically, a nonlinear procedure (like Levenberg-Marquard) is not necessary.

18) Page 5, lines 10, 11: The line integrals was already explained above (Eq. 5), delete sentence here.

19) Page 5, line 13: The matrix needs a thorough explanation, in particular since the reconstruction methods 'revolve around this matrix'. For instance: What are rows and columns? Also, 'detector' should probably read 'detector number'

20) Page 5, Eq. (7) and its explanation: This is very difficult to understand fort the reader, in particular since the coordinates X and Y are not given in Figures 1 and 2 (or any other Fig.). Probably a sketch of the geometry showing X1, X2, X1, ... would be very helpful here.

21) Page 6, 'Algorithm I': Is this a Table?

22) Page 6, lines 6-10: Neither the mentioned projection angles nor the parameter

't' are given in Figures 1, 2.

23) Page 6, line 18: The 'Fourier slice theorem' needs a literature reference.

24) Page 6, lines 21-23: Why are the images distorted and in which way and why only by chance? How are the projections weighted?

25) Page 7, fig. 1, 2: Angles are not given, coordinate system is not labelled.

26) Page 7, lines 3-6: The re-mapping of rays from a fan beam projection to a parallel projection needs to be explained better. Perhaps a sketch could help.

27) Page 7, line 8: What is iterated in an 'iterative algorithm'?

28) Page 7, lines 9-11: The description of the matrix needs to come earlier, see point 19), above.

27) Page 7, line 14: Define 'row' and 'column'

28) Page 8, lines 4-7: Is this treatise of the history actually needed in this publication?

29) Page 8, line 8: What is the meaning of 'exceedingly large'?

30) Page 8, Eq. (9): The meaning of pj and g(k) in the equation is not explained.

31) Page 8, line 24ff: NBP is not explained. Where is the RSNG coming from in this study where no measurements were made?

32) Page 9, section 2.3: What is the relevance of the Shepp-Logan Phantom in this context? Unlike the situation in biological objects in the atmosphere steep gradients in density are rare.

33) Page 9, section 2.4: Part of this information is already given in the introduction. The authors of this manuscript may also find relevant information in Hartl et al. 2006 (Atmos. Chem. Phys., 6, 847–861, 2006).

34) Page 10, 1st sentence of section 3.1: This sentence belongs in the introduction.

35) Page 10, line 27: A positioning error of 2 arc seconds (about 0.0006 degrees) appears extremely small, where does this figure come from?

36) Page 10, line 28: Probably 2048 spectral channels is meant here.

37) Page 11, line 9 and Fig. 5: The angular interval (Delta) is not shown in Fig. 5 (just a few 'Delta' symbols are shown).

38) Page 11, lines 11, 12: The elevation of the observation is not given. In which direction does the instrument look, to the ground to the sky or horizontal?

39) Page 11, lines 19, 20 and Figure 5: The location of the 'ROI' is not clear from Fig. 5. Also the points A, B and distance AB are not given.

40) Fig. 6: What is the meaning of the colour shades? Scales are missing.

41) Table 1: What are the units of C0, X0, Y0, a, b, and angle?

42) Section 3.4: The size of the pixels is given (1m x 1m), but not the angular interval (Delta).

43) Figure 7: All scales are missing (ordinate, abscissa, and colour scale).

44) Figure 9: Since the intensity scale is missing it is impossible to judge the error of the reconstruction.

45) Page 16, line 2ff: It is stated that the '. . . number of projections was adequate . . .'. What actually was the number of projections used? Different values are given in the text. By which standards is 'adequate' defined?

46) Page 22, line 30ff: Reference to Laepple et al. 2004 should be replaced by the final version: 'Atmos. Chem. Phys. 4, 1323–1342, 2004'.