

First and foremost, we would like to express our sincere gratitude to the two anonymous reviewers, whose extremely insightful feedback has enabled us to significantly improve this study. Below, we address each of the reviewers' comments. We hope that we have adequately addressed their comments and successfully incorporated the suggested improvements into the manuscript. For better readability, additions or changes to the manuscript text that address the reviewers' comments are written/highlighted in red.

RC1

It would be beneficial to include a table summarizing the boundary conditions applied to various surfaces of the computational domain (e.g., inlet, outlet, freestream, wall). Such a table provides clarity and helps the reader quickly grasp the simulation setup, especially when dealing with complex geometries or multiple flow regimes.

AC: We agree, a newly included table (Table 2) summarizes the boundary conditions applied to the surfaces of the calculation domain and is further illustrated in Figure 3.

While the use of a global Knudsen number is standard practice, it may obscure important local variations that are crucial in assessing the applicability of continuum-based or rarefied flow models. I suggest the inclusion of a figure illustrating the local Knudsen number distribution across the computational domain. This would serve as a more comprehensive diagnostic tool, offering insight into whether the flow remains within acceptable continuum or transitional limits throughout the domain, rather than only in an averaged sense.

AC: We agree with this important comment and have depicted the spatial distribution of the Kn -field near the instrument module in the new Figure 2 of the revised manuscript. Based on this, we also added discussions on the apparent flow regime based on the presented Kn -distribution. A discussion is implied about the appropriateness of the continuum modelling for our investigations including its extension via advanced approaches for slip-velocity boundary conditions to represent the slip- and the lower edge of transitional region (while global $Kn \approx 0.1$), see the beginning of Section 3.1, lines 167-199. Accordingly, we have extended our simulation model by (conventional) slip-velocity boundary conditions of the first and second order on the instrument module surface and present a sensitivity study w.r. to the boundary condition applied in the Appendix B, see also our further replies to the reviewer RC2.

These additions would not only enhance the scientific completeness of the manuscript but also assist readers and reviewers in better understanding the flow regime and the validity of the numerical approach.

In conclusion, I believe the manuscript is suitable for publication pending minor revisions as suggested above.

AC: We thank the anonymous referee for the valuable suggestion and the positive feedback.

RC2

General comments

[...]

The scientific quality of the work overall is fair, and although the introduction is of good quality, providing a solid overview of the current understanding of MSPs and NLCs and a good motivation, both verified by high-quality citations, the methodological, the results and the

conclusion parts need some substantial improvements. This, especially, applies to the structure, the choice to perform continuum simulations (e.g., the choice of the wall boundary model), the assumptions made for the particle tracking, its implementation and the discussions of how these considerations may influence the final results.

The form of presentation at the beginning of the manuscript is very convincing, with a decrease in quality (in terms of content and structure) at the end of the article.

AC: We would like to thank the second anonymous reviewer for the thorough and candid discussion of the critical aspects of the submitted manuscript, most of which we agree with and address in the revised version. We hope that the revisions we have made concerning

- the structure of the paper,
- the fluid wall boundary conditions taking into account prevailing flow regimes and ranges of Knudsen number,
- the robustness of our extended continuous simulation approach by comparisons of several surface boundary conditions available in Appendix B,
- the assumptions for particle properties and
- the revised discussion of our recent findings achieved

adequately address the concerns raised.

Specific comments

Before posting comments on the single sections of the manuscript, general comments on the outline of this manuscript: 1.) Avoid singular subsections. 2.) The article's outline misses a discussion section and has two conclusion sections ("4. Results and Conclusion" and "5. Final conclusions").

AC: Concerning 1) and 2), we agree and corrections are applied as suggested. Discussion and results are joined in Section 4.

1. Introduction:

This part is well written, with a good choice of references.

L35: NLC were measured by optical instruments (lidar, camera) not radar. The radar phenomenon related to ice crystals are called ((P)MSE, Polar Mesosphere Summer Echoes). Similar radar echoes in winter (PMWE, Polar Mesosphere Winter Echoes) involving tiny MSPs. See e.g., Latteck et al., 2021 (<https://doi.org/10.1016/j.jastp.2021.105576>); Staszak et al., 2021 (<https://doi.org/10.1016/j.jastp.2021.105559>)

AC: We agree and corrected the text accordingly.

L37: "b) particle [...] size distribution and c) shape, [...]" – Consider adding Asmus et al., 2017 (<https://doi.org/10.5194/angeo-35-979-2017>) and Kiliani et al., 2015 (<https://doi.org/10.5194/acp-15-12897-2015>) for reference.

AC: The suggested references are added.

L46/47: Referencing to comparable works does not motivate the work further. Consider demarcating this work from the work by Pineau et al., by the different design, etc.

AC: That's right – we rephrased the manuscript accordingly (see lines 54-58).

L47ff.: Here the goals of the work were mentioned: "analyses have the potential to provide information on whether MSP are involved in the processes of NLC formation", "provide

information on the morphology, size, and the chemical composition of the MSP.”, “sampling optimization” – Proof in your conclusions, if these goals have been reached.

AC: The text of the initially submitted manuscript states in one sentence: “The goal of this study is a proof of concept in the development process of a rocket-borne apparatus to sample NLC particles and embedded IN”, which was, in fact, the goal of the article presented and still is. In the revised version of the manuscript, more detailed explanations are provided immediately at line 53ff. Furthermore, the text has been supplied by references at the point (line 60ff), while their absence apparently caused a misunderstanding. The text is refined in that the analytical method is, in principle, capable of revealing physico-chemical properties of sampled particles (references are added). However, since the article does not discuss real in-flight particle samples and subsequent analyses, this cannot be the goal of the study; therefore, no proof is to be found in the conclusions to follow the reviewer’s request.

L58f: “where the presence of mesospheric ice particles during the rocket flight is ensured via back scattered radar sign” There might be radar echoes (occasionally in summer) that are not related to ice particles. (see Latteck et al.)

AC: We agree and have rephrased this statement by using the term ‘remote sensing techniques’.

L60: Not sure what this means: “stabilized against rolling” Do you mean de-spinned? Or spin stabilized? Using standard terminology makes this easier understandable (whole text).

AC: The word “stabilized” herein is used in a more general manner meaning there is a system, which is part of the rocket's support unit to prevent the vehicle from rolling around its longitudinal axis. This system is a so called rate control system based on the use of cold gas (compressed N₂). It is needed for the coast phase between booster stage burn out and HAS upper stage ignition as well as during the complete HAS upper stage burn, in order to support the thrust vector system. In contrast to usual atmospheric sounding rocket payloads a spinning payload would be a problem for a proper function of the thrust vector system needed for a hovering vehicle. However the detailed design of the HAS vehicle is not part of this paper, for more details, please refer to Naumann et al., 2020. The text is rephrased.

2. Instrument Design:

L70ff: Referencing to Figure 2: Which instruments were placed on the main deck? Or are these just mock-ups?

AC: For clarification, specific details and references are included in the revised text in latter part of paragraph 3.1. and the Fig 4 in revised manuscript.

L76: This is an interesting/critical part of the instrument design. It would be great to read more details to the design of the sealing mechanism.

AC: This is indeed a critical part of the instrument for sample preservation and conservation, but it is not part of the basic concept presented here regarding the effectiveness of particle collection in connection with the HAS carrier. Technical details of the instrument mechanics will be subject of a companion paper.

L94: Consider using AoA (angle of attack) term instead of attitude, as we are interested in the free stream velocity vector. (Whole text)

AC: We followed the suggestion and changed the text accordingly.

3. Numerical Simulations:

L109f: What about electro static forces? MSPs and NLC ice particles are part of the D-region plasma, and a substantial amount is likely to be charged. A comment to the expected forces, or the limitations of pure neutral simulations would be helpful.

AC: We thank the reviewer for this hint and have applied some considerations about electrostatic forces and charges of particles in the text of Section 3 in the revised manuscript, see lines 129-155.

L118ff: Dongari and Agrawal (2012) present an advanced version of a second order slip-boundary condition, not a “conventional slip boundary condition[s]” as is stated here. Further, your Fig. 6 suggest that a no-slip (with $u_{\text{wall}}=0$) was applied.

AC: We are grateful to the reviewer for this comment helping us to improve our modelling setting towards more realistic conditions. In our original study indeed the non-slip boundary condition was applied on the surfaces of instrument module and on the substrate mounts aof the SPICE booms. Based on this, the thickness of the boundary layer was investigated via a simulation-based velocity increase from zero value on the module surface (non-slip regime) to the fully developed free stream velocity on Fig. 8 (former Fig. 6). Indeed, the non-slip is an appropriate boundary condition to account for surface friction by viscous forces in continuum modeling of a dense fluid with nonzero viscosity, which is however arguable or even not appropriate assumption in the mesosphere conditions studied. Therefore, we validate the local Knudsen number to illustrate in detail the flow regime around the instrument module and the SPICE booms in the new Figure 2, and we add a new paragraph in Section 3.1, see lines 167-199 to discuss the necessary extensions of continuous flow models; see also further details in our response to the second point raised by reviewer comment RC 1.

Based on the new Fig. 2 we agree with the reviewer 2 concerning the necessity of slip flow regime modelling, especially for the representation of the upstream areas of the collection booms. Note that here the assumption of continuum regime is not affected, since here applies: $Kn < 0.1$. On the other hand, transitional regions are situated above and downstream of the substrate mounts and do not prevail upstream of the relevant impaction surfaces with substrate mounts, therefore do not affect the particle collection process. Moreover, as in the new parts of Section 3.1 argued, based on results presented in cited works, for regions upstream to the substrate mounts (which are relevant for the impaction surfaces), the continuous modeling in slip flow regime ($Kn \approx 0.04$) with conventional second order slip-velocity boundary conditions represents the measurements well. Accordingly, and in the view of reviewer's comment, we have extended our simulation model by the (convectional) first- and second order slip-velocity boundary conditions on the instrument module's surface, see Table 2. Moreover, we present a comparative **sensitivity study** for the velocity profiles ambient to the surface w.r. to the three boundary condition applied. The results on the velocity patterns are summarized in Appendix B and confirm, that imposing non-slip boundary conditions results, as expected, in lower speeds near the impaction surfaces, which potentially leads to fewer particle collisions due to lower inertia forces. This is also confirmed by the repeated particle tracing simulations and the particle impaction validations presented in the new Figure 13, compared for slip-velocity boundary conditions of second order (‘svbc’) and non-slip boundary conditions (‘nsbc’). Indeed, the slip-velocity boundary conditions (of the 1st or 2nd order), compare Fig. B4 in Appendix B, favor particle impacts due to higher inertia and even leads to a higher impact efficiency, as the new results in Fig. 13 confirm. The marginal differences in the velocity profiles along the chosen cut-lines or in surface distribution presented in Figs. B2, B3, B4, by imposing slip-velocity boundary condition of 1st order (formula B1) and of 2nd order (formula B2) are in accordance with the prevalent upstream slip-flow regime and low Kn . This suggests that

no advanced approaches to continuous modeling of boundary layers are required as it is the case when transitional fluid regime is prevalent, e.g. approaches based on the (effective) mean free path and effective viscosity under the 2nd order slip-velocity boundary condition, as investigated in Dongari and Agrawal (2012).

In addition, a new paragraph is added at the beginning of Section 4.1 (see lines 357–369) to comment on the surface boundary conditions imposed in the results of Section 4, and to highlight the relatively low effect by considered slip or non-slip boundary conditions on the thickness of the boundary layer, necessary for the development of the near free stream velocity in our settings. Lines 417–424 expand on this argument relating to comparisons presented in Appendix B on velocity profiles in the boundary layer above the head plate of a substrate mount. Below, in lines 441–451 of section 4.2 we also refer to results on the boundary layer, analogous to Fig.10, computed for slip-velocity boundary condition and their direct comparison to the non-slip regime by depicting the difference between the two velocity fields. This again confirms, that the boundary conditions applied do not significantly affect the identified thickness of boundary layer around the fuselage of the instrument module.

L127ff: The fact, that the simulations are done at the edge of conventional continuum mechanics and the huge errors of the field quantities mentioned here, need more investigations on the expected influence of the results (sensitivity study). Ultimately, this would to add robustness to this study and make the reader trust in the results.

AC:Based on the low local Knudsen number upstream the collection surfaces presented in the added Fig 2, we provide support concerning the appropriateness of our continuum mechanics modeling for slip to lower transitional regime in our settings to represent the areas of interest upstream the collection booms, whereas transitional regimes and the critical ‘edge of the continuum mechanics’ is present in the less relevant zones, e.g., in the slipstream zones to the impaction booms. From our perspective, this puts the reviewer's objection and the necessity of different (molecular kinetic or advanced macroscopic) approaches for transient modelling into perspective. We have extended the text of section 3.1, see lines 165-199, relating to this perspective. Moreover, since the air density and pressure values are marginal in mesosphere, the absolute deviations associated with the relative errors of the mentioned fields may not be significant in our study.

In accordance with the reviewer's comments and the cited results concerning extended continuous modelling for slip and lower transitional regimes we expanded our numerical study with regard to the slip-velocity boundary conditions considered, see the Table 2. We conducted a new comparative flow and particle simulations to provide a sensitivity analysis w.r. to the surface boundary condition in Appendix B and its impact on particle impaction efficiency in new lines of Section 4.4. We believe that in the revised manuscript we have **demonstrated the robustness** of our continuous modelling approach based on the presented effects on the speed profiles and patterns, as visible in Appendix B, see also above answers and new passages in Sections 3 and 4. The effect of differences in the near surface impact velocity profiles are however notable in the higher impact efficiency of particle collections (see Fig. 13) and confirm our hypothesis on higher inertia forces in slip-velocity case.

L131f: “can be compared with results from transitional flow regime modeling” From my point of view, a validation like this should be the start of the simulation work. If the results are similar, this is a rigorous proof for the validity of the continuum method (including appropriate boundary conditions).

AC: We agree with the reviewer's perspective on the validation of continuum simulations and have accordingly enhanced our study concerning this point. We have

adapted the corresponding text at the beginning of Section 3.1, see new lines 167-199 in the view of varying local Knudsen number as pointed out by the reviewer. Based on different Kn values around the SPICE module geometry, we validate our macroscopic approach at first, based on published simulation results for channel flows using continuum models, which are well working for rarified fluids up to low transitional regimes up to $Kn \approx 1$ by imposing the conventional second order slip-velocity surface conditions, see our argumentation in the beginning of Section 3.1. Accordingly, we extended our non-slip continuous model by slip-velocity (of the first and second order) boundary conditions and conduct a comparative fluid-flow and particle-impaction study as described in previous points and in the new parts of the manuscript. By the Appendix B, we believe we have demonstrated that the difference between simulations under non-slip boundary conditions and those under slip boundary conditions is only clearly noticeable in the very last step of the particles' approach towards the substrate surfaces; specifically, in the form of improved collection efficiency (compare new lines in Section 4.4). In view of the above arguments and our additional investigations related to the Knudsen number range and the appropriateness of continuous modelling, we have deleted the following sentence from the new section 3.1: 'The extent to which the resulting uncertainties quantitatively affect the simulation results presented herein ultimately remains open.'

In further analyses (Figs. 6.-11 & 14), concerning the boom length (boundary layer) necessary for the development of the 'free stream' velocity, the booms position along the fuselage, and the flow field at various AoA, however, the difference between a non-slip continuum analysis and analysis in the slip and prevalent transition region appears to play a subsidiary role, compare, e.g., Figure B1. We therefore assume that the repeated particle impaction efficiency analyses under slip-velocity boundary conditions (new Fig. 13) are sufficient and that, all other previous flow pattern analyses remain largely valid for their respective objectives even under non-slip boundary conditions. In line with this, we have added new text relating to these perspectives at the beginning of Section 4.1, above Figure 8 (lines 417-425) and in lines 441-451 in Section 4.2.

L136: "starting from zero velocity". What's the reason of doing this for steady-state simulations? From my view, this blows up the simulation time needed and may cause numerical stability issues due to the extreme (velocity) gradients at the inflow region. A short statement of the reason could help me to understand.

AC: In the numerical study, a stationary flow pattern around the instrument module is aimed for. In this case, however, it is difficult to define a consistent initial solution for the numerical stationary solver. Therefore, the zero initial state is considered, subsequently the incident/inlet velocity increases continuously over time up to the final (maximal) velocity value within a short time range. Afterwards, further computation is then necessary, with a steady incident velocity imposed at the inlet, in order to converge/develop the solution to a steady state. This is a simple approach to overcome the convergence difficulties of the stationary solver when inconsistent boundary or initial states are defined. We added lines 202-205 to give more explanation on this point in the manuscript.

L151f: "error of less than $\pm 1.1\%$ " This depends much on the temperature range. Consider, emphasizing the transsonic character of the flow, since for supersonic flows, readers might think of high temperatures in the shock.

AC: We fully agree and have rephrased the text at this point accordingly.

L154ff: Where were these variables set? Were they set as boundary condition? A schematic figure of the computational domain with set boundary conditions (u , p , T , ...) would be helpful to follow your setup explanations.

AC: For clarification the requested informations concerning the boundary conditions are provided in lines 210-214, 231-232 and given more schematically in the revised manuscript version, see new Fig. 3 and new overview Table 2.

Section 3.1: Why is the payload section completely free in the simulation volume, i.e. is decoupled from the rest of the payload (service module, recovery, aft deck)?

AC: We are confident that all rocket components located downstream of service module (which is included in the CAD model) would have no significant or, at most, a negligible influence on the flow pattern near the SPICE booms and the simulation result in terms of particle collection effectiveness and efficiency. For reasons of simplifying the rocket model, reducing the simulation domain and complexity, and ultimately saving CAD design and at all computing time, the above-mentioned rocket components after the service module were discarded from the numerical analysis. Indeed, for this study on the effectiveness and efficiency of particle collections at the SPICE booms, it does not appear advantageous or relevant to include more of the rocket structure, as this is not expected to yield any additional and decisive findings for the present study. We acknowledge the reviewer's comment and will emphasise this point more clearly in the article (introducing sentences at the beginning of Section 3).

L172: "in the relevant size range and mass of NLC particles and MSP" – The particle tracking simulations were performed only for a single size and mass ($r=0.6$ nm; 3 g cm⁻³). However, simulations for a range of radii/mass (similar to studies made for other detectors) would be very insightful, since the critical radius/mass could be deduced from that results. Moreover, please clarify, why the MSP tracking is considered to be valid for NLC as well (consider moving content from Appendix A to the beginning of section 3.2). What's the purpose in not using the mass/radii evolution term in the particle tracing simulations?

AC: In fact, we repeated this computationally intensive analysis for various particle radii, as the reviewer is correct on this point, see the revised Sections 4.3, 4.4. We also took this opportunity to thoroughly investigate the difference between "non-slip" and "slip-velocity" boundary conditions and their effects on the results, as this difference has here, at this point, the greatest influence throughout the entire study. Both findings have been incorporated into the revised manuscript, specifically in new Fig. 13 and the accompanying text, as well as in the conclusions. In Section 3.2 we added text referring to the content of Appendix A concerning the ice coat sublimation due to the heating in prevalent temperate distribution, see lines 273-290. The reason for not including the mass evolution model (A1)–(A2) in the particle tracing simulation model (8) is the additional complexity arising from the rigorous replacement of the constant mass of the MSP nucleus m_p in (8) by $m_p + m_{ice}(t)$, where the second summand is an instantaneous mass of the ice cote governed by the additional system (A1)–(A2). This would lead to a coupled system of three ordinary differential equations for each particle computation, which would significantly increase the computational complexity and expense of the particle tracing simulations for high number of particles. For this reason, this model extension is beyond the scope of this paper, nevertheless the reviewer's suggestion could be considered for future perspective on more detailed analysis of particle collection processes in mesosphere.

L174ff: The aerodynamic simulation results have been stated to be from steady-state. Now, there is stated that the "short excerpt" of 0,021 s was used for the particle tracking. Please

clarify your experimental setup for the particle tracking. If one-way coupling is assumed and the flow is considered steady-state for a single altitude, field variables remain the same for each time step at each grid point, or do I misinterpret something?

AC: The reviewer is right concerning aerodynamic conditions considered as steady-state, meaning that the field variables such as the air velocity (the transport velocity for particles), ambient pressure and density remain the same at a chosen grid point throughout the entire computational time for the particle simulations. These fields (non-uniformly distributed in the computational volume) are drivers of non-constant particle movement. Therefore, the particle tracking modeling (of particle velocities and positions) is instantaneous by nature and in our study as well, even for the stationary but spatially non-uniform driving forces including air velocity or the temperature field. In the implementation of particle simulations we consider an initial particle velocity, which is consistent with the ambient, simulated, non-uniformly distributed air velocity field. In the simulated time, the particle velocity is adapted according to the influence of local forces including air velocity or density/pressure, based on the Newton's law (8) by instantaneous particle simulations.

L199f: Please, rephrase to clarify that the original Stokes' drag force expression is known to be massively incorrect for $Kn > 1$ and therefore a correction needs to be applied. (As you did). For high aerosol- Kn -numbers (~ 44000), the drag-force is to be formulated as free molecular drag force. Proof that the Stokes drag with the Cunningham slip corrector converges to the free molecular formulation. (e.g., by reference)

Just for reference:

W.F. Phillips 1975 (<https://doi.org/10.1063/1.861292>) provides a convincing model to describe the drag forces on droplets of mercury, oil and shellac in air. He also showed, that Millikans formulation is erroneous for droplets other than oil in air.

AC: The reviewer may rightly point out that certain assumptions no longer hold for $Kn > 1$. However, since our simulations are in the lower transition region considering local Knudsen number ($0.04 < Kn < 2$, or global $Kn \approx 0.1$, cf. Fig. 2) and by no means clearly fall within the range mentioned above (" $Kn > 1$ "), any inclusion of a statement into the article as requested would represent an excursion away from the article's main topic that neither makes a significant contribution to our study nor is relevant to it. See also our above responses on local Knudsen number and associated slip to transitional flow regime.

Table 2: Temperature and dynamic viscosity are missing. Remove items that were not used in the simulations presented in the simulations (e.g., NLC parameters).

AC: We have removed irrelevant NLC parameters and added the free-flow temperature for the ambient conditions. We have also included the temperature reference in the calculated viscosity (now Table 3).

L211: The phrase "sensitivity study" is misleading here. What I believe to understand is, that the sensitivity limit should be investigated. In my view, this limit should describe the probability to catch at least one MSP and might be deduced from analytical considerations (number concentration, detection efficiency, collector area, rocket velocity, (NLC) layer thickness) or something similar...

AC: One of the questions addressed in this study was how many particles would be expected to be collected for a given ambient particle concentration. In this study we investigate the lower limit of the estimated particle concentrations and demonstrate

almost constant collection efficiency based on our simulations for considered particle concentrations (PCs), see Fig. 13 a), which implies a linear increase of particle impactions with increasing PC. This independence of collection efficiency from ambient MSP particle concentration allows - theoretically - the collection efficiency results to be extrapolated to higher concentrations. Therefore, in fact we conduct a critical/extreme case simulation study in this regard; accordingly we have replaced the expression 'sensitivity' in this text passage to 'extreme-value analysis'. However, we have meanwhile amended the study with a test of collection efficiency as function of particle size, which adds up to a sensitivity analysis.

L118ff +Table 4: I doubt, whether this setup is meaningful to investigate the sensitivity limit. If "particle number" describes the number of particles inside the simulation (i.e. are test particles), this study only investigates the statistical error of the sampling related to the number of test particles. I expect the efficiency (ratio of released particles to particles impacting the sensor) for all runs to be constant, with larger errors for less simulated particles.

AC: We agree with the reviewer regarding the statistical error in the simulated collection efficiency resulting from different particle concentrations, and in our new particle simulations (with lower incident velocity and under both non-slip and slip boundary conditions), we estimate the efficiency based solely on the three lowest test particle numbers in order to reduce computational effort. Table 5 (formerly Table 4) shows the applied particle concentrations (PCs) for the respective numbers of (test) particles in simulations with an incident air velocity of 300 m/s, which actually results in higher PCs compared to former 400 m/s for identical number of particles, since the three numbers of particles in the (smaller) volume occupied by the (slower) rocket during the simulation time remain unchanged for both incident velocities in our simulations. As next, we have amended the study with tests of collection efficiencies as function of particle size regarding the above reviewer comment on L172 and on L122ff.

L122ff: To design an instrument able to prove that a detected MSP was a former nucleus of NLC, simulations for a range of radii/masses would have been performed to find a position of the sensor on the rocket payload, that is unable to collect MSPs, but has a high enough collection probability to catch NLC ice particles. A variation of the number concentration does not do that.

AC: We have amended the study with tests of collection efficiencies as function of particle size. However, this does not address the fundamental question raised by the reviewer. We agree that such a dedicated instrument design study would be an interesting approach. But even if an instrument part were designed to preferentially collect NLC ice particles while avoiding direct MSP collection, the mere simultaneous or selective collection of NLC ice and MSP material would still not unambiguously prove that a specific MSP acted as the nucleus of a specific NLC particle. We think that such a conclusion would require additional constraints beyond collection probability alone. However, this was not within the scope of the present work. Our study was limited to assessing whether the collection probability would be suitable for the collection of MSPs under plausible atmospheric conditions. Thanks to the reviewer's advice, the study now also demonstrates the suitability for various MSP sizes, which represents a significant improvement to the study. In addition to the fact that even small particles ($r \approx 0.4$ nm) impact with considerable efficiency, this also supports our assumption that, in principle, the larger the particle (and thus its inertia), the more efficiently it impacts, which is also confirmed in Fig. 13 b).

L232f: A quantitative answer to this speculation can be derived by running the particle tracking with different radii.

AC: We have amended the study to include the tests of collection efficiencies as function of particle size, see the revised Sections 4.3, 4.4, which supports the presented hypothesis, see also our response in the point above.

My major points of criticism of section 3 are:

1. It's not clear whether the temperature and density, (or viscosity) as a field, from the former simulations were used for the particle tracking. In the shock, these variables change much and should not be a constant, as Table 2 suggests.

AC: Naturally, the previously calculated flow field variables presented e.g., in Figures 2 b), 10, 11, 14 (including the shock regions) were used in the particle simulations as driving forces by imposing one-way fluid-particle coupling (see also our response to comment on L174ff) and no constants were employed, as Table 3 may suggest. The values shown for viscosity or density or pressure gradient were intended to reflect orders of magnitude in order to characterize the mean flow conditions involved. Moreover, based on these characterizing parameters presented in Table 3, the force magnitudes acting on particles are evaluated in Table 4 to give the reader an idea of their orders of magnitude and to argue the disregarding of some of them. However, as this could lead to misinterpretations, we have removed the density variable and added the reference temperature for the calculation of dynamic viscosity.

2. the variation of simulated particles is not expected to deliver insightful results, besides a variation of the statistical error (efficiency is expected to be independent of number of released particles)

AC: The reviewer is correct on this point. Therefore, we have limited the tests on released particle number (analogously particle concentrations) to three cases, see Table 5. Instead, we focus on testing with differently large particles and we have amended the study with tests of collection efficiencies as function of particle size, see the revised Sections 4.3, 4.4 and our responses to the comment on 'L118ff + Table 4', or on L172 and L122ff.

3. the probability of catching at least one particle can be determined by use of these results (i.e., efficiency).

AC: We agree with the reviewer, using the simulation based efficiency, the number of test particles/particle concentrations can be derived, necessary for a successful particle sampling, see also our response to comment on L211.

4. Instead of performing many simulations with different numbers of test particles, a study with different radii would be insightful.

AC: We have amended the study with tests of collection efficiencies as function of particle size, see above responses and the revised Sections 4.3 and 4.4.

5. Taking a radius of 0.6 nm to simulate NLC impact, by claiming the total melt of the ice particle in the shock/in vicinity of the collector is a huge assumption and must be discussed (at the beginning of this section, or in a discussion part).

AC: We have amended the study with tests of collection efficiencies as function of particle radius from 0.4 through 25 nm, see the revised Sections 4.3 and 4.4 and above responses.

4. Results and Conclusions:

I suggest dividing the results from conclusion. Maybe a joined "Results and Discussion" would make more sense, since there already is another "Final Conclusions"

AC: We understand the point raised here by the reviewer and have made structural changes as part of the manuscript's revision. In doing so, it turned out as useful to embed discussions and interpretations within the context of the presentation of the results, since the aspects examined are complex and multifaceted, and the reanalysed simulations have different effects on individual subjects analysed. In principle, we therefore follow the reviewer's suggestion by renaming Section 4.

L252ff: Methodological information like, domain and boundary information, type of FEM, spatial and temporal discretization schemes, belongs to the methodological part (section 3.1).

AC: We agree and describe the methodological information in Section 3.1, see lines 248-255.

Figure 4: Instead of mesh size, a plot of local Kn-number would be more insightful.

AC: Please, see the new Fig. 2 in the revised manuscript, which exhibits the local Knudsen number and we have removed the image of the mesh size here in Fig. 4 of the initially submitted manuscript (now Fig. 6 in the revised version).

Consider adding another plot with density, since it influences the local viscosity. Consider plotting fields for different AoA (angle of attack).

AC: The Fig. 11 depicts the three different simulated AoAs. Moreover, we have added a density plot in Fig. 2 b) for AoA of 0°.

L269f: "[...] SPICE booms unaffected by any flow disturbance caused by the m-NLP [...]" – Plots of the flow pattern (on slices/ or as iso surfaces) could give more support to the claim that differences are mainly caused by the front deck instrumentation.

AC: This was indeed illustrated in the figures (Fig. 4, panels b and c of the submitted manuscript), but we admit that it was not highlighted clearly enough, which is what we would like to correct with the revision. Given the flow pattern depicted in the submitted manuscript (Fig. 4b), the flow conditions reach near-free flow velocities shortly downstream of the m-NLP. Hence, there appears to be little reason to assume that the two downward facing SPICE booms (boom #2 and #3, see also submitted manuscript's Fig. 1) are directly affected during a normal flight. From a geometric point of view, the substrate surface of the two SPICE booms would only be located inside the wake of the m-NLP at an extreme negative angle of attack ~38°-40° (see following Fig. 1, right after this comment) that is very unlikely to be reached during a sounding phase of a flight with the HAS vehicle – and is therefore also out of the range of simulated AoA. However, to better emphasize this point, a corresponding sentence has been added at here in the revised manuscript, see lines 377-381.

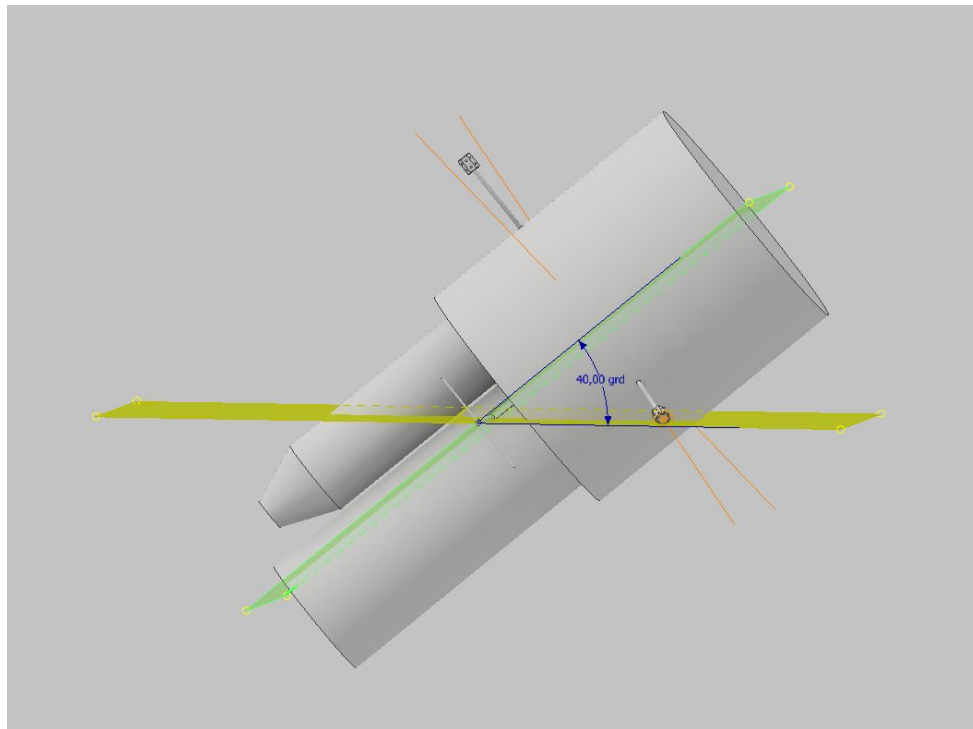


Fig 1.: With flow from the left (in parallel to yellow plane), negative AoA of ~38-40° were required to have SPICE booms aligned with the wake of the m-NLP.

L272: Good idea to investigate the sensitivity to velocity! This should be pronounced more prominent in the methodological part.

AC: Following the reviewer's suggestion, we have added a highlighting statement at the beginning of Section 3, lines 119-120.

L279f: This is not a strong argument. Please show the data samples up to a radius, where velocity approaches free stream values.

AC: We have added data points extending up to the velocities in the free stream, as shown in the following two figures. Please note that data points on line 2 end well before reaching the graph's scale limit since the boundary of the simulation geometry is reached. However, Figures 8(a) and (b) in the revised manuscript are used to determine the boundary layer thickness with the aim of sampling particles in the "free stream" (which is considered achieved upon reaching 90–95% of the main flow, which prevails far from any wall effects), i.e. to determine the position of the collection surfaces and thus the distance to the rocket envisage. To this end, we considered it necessary to provide an enlarged view focusing on the boundary layer region in the manuscript. We have also included a note in the text (without an additional figure, see lines 391-394) indicating that the background (or incident) flow velocities of 300 m/s and 400 m/s are only reached at 1200 mm and 650 mm, respectively; however, there are design constraints that prevent the booms as long as that.

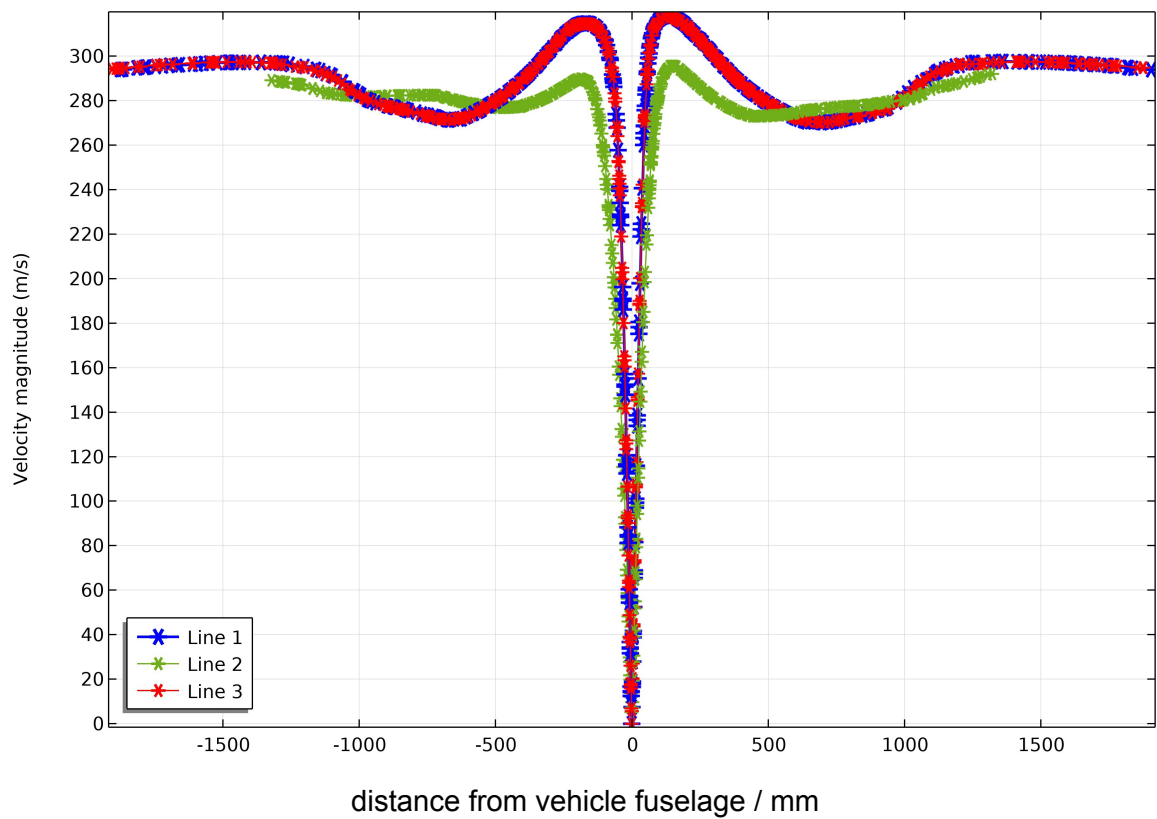


Figure 2: Flow velocity as a function of distance to the rocket's fuselage surface (0 mm) at incident flow velocity of 300 m/s.

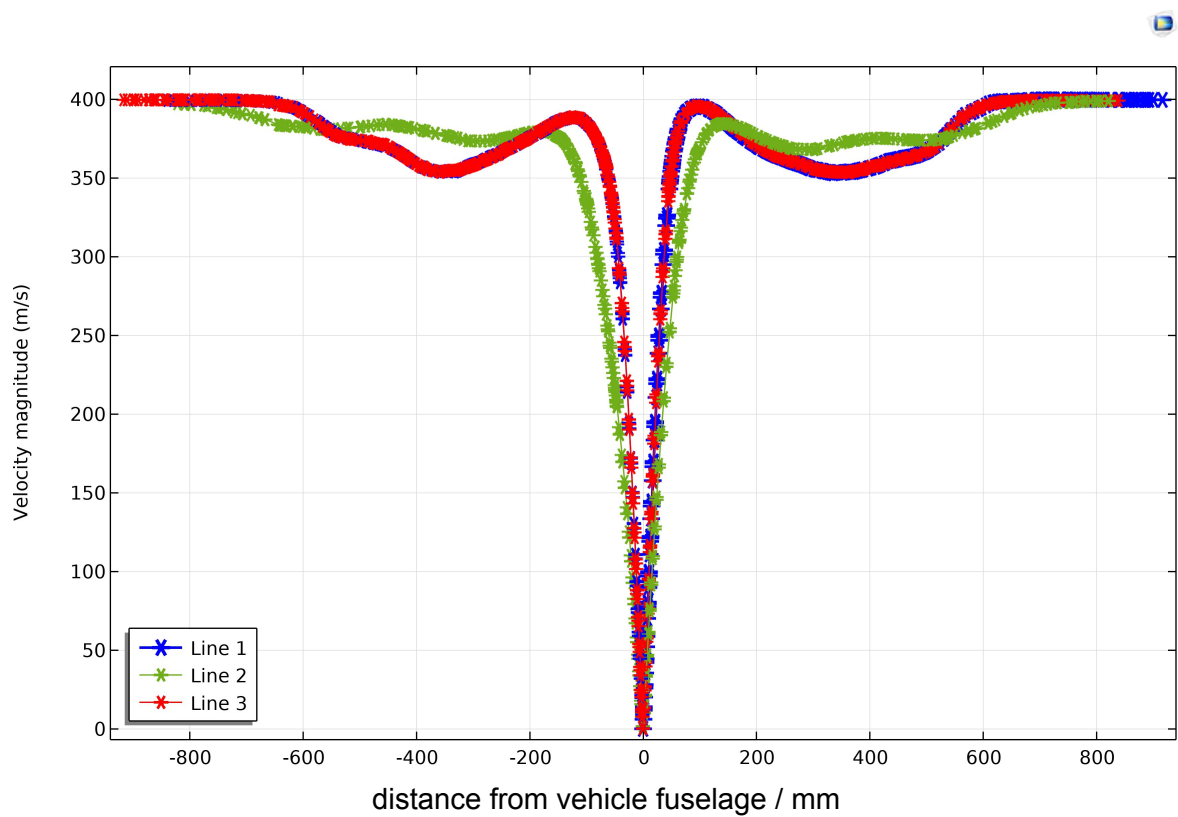


Figure 3: Flow velocity as a function of distance to the rocket's fuselage surface (0 mm) at incident flow velocity of 400 m/s.

L284f: The cause of differences of the sample lines is not clear from Fig. 6. Additional plots (e.g., iso-surfaces of the shock, induced by the front deck instrumentation) would allow following your argumentation.

AC: Fig. 7 (revised manuscript) shows that the red and blue cut-line are nearly mirror images of each other with respect to the rocket's symmetry, particularly regarding the geometry of the instrument bay in the nose cone. This could be the main reason why the two velocity fields along these cross-sections (blue and red) are nearly congruent (see Fig. 8), though not perfectly symmetrical. The flow along the green cut-line, however, is more significantly influenced by the asymmetry caused by the more cylindrical ECOMA instruments and the tapered CONE instruments. The asymmetrical arrangement of the instruments in the main instrument compartment also leads to an asymmetrical distribution of the velocity field at the point where the SPICE booms protrude from the rocket body. Consequently, the thickness of the boundary layer along the green cut-line is slightly enhanced (as also indicated in Fig. 6b of the revised article) and not completely symmetrical; however, with an estimated boom length of 120 mm, 90–95% of the free flow (far removed from any wall effects) should be achieved, so that the sampling likely takes place essentially outside the boundary layer. We have added a note to this effect in the revised manuscript version (lines 394–402).

L287f: It seems that a no-slip boundary was applied to these simulations. In Sec. 3.1., where the validity to use continuum mechanics, it was stated that the slip boundary should be applied in this Kn- regime. Dongari et al. (from your references) applied an advanced second order slip boundary. I expect that a no slip boundary condition will raise large errors.

AC: The revised manuscript version contains extended simulation results for slip-velocity boundary condition of 1st order and 2nd order. Please refer to our responses on comments L118ff, L127ff, L131ff concerning the impact of no-slip boundary condition on flow pattern in near field around the SPICE structures and substrate-mount surfaces and on its impact on particle impactions. Please refer to Appendix B and Section 4.4.

L290f: This point can be merged with #2.

AC: In our view, these are two separate issues, since point #2 concerns the main flow field around the fuselage along the cut lines, and we would like to clarify here (#4) that, apart from these cut lines, virtually no local influence of m-NLP sensors on the SPICE sampling position is to be expected. We think this deserves its own mention.

L297: "Sensitivity test" is too general. Choose a title that directly refers to the influence of AoA variation.

AC: The title is changed in the revised manuscript version.

L299f: Check terminology.

AC: Sentence is rephrased in the revised version.

Figure 7: Plotting the local Knudsen number, instead of mesh element size, would add rigor to the simulation results.

AC: Please, see Figure 2 for a now analysis of the local Knudsen around the flow obstacle. To ensure the accuracy of the simulations, however, the mesh size shown is related to discretization error and is important, which may indeed be of interest to the reader as well.

L311: The critical (larger) boundary layer is expected to develop at the lower velocity (300 m/s), a comparison to this simulation would strengthen your claim, that 120mm is a sufficient boom length.

AC: We believe that we have clearly illustrated this point in Figures 6a and 6b of the submitted article. In the revised version (lines 413-417), we have added a new reference to emphasize this point. In addition, analogous boundary layer to Figure 10 a) however for 300 m/s incident flow speed under slip-velocity boundary conditions can be found in Appendix B, Figure B1 as well as the deviation analysis of the resulting flow patterns. This new result demonstrates once again that the thickness of the boundary layer does not differ significantly at a flow velocity of 300 m/s and that, in both cases, the impact surfaces lie outside this boundary layer.

Figure 9: Consider using the same camera angle for the different AoA.

AC: In Fig. 11 (previously Fig 9), we have maintained the camera angle relative to the direction of flow (inflow on the left-hand side in each image). The cross-sectional planes shown - which intersect the positions of the SPICE booms (offset by 120° from one another along the module's longitudinal axis) and on which the flow velocities are overlaid - create a complex image that is best represented in such a 2D projection through the slightly different tilts. A constant camera angle would not adequately capture the image's level of detail. Therefore, we decided to retain these perspectives because, in our view, they provide the optimal representation of the result.

L321: From my view, the term "undisturbed" is misleading, the SPICE sensors are downstream the main shock. Consider using a term like: 'similar to the free stream condition' or similar..

AC: In the revised version the term "undisturbed" was avoided entirely and replaced.

L323: "are consistent at the three boom positions." Do you mean symmetric?

AC: This sentence was rephrased in the revised manuscript version, see line 461.

L340: This sub subsection is singular.

AC: We agree and corrected the text accordingly.

L350: What is 'impaction frequency'? Do you mean 'number of impacted particles'?

AC: We see that this term was misleading, instead of 'frequency' we apply now 'efficiency'. We have corrected the text accordingly in the first paragraph of Section 4.4 and text below.

L456f: This is precisely what is expected. Varying the number of particles only changes the statistical error on these results.

AC: We agree with this comment. In Section 4.4. we have adapted the corresponding text and we focus also on new findings concerning the deviation between the results based on the different boundary conditions imposed. Moreover, we have amended the study with tests of collection efficiencies as function of particle size, as described in above points.

L363ff: These are not new findings. In this paper, the term "concentrations" is misleading, since here it means 'number of test particles', only. The observation that using more test particles N , does not change the efficiency, but the statistical error is a basic $1/N$ behaviour of the expected value.

AC: A number of particles in a volume element, one would call it concentration. We agree that the behavior is generally expected, but it yields an estimate of required concentrations for a minimum number of particles on the substrate. In practice, we have used the term particle number concentrations, but for the reason of simulation implementation, the total particle number as an input parameter is required. We have therefore converted the particle concentrations into total particle numbers (Table 5) by a formula accounting for an air volume filled by particles during the flight simulation time considering incident speed.

This said, plus the new efficiency studies with different particle sizes, plus the conversion Table 5 in the revised manuscript version should make this clearer.

L369ff: Interesting: I wonder if the steep density increase and subsequent collisions were considered by any means, and if this finding would still hold? I did not definitively understand, if you use the dynamic viscosity and temperature as local variables.

AC: Yes, we confirm that density (see Figure 2b), temperature and viscosity were calculated as local variables (fields) in the fluid flow simulations. The particle simulations are based on the results of the flow calculations for background dynamics; accordingly, the particle simulations also include the local variables density, temperature and viscosity, see our response to the previous major points of criticism of section 3, Nr.1.

L371ff: How different?

AC: We have added a clarifying statement at this point in the revised paper version, lines 525-527.

Figure 11: The efficiency (Eq.9) is expected to be constant for each AoA and mount. These plots should be concentrated in a single diagram (collection efficiency vs AoA). Plotting over "particle number concentration" (i.e. number of test particles) These plots barely carry any further information besides the decrease in statistical error with increasing N.

AC: This figure (Fig 13 in the revised manuscript version) is entirely replaced by a new more compact Plot that also includes the particle size dependent collection efficiency calculations.

L388f: What's the information of this sentence?

AC: Due to extensive revisions made in response to the reviewer's earlier comments, large portions of the text including this sentence are no longer included in current version of the manuscript.

Summary of comments to 4.2:

This section can be condensed to two figures and their discussion.

-Fig11: A simple "collection efficiency vs AoA" would hold the same information as the 6 sub figures in the current version.

AC: The Figure 13 is refined in the revised version of the manuscript and include additional information on impaction efficiency dependent on particle size.

It seems the concept of "concentration" and "number of test particles" have been confused. This makes the discussion of "particle number concentration" vs. "impacted particles" basically obsolete. Same for the efficiency plots: They are thought to be constant and the number of test particles only influences the statistical error.

AC: A number of particles in a volume element one would denote as concentration. We agree that the behavior is generally expected, but it yields an estimate of required concentrations for a minimum number of particles on the substrate. In practice, we have used the term particle number concentrations, but for the reason of simulation implementation the total particle number as an input parameter is required. We have therefore converted the particle concentrations into total particle numbers (see Table 5). This said, plus the new efficiency studies with different particle sizes, considering the conversion Table 5 in the revised manuscript version should make this clearer. Moreover, the new Figure 13 includes the results for collection efficiency calculations as a function of particle size.

For the part discussing the streamlines, it is not clear if the density and temperature field (which are subject to strong gradients in the shock) derived from the simulations were input to the particle tracking algorithm. If not so, this should be discussed properly, including possible influence in the finding that higher free stream velocity increases the collection efficiency.

AC: Yes, we confirm that density, temperature and viscosity were calculated as local variables (fields) in the flow calculations. In the implementation of particle simulations we consider the results of the flow field calculations for the background fluid dynamics; accordingly, the particle simulations also include the local variables density, temperature and viscosity, which are non-uniformly distributed and consistent with the ambient simulated temperature, viscosity and density field *inter alia*.

5. Final Conclusions

Consider changing the title to “Conclusions” only.

AC: We renamed Section 5 to ‘Summary on flow simulations and particle collections’. Parts of this manuscript's end have been changed or even omitted, such as the “Outlook” section from the initially submitted version of the article.

L397f: “The simulated particle collection occurs mostly unaffected by the shock wave evolving at the tip of the instrument module.” – This contradicts e.g., findings by Hedin ACP, 2007, or Asmus ANGEOS, 2017. Please discuss the main differences to their setups.

AC: We have deleted this sentence and rephrased the section in the revised manuscript, see lines 569-570.

L409f: “Pineau et al. (2024) states that lower velocities result in more efficient particle collection” How does that relate to your finding, that the efficiency is higher for higher velocity?

AC: In Pineau et al. (2024) different velocity range and conditions were investigated, a clarifying sentence was added in the revised version of the manuscript, lines 573-578.

L412: “compared to the MESS rocket” – MESS is the name of the instrument. You should compare instrument with instrument, not instrument with rocket, on a specific rocket flight with a specific trajectory. However, it's good to discuss the special flight pattern of HAS and its advantages over the Maxi-Dusty 2 (with MESS onboard) trajectory.

AC: We have corrected the admittedly misleading wording, lines 573-578 and 579-580.

6. Outlook:

L423: From my perspective, this step should not be in the outlook, but should be the beginning of this work. This would make readers and the community trust in the reliability of the simulation results. Two possible ways (I imagine, there may be others):

AC: As the revised version of the article has grown significantly not only in terms of substance but also in length, the “Outlook” section was removed from the revised manuscript.

A) Do the verification yourself: with high-quality wind tunnel measurements (e.g., by Allègre, Bisch and Lengrand, 1997), or simulations (e.g., DSMC flow around cylinder)

AC: Major parts of this objection may have been addressed by the additional simulation using slip-velocity boundary conditions of the second order we added to the manuscript in Appendix B during the review process. Undoubtedly, further simulations using other tools could confirm or refine this investigation, but, as we hope to have demonstrated, no substantially different results are to be expected in this range of Kn indicating lower

transition range. Ultimately, the experiment itself must show how effective the collection with SPICE is in reality. That said, it may be a challenge to find a suitable wind tunnel capable of generating wind speeds of 300–400 m/s under mesospheric conditions, and alternative scaling methods would still introduce enough uncertainty regarding how well they reflect a real collection in the NLC target area.

B) Apply appropriate boundary conditions, that have already been verified to deliver to a certain extent reliable results (e.g., Dongari and Agrawal, from your references).

AC: We have improved our modeling settings towards more realistic conditions representing the slip- and lower transition region of rarefied fluids characterized by Knudsen numbers of up to $Kn=1$. As already mentioned in our response to reviewer's comment on L118ff, L27ff and L131f, we replaced the previously applied non-slip boundary condition with (conventional) first- and second-order slip velocity boundary conditions at the surfaces. The corresponding simulations and the resulting changes in the flow field and particle impaction are discussed in the revised manuscript. This provides a more appropriate representation of the gas–surface interaction under the considered mesospheric conditions while retaining the continuum modeling framework.

Appendix:

L457: Wrong reference. Pages 1-9 only contain a historical review. (I looked up the edition from 2000, but the general structure of the textbook did not change for the 2010 version.). Please correct.

AC: It turned out this was a copy-and-paste error. The page number has been removed.

L474ff: These statements are not supported by the referenced figures, since the figures show a simulation time (or time of flight?) on the x-axis. For the reader, it remains unclear where (in the simulation volume) the sublimation process happens.

AC: To supplement this, we no longer presented the graphs solely as time series but as a countdown to the time = 0 when the particle impacted the surface of the substrate mount. In addition, the corresponding distances between the particle and the impact surface were introduced as an additional x-axis. This should make it easier to determine at what distance upstream from a relatively small flow obstacle, such as the SPICE booms, the sublimation of water ice particles is already occurring, depending on the actual deposition coefficient α_d .

Technical corrections

Overuse of weak connectors like "hence" and "thus" — more formal structuring is advised.

AC: we reduced the number of "thus" throughout the text.

Some sentences are long and convoluted. These should be split for clarity.

AC: We agree with the reviewer and shortened most of the critical sentences.

Technical terms (angle of attack, attitude, orientation) are mixed up. This needs strict distinction throughout the manuscript.

AC: The term 'orientation' was used consistently and exclusively in relation to the SPICE booms. We agree that the terms 'attitude' and 'angle of attack' (both of which refer to the rocket module during flight) were occasionally used interchangeably. We have revised the text accordingly to ensure a more consistent use of the term "angle of attack" or "AoA" and to use the term "attitude" only when referring to the general flight behaviour of the rocket module during flight.

There's a tendency to hedge strong conclusions ("may", "possibly", "suggest"), which weakens scientific rigour.

AC: We agree with the reviewer and have limited the use of 'may' to a single instance, removed the word 'possibly' from the entire text, and the word 'suggesting' does appear in the text only once in connection to Knudsen number.

L2: "in about" → "at about"

AC: We agree and corrected the text accordingly.

L4: "...an inertia-based particle collector, which allows for sampling NLC particles during a sounding rocket flight for off-line single particle physico-chemical analyzes." → "...an inertia-based particle collector that enables sampling of NLC particles during a sounding rocket flight for offline single-particle physicochemical analyses."

AC: We agree and corrected the text accordingly.

L12: "confirm possible impactions on the collector surfaces." → "confirm impactions on the collector surfaces."

AC: We agree and corrected the text accordingly.

L14: "investigation on the morphology" → "investigation of the morphology"

AC: We agree and corrected the text accordingly.

L32: "Little is known about MSP aside..." → "Little is known about MSP beyond their presumed role in mesosphere ice particle formation"

AC: We agree and corrected the text accordingly.

L42: "are lacking to date" → "are still lacking"

AC: We agree and corrected the text accordingly.

L61: "expected radius" → "...expected particle radii below 100 nm..."

AC: We agree and corrected the text accordingly.

L64: "... out test flights numerical.." → "test flights, numerical ..."

AC: We agree and added the comma.

L73: "Two transmission electron microscopy (TEM) grids each are embedded " → "Two transmission electron microscopy (TEM) grids are embedded as substrates on each side panel of the prisms (substrate mounts)"

AC: We agree and corrected the text accordingly.

L74f: " at different exposure direction with respect.." → "at different exposure directions regarding the outside airflow, resulting in varying collection efficiencies."

AC: We agree and corrected the text accordingly.

L77: "underneath each TEM grids, for the case that the thin.." → " underneath each TEM grid, for the case that..."

AC: We agree and corrected the text accordingly.

L82f: "Due to the non-aerodynamic design." → "Because of its blunt design"

AC: We agree and corrected the text accordingly.

L151ff: “, and the specific gas constant R_s ” Is incomplete.

AC: Here, we've moved the quoted phrase to the previous sentence, where it fits better, and made some minor rephrasing changes, see lines 225-228.

L176: “it seems justified” → “Since the fraction of particles (NLC/MSP) is low compared to the constituents of the surrounding flow, a one-way coupling mechanism is applied. Consequently, the fluid ...”

AC: We agree and corrected the text accordingly.

L228f: “only the desired ice nucleus” → “only the desired ice nucleus (i.e., MSP) may remain available for collection in extreme cases.”

AC: We agree and corrected the text accordingly.

L331f: “remain as unaffected as possible” → “remain minimally disturbed over a wide range of angles of attack.”

AC: We agree and corrected the text accordingly.

Since the content of this manuscript is of great interest and the general concept promises to deliver solid results if the points concerning the methodologies of the aerodynamic simulation in the Kn-number regime and the particle tracking part have been improved, I want to encourage the authors to work on a revised version of this paper.

AC: We truly appreciate this feedback and are happy to follow the reviewer's suggestion by resubmitting the manuscript.

AC MOREOVER:

We have expressed our gratitude to both anonymous reviewers in the newly added acknowledgments section and kindly request both reviewers to identify themselves so that their contribution to crucial improvements of this article can be appropriately acknowledged.