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Atmospheric Measurement Techniques Discussions

Interactive comment on "Particle Loss Calculator – a new software tool for the assessment of the performance of aerosol inlet systems" *by* S.-L. von der Weiden et al.

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We thank the reviewers for their detailed and useful comments on the manuscript. We have attempted to improve the paper by implementing the given suggestions. In the following we respond to the individual detailed comments and describe their realization.

Comments on the review by C. Twohy:

General Comments

This describes a useful new tool for quickly calculating expected passing efficiencies of particles through different inlet and tubing geometries. The program uses standard

equations not only to calculate losses in existing geometries, but also can be used as a tool to aid in design of new measurement systems. This should be a valuable community resource that extends the Excel-based "Aerosol Calculator" that has been available for a number of years. This paper describes the equations used in the "Particle Loss Calculator," how to use the program, and some validation of its performance. Overall the document is well written and appropriate; below are minor specific suggestions to fine-tune it.

Specific Comments

p. 1102, lines 10-11. As it is not specified, I suggest noting here and on the download page that this is an IGOR program, and IGOR is necessary to run it. Also it would be useful to note on the download page that users can get a free IGOR trial on the Wavemetrics website.

We mentioned the necessity of IGOR Pro and the link to the free IGOR Pro trial on www.wavemetrics.com in the paper as well as on the download page.

p. 1103, line 8: Most equations are only valid for a specific range of conditions which, while usually described in this paper, are not readily apparent when running the PLC program. A desirable upgrade would be to include pop-up windows that alert the user whenever the conditions are violated (for example, when a critical Re or Stk is exceeded). This is not required for publication; just a suggestion for future improvement.

We agree with the reviewers suggestion that it is useful to specify which values and equations violate the validity conditions. This upgrade will be included in the Particle Loss Calculator as soon as possible. At the moment the exceeding of the range of validity in the calculation is only marked by a dashed instead of a solid line in the output graph (see Section 3.1). We added a table containing all implemented sampling and transport effect parameterizations and their range of validity to Supplement 1.

Equation 1: I think it would be clearer, and less redundant, if this initial equation just *defined inlet efficiency as the product of sampling efficiency and transport efficiency. The latter two quantities are already defined separately as Equations 2 and 19.*

We reduced this equation to the product of the sampling and the transport efficiency as suggested.

p. 1103, line 19: I found the implementation of particle size, dp, a little confusing. Here it is defined as just "size", while on line 9 of p. 1104 it is "aerodynamic diameter". In the program, it seems to be physical diameter, since the particle density is a chosen quantity. Please clarify and use appropriate symbols throughout.

We clarified, that "d_a" is the aerodynamic particle diameter, which is the quantity that characterizes the particle size in our calculations. In the program the aerodynamic particle diameter is used for all calculations. However, if the user sets the particle density to the standard density of 1 $\mathrm{g\,cm^{-3}}$, the aerodynamic diameter equals the physical diameter d_{phys} of the particles. This notation is now used consistently in the text.

p. 1103, line 19. "Efficiency" should be defined here at the beginning. Also, the later definitions of efficiency are inconsistent–on p. 1105 it is given in terms of "concentration", on p. 1107 in terms of "number density" and on p. 1107 and 1122, in terms of "number". Suggest using "number concentration" or "number density" consistently throughout.

We added the definition of "efficiency" at the beginning of section 2.1 and modified all further definitions of efficiency using “number concentration” to be consistent throughout the paper.

p. 1105, line 3: Something should be said about the "sampling in moving air" conditions for which the equations are likely to be invalid–for example during high-speed aircraft sampling.

We added the advice, that the PLC should not be used for wind speeds U_0 much larger than 30 $\mathrm{m\,s^{-1}}$. This velocity is a suggestion, there are no commonly agreed guidelines

for sampling in moving air conditions.

p. 1105, line 23: Move (Stevens 1986) to the end of the equation.

We moved this reference to the end of the equation.

p. 1106, line 16: Perhaps the dynamic shape factor should be defined, or at least the reference given later (Seinfeld and Pandis) should be included here.

We included the reference "Baron and Willeke, 2005" for the dynamic shape factor here.

p. 1107, line 10: A quantitative definition of thin vs. thick walled probes would be useful here.

We added the definition of a thin-walled sampling probe from "Belyaev and Levin, 1972".

p. 1107, elsewhere: A single figure showing all the different angles invoked (angle of inclination, aspiration angle, angle corresponding to the vertical, and half-angle), while not essential, would be valuable.

We added two figures to Supplement 1 showing all angles invoked.

p. 1109, line 21-22: It would be appropriate to mention here that there is an option in the program to extend the laminar equations through the transition regime.

We we added information on this option of the Particle Loss Calculator to the text.

p. 1112, Eqn 27: Is this valid over the full Re range? Also, in section 2.3.6, wouldn't the half angle for eddy formation also depend on Re?

We added the information, that Eq 27 (now Eq 28) is valid in the turbulent flow regime up to a Reynolds Number of 15600 to the text. Particle loss caused by eddy formation in tube enlargements is difficult to determine mathematically. In the common literature only general advices can be found how to avoid losses in enlargements. One of these experiential advices given by Schade and Kunz (1989) is to reduce the half-angle below 4°. They give no information about a dependence on Re. The general advice is to experimentally determine occurring particle losses if it is not possible to avoid an enlargement in an inlet system.

p. 1112, section 2.3.4: Are these completely independent of the radius of curvature? If not, the applicable range should be specified.

We added the information to the text that the effect of the curvature ratio (R_0) is insignificant for R_0 between 5 and 30. We also added a definition of the curvature ratio R_0.

p. 1114, lines 13-15: This statement should have a reference.

We did several calculations including different temperature gradients and air thermal conductivities to estimate the influence of thermophoresis. The conclusion is that this process is negligible for ambient aerosol particles, if the temperature gradient is smaller than 40 K.

p. 1115, line 5: Who has this been confirmed by? The authors?

We confirmed this by calculating the magnitude of coagulation for several particle number concentrations and residence times.

p. 1116, section 3: I think the paper would read better if this introductory section (through approximately line 22 on p. 1117) was moved up, before the equation details currently given in Section 2.

We moved up this introductory section to Section 2 before the part where the equation details are given.

p. 1117, line 5: Delete "to" before "preferable". Line 11: I believe "emitted" should be "omitted".

We corrected these typos.

p. 1118-1120: This is a nice discussion of the working details of the program, and the ability of the user to select various options should be quite useful. If this is to be a community resource, I would suggest that the download page also have a link for comments or corrections to be submitted to the authors.

As soon as possible, we will add to the download page the option to submit comments or corrections to the authors. At the moment comments can be sent by e-mail to the first author. The e-mail address is given in the paper.

p. 1123, line 6: Delete or change the word "widespread", which seems vague. Line 13: what do you mean by "partial" sedimentation?

We changed "widespread" to "large"; the range of the size dependent discrepancy is given later in the same sentence. We changed "partial sedimentation" to "to some extent sedimentation" to make clearer what is meant.

p. 1124, lines 7-9: There is something wrong with the grammar here–as written, it indicates that you do NOT recommend that inlet designs be kept simple.

We rephrased this sentence.

Fig. 2: It would be useful if the symbols used in the equations for the various Sampling and Tubing Parameters were included in the two boxes at the top of the figure.

We added the symbols used for the sampling and tubing parameters to the green input boxes at the top of Figure 2.

Comments on the review by J. C. Wilson:

The authors have presented a description of a Particle Loss Calculator (PLC) that facilitates the analysis of particle losses in sampling and transmission to instruments. The objective is to provide a tool to those utilizing sampling and transport systems while making aerosol measurements. The PLC permits users to quantitatively evaluate the losses of particles in sampling and transport systems. They also present experimental *data acquired in lab measurements of particle penetration through various transport geometries which they then compare to the output of the PLC. The comparison is presented as a validation of the PLC. In my opinion this manuscript is appropriate for publication in AMTD. The tool that is presented here will be of use to those designing sampling and transport systems. The review criteria for AMTD ask: "Does the manuscript represent a substantial contribution to scientific progress within the scope of Atmospheric Measurement Techniques (sub- stantial new concepts, ideas, methods, or data)?" I am unaware of other compilations of the literature results that facilitate the calculation of end-to-end losses in a sampling system. Substantial new results concerning sampling and transport are not presented here, but the method presented will assist members of the aerosol community. (I have collaborated with one of the co-authors, but decided that the conflict of interest require- ment, #5 in Reviewers Obligations, is met in this case and that this collaboration does not bias my judgment.)*

The following comments are indented to aid the authors in improving the manuscript.

1) The introduction states that the PLC addresses conditions typical of ground based sampling. But this qualification is not specific enough. This might be dealt with by adding the qualification "through a constant-diameter tube" to the description of the sampling cases covered by the PLC (Intro and lines 16 and 17 of page 1117). This would help the user avoid the temptation of applying the PLC to other types of inlet geometries such as shrouded or diffusing inlets.

We added the information to the manuscript, that the PLC is only applicable for constant-diameter sampling probes.

2) Although CFD calculations of particle loss are not the subject of this paper, the authors offer some opinions concerning the usefulness of such calculations. And they leave the reader with the impression that CFD calculations might in fact be superior to the relations used in the PLC. I suggest that those comments be dropped. In fact, CFD calculations of turbulent sampling or turbulent transport are often not reliable (Tian,

L. and G. Ahmadi, 2007. Particle deposition in turbulent duct flows - comparisons of different model predictions. J. Aerosol Sci. 38:377-397.) But many of the relationships used in the PLC capture the impact of turbulence since they describe the results of experiments done with turbulent flows.

We cited "Tian and Ahmadi, 2006" to show, that CFD calculations of turbulent effects on particle sampling and transport are often not reliable. We mentioned, that the equations implemented in the PLC are the results of experiments with turbulent flows and therefore are likely more reliable for those conditions.

3) The text lists many relationships used to calculate losses and provides conditions under which the relationships are valid. To help the user avoid misuse of the relationships, it might be helpful to tabulate the mechanisms treated with the range of validity for each one. (Or the software could issue a warning if the parameters entered are outside of the validated range.)

In the current state the software warns the user that the calculations are not within the validity range by plotting the output graph with a dashed instead of a solid line. This information is given in Section 3.1. If the experience shows that this warning is too weak and contains too little information we will add additional warnings to the software containing details about the values and equations, which are not valid. Furthermore, we added a table to Supplement 1 containing the range of validity for all implemented mechanisms.

4) Many aerosol sampling and transport systems use flow splitters. Losses in flow splitters have been studied and are not mentioned: Gupta, R. and A. R. McFarland. 2001. Experimental study of aerosol deposition in flow splitters with turbulent flow, Aerosol Sci. Technol. 34: 216–226.

We are aware of the large number of studies performed to investigate particle loss in a variety of inlet elements under most different sampling and transport conditions. The PLC will continuously be further developed to improve the already available functions.

Furthermore, we indent to implement more features to extend the applicability of this software to additional inlet elements. Aerosol deposition in flow splitters and sampling with blunt samplers, for example, are two options, which can be included in the PLC. We are thankful for any feedback on how to improve the PLC. We added to the conclusion of this paper, that the PLC is software under continuous development and ideas for its improvement are welcome.

5) The claim that the reported measurements validate the accuracy of the PLC is not justified and should be dropped. (a) The accuracy of the PLC depends on the accuracy of the primary literature which is compiled in the PLC. Note that figure 5 shows calculations of loss that are outside of the error bars of the measurements, but the text claims consistency of the measurements and calculations. The text does not present a careful discussion of accuracy. The only possible discussion of accuracy would be to state the accuracies found in the primary literature describing the formulas that are used. The functionality of the PLC is demonstrated in some interesting cases and those results are informative, so I am not suggesting that the results be eliminated from the paper. (b) the ranges of variable values and geometries that have been tested are small compared to the ranges to which the PLC might be applied.

We agree that the described measurements do not validate the accuracy of the PLC. We changed our statement to express that we only validated the functionality and practicability or applicability of the software. As mentioned by the reviewer the accuracy is limited by the implemented formulas and is not easy to determine with appropriate efforts. The number and variety of tested cases is indeed small. However, we think the presented examples demonstrate that the PLC can be used to estimate occurring particle losses for commonly used aerosol inlet systems. Recently, we got some feedback from Dan Dodier (Application Engineering Manager, Particle Measuring Systems, Boulder, Colorado USA). He compared the results of the PLC to empirical data for particle losses through straight tubing and found consistence for most conditions. (The discrepancy for large particles mainly caused by particle re-entrainment is now

also discussed in Section 2.3.7.) So we are assured that the PLC can be used for a large variety of (not too extreme) aerosol inlets, even beyond the tested and presented geometries and conditions.

6) The authors might wish to address the accuracy of the calculations done in the PLC. As stated in 5) these comments would be based on the primary literature. Would the authors suggest that users apply corrections to measurements based upon on calculated losses in sampling and transport? (For example, would they recommend dividing measurements by the sampling efficiencies shown by green line in figure 7 in a case where the line described the performance of the transport system?) Or would the authors only recommend that the PLC be used to avoid large losses such as are presented in figure 6 for particles larger than 6 microns by altering the design of the system? I recommend the second strategy over the first.

We think that the PLC is on the one hand a tool to optimize new and also existing inlet systems. Sources of large particle loss can be identified and the quality of an inlet system can be characterized using this tool. On the other hand it is also possible to correct measurement data by applying the PLC results. Of course there is a certain range of uncertainty of the calculated results which will then be included in the resulting data. However, for an estimation of the error of measurement data caused by particle loss the calculated results are suitable. A correction of data by multiplying with the calculated efficiency can be done if the user keeps in mind that this estimated correction factor has an uncertainty and it is not an exact factor.

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