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Peer Review File

Threshold for entrainment of mineral aerosols from grain-scale simulations.

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This file contains all reviewer reports in order by version, followed by all author rebuttals in order by version.

Attachments originally included by the reviewers as part of their assessment can be found at the end of this file.

Version 0:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
My comments for the authors are provided in an attached pdf.

Reviewer #2

(Remarks to the Author)
Review of “Grain-scale soil topography boosts emission of mineral aerosols”
This paper employs the Discrete-Element-Method (DEM) to numerically simulate mineral dust emission, addressing limitations in current Earth System Models (ESMs) that rely on empirical parameterization for dust flux, leading to large discrepancies in field measurements. They found that Natural soils' grain-scale topography drastically reduces dust entrainment thresholds. For 10μm dust in mixed sand-dust beds (10μm dust + 100μm sand), the threshold wind shear velocity is only 0.05m/s—an order of magnitude lower than in monodisperse dust beds and 1/5 of sand's threshold (≈0.25m/s). This challenges the traditional view that dust emission mainly depends on saltation bombardment (sand grain collisions). Besides, this study also clarified that dust emission modes vary with particle size: 10μm dust is mostly emitted as single grains, 5μm dust via mixed modes, and 1μm dust mainly coated on sand grains. The study suggests future climate models must incorporate the grain-scale topographic effect to improve dust cycle simulations, though it notes unconsidered factors like humidity and vegetation that need further research. This study is of great significance for understanding dust processes and researching aeolian geomorphology. Therefore, it is recommended to make moderate revisions before publication.
General comments:
1. The study highlights that grain-scale topography reduces dust entrainment thresholds, but it does not quantify how soil roughness (e.g., size difference between sand and dust, dust proportion) quantitatively modulates this threshold reduction. For example, is there a linear or nonlinear relationship between the sand-dust size ratio (or dust proportion) and the percentage decrease in entrainment velocity? In this paper, a fixed number of 50,000 dust particles were used to cover the surface of 10,000 sand grains. The rationale for adopting this fixed ratio requires further explanation: is it because the critical wind speed for emission reaches a minimum (or holds other representative significance) under this coverage condition, or because the critical wind speed for emission is insensitive to the dust proportion?
2. There is confusion between the calculation of vertical dust emission flux (Figure 2 and Equation 18) and the sophisticated DEM simulation: This study elaborately designed a DEM model that accounts for various interparticle forces and flow field feedback. Based on this model, the complete motion process of dust particles can be accurately calculated (theoretically, the vertical dust emission flux can also be derived, though this requires clarifying the criteria for determining dust emission—e.g., the height or conditions that signify the occurrence of dust emission). However, the formula for calculating vertical dust flux appears to have no direct connection with the DEM model. If the dust flux is calculated using Equation 18, only the dust content and flow field characteristics need to be known—so what is the relevance of the DEM simulation and the series of corresponding settings?
3. Admittedly, the discovery that critical wind speed is far below the known dust emission threshold is of great significance. However, several questions require clarification: Is this mechanism a universal phenomenon (e.g., within what range of dust content does this mechanism exist significantly, and under what natural environments does this situation typically occur)? Meanwhile, is this emission pattern sustainable (as observed in Figure 2b, dust emission only occurs in the initial fraction of

a second)? What is its contribution to the total dust emission (or its contribution under specific conditions)? These questions directly relate to whether we should emphasize this mechanism and its impacts in the study of dust emission processes.

Reviewer #3

(Remarks to the Author)
The authors present a new dust emission mechanism, namely the direct entrainment of loose dust particles by micro-accelerations of surface shear stress through grain-scale topography. Using grain-scale modeling, they demonstrate that this mechanism is effectively leading to dust emissions (a) already at shear stresses considerably lower than what is usually throught of as the threshold shear stress for dust uplift; and (b) without saltation as a trigger.

The theoretical considerations of the process and its numerical modeling are convincingly presented and clearly show its effect. Support of the validity of their methodology is achieved by initially reproducing state-of-the-art understanding of the aerodynamic dust emission threshold and its dependency on particle size. The study is novel and provides a fresh perspective on the challenging problem of theoretically describing dust emission.

The one major aspect that is left unanswered in the paper is that of the relevance of the process in a natural environment. In the present manuscript, dust emissions through the new mechanism are quantified for a bed of loose particles. In nature, desert surfaces are often strongly consolidated, leaving only a very thin layer of loose sand and dust on top. This would arguably severely limit the amount of dust that can be emitted via this process. However, the authors clearly state that they intentionally ignored such kind of effects in their initial study, leaving their quantification for future research.

In summary, although the importance of the process described in the paper is as yet unclear, the manuscript presents novel insights into the emission of mineral dust - a dominant type of atmospheric aerosol. The methodology is sound, results are well presented, and conclusions are supported by the results. I therefore recommend publication of the paper.

Version 1:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
My comments for the authors are provided in an attached pdf.

Reviewer #2

(Remarks to the Author)
Comments to the Author
Review of manuscript COMMSENV-25-4963A
'Threshold for entrainment of mineral aerosols from grain-scale simulations'

The author has addressed and resolved most of the issues I raised, and the quality of the manuscript has been substantially improved. I recommend publication after the following minor revision:
(1) The unit formats are inconsistent. In the title of Figure 1, both "kg s^{-2}" and "kg/s^{-2}" are used, while slashes (e.g., m/s) are predominantly adopted elsewhere in the text. It is recommended that the entire manuscript be revised to a uniform unit format.

Reviewer #3

(Remarks to the Author)
I thank the authors for considering and addressing my comments. However, I would like to clarify one important point: What I consider a consolidated soil is by no means "perfectly non-erodible", contrary to what the authors specify in their rebuttal letter. There are many hard surfaces, for example, crusted and paved sediments, which are very erodible (e.g. Gonzalez-Romero et al., 2023). Perhaps there are different interpretations of what is a "consolidated" surface. In this context, it would be good to clarify what the authors consider "consolidated, shallow erodible soils" as in their revised manuscript (l. 292).

Reviewer 1

The authors use simulations of particles exposed to a boundary layer flow to study dust emission. The monodisperse particle bed simulations align well with previous observations for a range of particle sizes and cohesion. Simulations with a bidisperse particle mixture reveal that small dust particles can be exposed to higher positions within the flow when "stuck" to the tops of larger sand particles through inter-particle interactions. The exposed dust particles are subjected to higher wind speeds owing to their higher position, leading to enhanced emissions of dust in the bidisperse mixture.

The interpretation makes sense, and I suspect there is a real enhancement of dust emissions due to grain-scale topography in mixtures with larger particles.

Reply: Thank you, we are glad that the reviewer agrees with our interpretation that grain-scale topography in mixtures with larger particles may truly enhance dust emissions, as observed from our numerical simulations. Thank you also for the very constructive comments, which helped us to improve our manuscript. Below we provide a point-by-point reply to these comments, thereby specifying where changes were made in the manuscript to address each point raised.

However, the result is also in part due to limitations of the stochastic model for representing the flow. It cannot be discerned from the present results how much of the outcome should be attributed to a real mechanism versus limitations in the methodology. I therefore recommend the article not be published, and encourage the authors to either validate the simplified two-way coupling in the bidisperse mixture or employ a more sophisticated flow model.

Reply: We have now clarified how much of the outcome should be attributed to the real mechanism of the flow modification due to grain-scale topography, while emphasizing the limitations in the methodology and the significance of this limitation for the interpretation of our results, as discussed in our reply to your comments on the flow simulation (see below). In short, we explain why our model, which indeed accounts for a representation of the grain-scale boundary layer of a protruding sand particle, is correctly predicting, in a qualitative sense, the effect of the sand bed topography on the dust threshold, and we now emphasize in which sense a more sophisticated flow model will help to improve the quantitative predictions on single dust particle trajectories (not the scope of our study) in future work (see below).

Further details on my main criticism are discussed below, followed by minor line-by-line comments.

Reply: Thank you, we have revised our manuscript substantially by considering all issues raised in your report, including the minor line-by-line comments as addressed below in our point-by-point reply.

As an aside, if the results can be properly validated, it would be interesting to compare the findings with fluvial sediment transport in mixed-size beds. In that case the smaller particles mostly "hide" in the interstitial space between larger particles, leading to a reduction in transport of the small particles (Wilcock & Crowe, *J. Hydraulic Eng.* 2003). The opposite finding in this study appears to be due to inter-particle attractions which allow the smaller particles to remain at the top of the bed exposed to the flow.

Reply: This is exactly what happens in our numerical simulations – thank you very much for this remark. Micrometer-sized Aeolian dust particles do not fill the pores between large sand grains because cohesive van der Waals interactions prevent them from rolling or sliding down into the interstitial space between the sand grains. As a result of this adhesive interaction between dust and sand particles, the dust grains remain exposed to boundary layer flow atop the sand particles, as noted by the reviewer.

We have now introduced a comment that highlights this difference in the manuscript, thereby referring to the work by Wilcock and Crowe (2003) as suggested by the reviewer (see lines 176-183 in the revised manuscript).

Flow simulations

The flow model imposes a mean velocity profile that varies with height above the bed according the fundamental theory for boundary layer flows. The velocity fluctuations around the mean are also imposed using stochastic generation based on an assumed Gaussian distribution of the fluctuations. The only impact of the particles on the flow is to modify the mean velocity profile based on the total drag and volume on the particles (Eq. 13).

Accordingly, for a larger particle extending farther into the flow as seen in Fig. 2(a), the modelled flow velocity through the particle will correspond to the mean $\overline{u}_x$ at that height and a random fluctuation. In this case, the local smaller particles will almost certainly be exposed to a high velocity as noted in line 167.

In reality, the flow will be displaced around the protruding particle, introducing local fluctuations highly coupled with the particle location and an internal boundary layer forming around the particle. Due to this, the velocities around the protruding particles will be reduced compared to the mean. This reduction, due the coupling between the particle and the local fluctuations, is missing from the model.

Reply: We fully agree: However, our simulations **already consider the reduction in wind speed owing to the internal boundary layer, highlighted by the reviewer**. Better yet: Our model does not simply reduce the wind velocity, it rather **sets the velocity of the wind as zero in the lee side of the sand grain**. This simple but efficient model is described in the subsection entitled "Wake effect in the lee of soil particles", within section 3.1.3 (see chapter Methods), but we recognize that it should have been mentioned in the main text of the original version explicitly too.

Therefore, in the revised version, we now emphasize this very important aspect of our model in the main text too (see lines 90-93 of the revised manuscript) – thank you very much for calling our attention to this point.

Furthermore, we would like to add a couple of remarks on this very important topic of the flow modeling through the mixed-bed soil in our manuscript.

Three additional remarks on the flow characteristics over mixed-beds (including associated discussion added to the manuscript):

Wake zone of sand grains: We note that a more accurate model of the wake zone effect would require knowledge of the exact shape and size of this wake zone, which extends up to a reattachment point downwind of the grain and further depends on non-local effects which cannot be captured in an analytical model. We agree with the referee that a much more complex numerical tool that captures such hydrodynamics will be needed to improve the quantitative assessment of the flow in mixed beds. However, for the purpose of our work, the only relevant ingredient is the wind profile around the dust grains that are directly in contact with the (protruding) sand grains, since our model aims at investigating the *initiation* of motion of the dust grains (which are in the uppermost dust layer). And since the wind velocity over these grains is set as zero in the wake, including the turbulent wind patterns in the wake zone of sand grains would not reduce the emission rate, instead it would, at most, *enhance* even further the vertical dust flux. Nevertheless, we agree that full consideration of turbulent wind patterns in the grain-scale boundary layer will be important for improving the quantitative assessment of grain trajectories and is an excellent point for future work.

Wind speed-up owing to compression of the streamlines on top of sand grains: Moreover, in addition to the increase in wind speed with vertical distance from the bed height owing to the atmospheric boundary layer wind profile and the reduction of the wind speed in the wake zone of soil sand – both effects considered in the paper – there is one further effect that is not explicitly modeled in our simulations, but which should enhance the overall trend of the grain-scale topography in lowering the entrainment threshold over natural mixed-beds substantially. The reviewer noted well that the flow is displaced around the protruding particle, and this displacement leads – as well known from boundary layer theory – to an ***enhancement*** of the ***mean*** flow speed **at the top of the protruding sand grain**. This effect further enhances the wind drag force on a small dust particle located on top of a sand grain, thereby further enhancing, as well, the overall effect of reducing the minimum upwind shear velocity required to initiate dust emission.

The flow model is therefore missing crucial dynamics occurring locally around the particles that will be very consequential to the quantitative emission outcomes. The simplified flow model thus makes it difficult to trust the conclusions of the study. The validation of the flow model is unfortunately limited to the monodisperse case (Fig. 1). The simplified model is acceptable for the monodisperse case when the topography effects are the same size as the dust (Fig. 2a left side), but in the bidisperse case the topography induces much larger fluctuations and flow deformation around the large particles (Fig. 2a right side) that needs to be incorporated into the model to accurately predict the dust emissions.

Reply: Since our model *does* account for the reduction of the wind velocity in the internal boundary layer of the sand grain (see above), our model is *not* missing the crucial dynamics referred to by the reviewer. Indeed, we can say that our model is overemphasizing these dynamics as in our simulations the wind flow is completely turned off around any dust grain located in the wake of a sand grain. Moreover, although we recognize that a more sophisticated model will be required to further improve the quantitative assessment of sand and dust transport (out the scope of our manuscript, which focuses only on the initial process of direct entrainment of dust particles in direct contact with sand grains), more sophisticated models will further include the compression of the flow streamlines with the concatenated shear stress increase on the top of the sand grains. Because such a compression of the flow streamlines is associated with an increase of the shear stress on top of a protruding grain, the effect should rather enhance the overall topographic effect on reducing the wind threshold for dust entrainment (the main conclusion of our manuscript) even further.

We have now incorporated the discussion above into the manuscript. The associated text can be found in lines 232-245 of the revised manuscript. Furthermore, in consideration of the reviewer's excellent observation that our model successfully reproduces the entrainment threshold in the monodisperse case (Fig. 1), and to more emphatically remark on the groundbreaking insights gained from Fig. 1 – that van der Waals cohesive forces are the main underlying factor for the increase in threshold with decreasing particle size, and that stochastic particle-particle interactions can explain, to a large extent, the scatter in the experimental data, with turbulent wind fluctuations playing rather a subordinated role – we have now changed the title of our manuscript to "Threshold for entrainment of mineral aerosols from grain-scale simulations".

Minor comments

1. Line 18. It is misleading to use the phrase direct numerical simulation here, given that this term is usually reserved for fully-resolved simulations of the Navier-Stokes equations in fluids literature.

Reply: We now use “discrete element simulations”, “particle-based simulations” and “granular simulations” throughout the paper instead.

2. Line 71. “Stable” boundary layer may be confused with a stably-stratified atmospheric boundary layer. Would “stationary” be a suitable descriptor?

Reply: We agree that the boundary layer may be regarded, statistically, as stationary, since mean velocities are treated as constant over time and modulated by turbulent fluctuations. We now use the descriptor “stationary” in the manuscript, as suggested by the reviewer.

3. Line 87. The assumption of isotropic turbulence is inconsistent with the fluctuation amplitude varying across directions (line 376).

Reply: Thank you for noting this. Although we assume the same model for the statistics of turbulent fluctuations in all directions, we indeed apply the values of fluctuation amplitude as determined from measurements on the initiation of particle motion in wind tunnel simulations. We have thus removed the mention to “isotropic” from the sentence and now cite, instead, the previous work from which the values of the fluctuation amplitudes were taken.

Reviewer 2

This paper employs the Discrete-Element-Method (DEM) to numerically simulate mineral dust emission, addressing limitations in current Earth System Models (ESMs) that rely on empirical parameterization for dust flux, leading to large discrepancies in field measurements. They found that Natural soils' grain-scale topography drastically reduces dust entrainment thresholds. For 10µm dust in mixed sand-dust beds (10µm dust + 100µm sand), the threshold wind shear velocity is only 0.05m/s—an order of magnitude lower than in monodisperse dust beds and 1/5 of sand's threshold (≈0.25m/s). This challenges the traditional view that dust emission mainly depends on saltation bombardment (sand grain collisions). Besides, this study also clarified that dust emission modes vary with particle size: 10µm dust is mostly emitted as single grains, 5µm dust via mixed modes, and 1µm dust mainly coated on sand grains. The study suggests future climate models must incorporate the grain-scale topographic effect to improve dust cycle simulations, though it notes unconsidered factors like humidity and vegetation that need further research. This study is of great significance for understanding dust processes and researching aeolian geomorphology. Therefore, it is recommended to make moderate revisions before publication.

Reply: Thank you very much for this positive evaluation of our manuscript. We are glad that the reviewer considers our study of great significance for dust processes and aeolian geomorphology research, and that the reviewer recommends our manuscript for publication after moderate revision. Below we provide a point-by-point reply to the reviewer's comments, thereby indicating where changes were implemented in the manuscript to address every single comment.

The study highlights that grain-scale topography reduces dust entrainment thresholds, but it does not quantify how soil roughness (e.g., size difference between sand and dust, dust proportion) quantitatively modulates this threshold reduction. For example, is there a linear or nonlinear relationship between the sand-dust size ratio (or dust proportion) and the percentage decrease in entrainment velocity?

Reply: Excellent question. Since the resistance to drag and lift forces depends on the interparticle cohesive forces, and because these are affected by the relative diameter of the particles in the mixed bed, the surface roughness would not capture completely the physics of dust entrainment. In our study, we thus focused on representative values for sand particle sizes (100, 200 mu) and dust grain sizes that are expected to undergo pure suspension transport (d < 20 mu), to focus on the qualitative discussion of the topography-induced flow effect. Nevertheless, we have followed the reviewer's suggestion and added a discussion (lines 253-268 in the revised manuscript) on the possible quantification of surface topography in terms of roughness – defined as the standard deviation of the local bed elevation at time $t = 0$ (Parajuli et al., 2016) – for the sake of future modeling. We have now also added a new Section to the Supplemental Material (Section S3), in which we provide the mathematical definition of roughness and the values of the roughness associated with the soil bed topography both in the pure dust scenario and in the mixed bed-scenario.

In this paper, a fixed number of 50,000 dust particles were used to cover the surface of 10,000 sand grains. The rationale for adopting this fixed ratio requires further explanation: is it because the critical wind speed for emission reaches a minimum (or holds other representative significance) under this coverage condition, or because the critical wind speed for emission is insensitive to the dust proportion?

Reply: Thank you very much for this very important question. The exact value of this ratio certainly does not play, per se, a major role for the main conclusions of our simulations, and our model indeed does not rely on keeping the ratio fixed. What matters for choosing the value of this ration in Fig. 2 is that we achieve a situation of sparse dust coverage over a dense bed of sand grains, to focus on the topographic effect. Specifically, our study can be divided in two parts – or cases – with regard to the type of sediment bed considered: In case (i), we focus on a dense monodisperse bed (Fig. 1), and study dust emission considering a thick layer of dust on the ground. By contrast, in case (ii) we consider the opposite, complementary scenario, in which the dust amount is low and the underlying topography associated with the presence of much larger sand grains affects the entrainment of the much smaller dust particles. Of course, case (i) is recovered from case (ii) as the dust to sand grain number ratio is increased to values much larger than 5. We can thus say that the value of "5" is a compromise between a dust to sand grain number ratio that is sufficiently large to yield a statistics of dust emission, and one that is small enough to emphasize the scenario associated with case (ii).

This explanation is now provided in a new sentence added to the caption of Fig. 2 of the revised manuscript.

There is confusion between the calculation of vertical dust emission flux (Figure 2 and Equation 18) and the sophisticated DEM simulation: This study elaborately designed a DEM model that accounts for various interparticle forces and flow field feedback. Based on this model, the complete motion process of dust particles can be accurately calculated (theoretically, the vertical dust emission flux can also be derived, though this requires clarifying the criteria for determining dust emission—e.g., the height or conditions that signify the occurrence of dust emission). However, the formula for calculating vertical dust flux appears to have no direct connection with the DEM model. If the dust flux is calculated using Equation 18, only the dust content and flow field characteristics need to be known—so what is the relevance of the DEM simulation and the series of corresponding settings?

Reply: Thank you for this remark. The information obtained from the DEM simulations that is inserted in Eq. (18) is the particle concentration profile, $C(z)$. The state-of-the-art scheme for determining dust emission fluxes from wind tunnel experiments consists in using Eq. (18) with the experimentally measured values of $C(z)$, while in our work, the dust concentration at different heights above the soil is obtained from the particle-based numerical simulations (i.e., $C(z)$ is not an assumption but a calculation result from the DEM simulations).

However, in the revised manuscript, we have now further included results obtained from an additional scheme that incorporates the information from the individual particle momenta obtained from our simulations. Specifically, while Eq. (18) scales the flux by using a pre-factor proportional to the wind shear velocity, using our DEM simulations we can obtain the momentum flux density by integrating the contribution of all particles crossing a given plane above the ground. Despite the arbitrariness inherent to such a scheme – associated with assumptions like the measurement height, as well noted by the reviewer – and the fact that it is difficult to compare results obtained from such a numerical scheme with outcomes from wind tunnel experiments, we have now added a new section to the Supplemental Material (see Section S4) describing this scheme and displaying the associated results. As we also discuss in Section S4 and in a new paragraph added to Section 3.1.8, the results for the dust flux using this scheme follow the same qualitative trend as the ones obtained with Eq. (18). The reason for this behavior is that, differently from the situation of dense saltation layer, the cloud of emitted dust grains has a rather low volume concentration and affects, thus, little the wind profile. Therefore, particle velocities scale roughly with the wind shear velocity, and thus the same scaling with u_* (Gillette and Passi, 1988) is obtained regardless of the scheme employed. The information has been now added to Section 3.1.8 (lines 524-542) and Section S4 (Suppl. Mat.).

Admittedly, the discovery that critical wind speed is far below the known dust emission threshold is of great significance. However, several questions require clarification:

Reply: Very important questions, thank you. We address them point-by-point below.

Is this mechanism a universal phenomenon (e.g., within what range of dust content does this mechanism exist significantly, and under what natural environments does this situation typically occur)?

Reply: Yes, this is definitely a universal phenomenon that should decrease the threshold for dust particles resting atop larger particles. As such, the topographic effect is important for all natural environments of our planet, because natural soils commonly display some degree of polydispersity. Indeed, as granular soils display often a very broad particle size distribution, our results suggest that the smallest particles in these soils may be associated with lower-than-predicted thresholds owing to the topographic effect elucidated in our manuscript.

We also remark that, while we have focused on a bidisperse mixture with two particle sizes separated by a factor of 10 only, in natural environments there will be both a larger difference in orders of magnitude between the lowest and biggest particle size in the soil and a distribution of particle sizes encompassing intermediate values. Therefore, quantitatively, the influence of the topographic effect on the particle-size-dependent threshold will need to be further elucidated in future work. We very much hope that the discovery reported in our simulations will now trigger this further work, as we now also remark in the manuscript (see also our reply to the next point).

Meanwhile, is this emission pattern sustainable (as observed in Figure 2b, dust emission only occurs in the initial fraction of a second)?

Reply: Yes, the emission pattern is sustainable because once the upper, thin layer of dust has been washed out (the process investigated in our simulations, as noted by the reviewer) and saltation of the much heavier sand grains has begun (the next stage of soil erosion, which has been treated in previous publications of sand transport but is out of the scope of the present paper), layers of buried dust grains will become exposed – this process is known as "surface renewal" and has been shown to provide one major factor for dust sources in natural environments (Refs. 10 and 38 of our manuscript). In summary, the emission partner is self-sustained as the mobilization of sand grains and the saltation transport process exposes inner layers of finer material, a process intrinsic to sediment transport in natural soils that leads to inherent "reposition" of exposed dust sources for aerodynamic entrainment.

This explanation has been now added to the manuscript and can be found in lines 290-298 of the revised version.

What is its contribution to the total dust emission (or its contribution under specific conditions)? These questions directly relate to whether we should emphasize this mechanism and its impacts in the study of dust emission processes.

Reply: The contribution of different species to the total dust emission and to the total dust budget in the atmosphere is certainly an open problem that depends on various factors and will demand much further research. Indeed, both entrainment processes through aerodynamic forces and saltation bombardment can occur concomitantly during sediment transport. Therefore, the question of the total contribution to dust emission must be addressed in long-scale simulations of the whole sediment transport process, including direct entrainment of dust and sand, entrainment of dust through saltation bombardment and dust source evolution through processes like surface renewal.

However, what we have shown in this paper is that the most basic quantity used to estimate the aerodynamic entrainment of dust must be revisited in the various models. Owing to the strongly non-linear scaling of dust emission flux with the wind shear velocity (see e.g., Fig. 2 of our manuscript with the various models adopted in climate simulations), the implications are substantial and may affect predictions on the contribution of the dust phase to various components of the Earth system (from atmospheric geochemistry to radiation balance and climate) by a considerable amount.

We have now added the discussion above to lines 298-307 of the revised manuscript to address this very pertinent comment raised by the reviewer.

Reviewer 3

The authors present a new dust emission mechanism, namely the direct entrainment of loose dust particles by micro-accelerations of surface shear stress through grain-scale topography. Using grain-scale modeling, they demonstrate that this mechanism is effectively leading to dust emissions (a) already at shear stresses considerably lower than what is usually throught of as the threshold shear stress for dust uplift; and (b) without saltation as a trigger.

The theoretical considerations of the process and its numerical modeling are convincingly presented and clearly show its effect. Support of the validity of their methodology is achieved by initially reproducing state-of-the-art understanding of the aerodynamic dust emission threshold and its dependency on particle size. The study is novel and provides a fresh perspective on the challenging problem of theoretically describing dust emission.

Reply: Thank you very much for this positive assessment of our work and for highlighting that our study is novel and provides a fresh perspective on the dust emission problem. We have now revised our manuscript by incorporating the comments and suggestions of other two reviewers and by addressing the criticism raised in your report, as we explain next.

The one major aspect that is left unanswered in the paper is that of the relevance of the process in a natural environment. In the present manuscript, dust emissions through the new mechanism are quantified for a bed of loose particles. In nature, desert surfaces are often strongly consolidated, leaving only a very thin layer of loose sand and dust on top. This would arguably severely limit the amount of dust that can be emitted via this process. However, the authors clearly state that they intentionally ignored such kind of effects in their initial study, leaving their quantification for future research.

In summary, although the importance of the process described in the paper is as yet unclear (…)

Reply: We fully agree that this major aspect was left unanswered in the original version of our manuscript – thank you for raising this very important point. In natural environments, the amount of dust available for emission remains significant due to a process known as surface renewal. Such process consists in the exposal of buried sediment layers (including buried dust grains) following a wind-blown transport event with the concatenated removal of coarse sediment particles through saltation or creep from the uppermost surface soil layers (Refs. 10 and 38 of our manuscript). Given that the impact of surface renewal for the atmospheric dust budget in natural soils has been demonstrated experimentally in previous work, the insights gained from our study are of utmost relevance for future investigation of dust emission in natural environments.

We also note that surface renewal does not occur if the surface is consolidated, i.e., if the soil is perfectly non-erodible. Nevertheless, as shown in Figure 2 of our manuscript, the vertical dust flux associated with direct entrainment does not depend on the degree of consolidation, i.e., the emission rate due to direct entrainment of dust is the same regardless of the consolidation degree of the subjacent soil. Moreover, we emphasize that our study focuses on the emission rates of the exposed dust layers (once these have been exposed by deposition and/or by surface renewal), and on the important message that the emission threshold can be much lower than previously thought owing to the topographic effect. However, future research should focus on longer-term dynamics that includes the saltation and creep transport of the sand grains and the concatenated renewal of surface dust owing the exposure of buried dust particles.

We have now added the discussion above to the manuscript. The corresponding text can be found in lines 290-307 of the revised version.

(…) the manuscript presents novel insights into the emission of mineral dust - a dominant type of atmospheric aerosol. The methodology is sound, results are well presented, and conclusions are supported by the results. I therefore recommend publication of the paper.

Reply: Thank you very much for this excellent evaluation of our manuscript and for recommending our paper for publication. Thank you also for the very important note on the relevance of our work for natural environmental soils. We hope to have addressed satisfactorily your comment in the revised version of our manuscript, and that our study can be now accepted for publication in *Communications Earth & Environment*.

Reviewer 1

The authors have adequately addressed the minor comments. They also emphasized the conservative assumptions employed in the model:

1. Velocity on the leeward side of the protruding sand is set to zero, thus neglecting any possible initiated motion in this region.

2. The acceleration of the flow over the protruding sand (corresponding to compression of the streamlines) is neglected, such that the enhanced drag and lift on the protruding sand is not reflected in the results.

I acknowledge #1, and I understood this point in the original review comments. My concern is the windward side of the sand grains. I agree with the #2 point that the flow speed is enhanced over the top of the sand, but crucially this is with respect to two points along the streamline, which approximately follows a relative height zrel as shown in the right of the figure below.

My understanding of the simulation is that the force on the dust is based on the absolute coordinates shown in the left of the figure, where I expect the force from u(zabs) is a multi-fold increase above u(zrel). The model reduces u(zabs) according to drag feedback from the particles (equation 13), but this correction appears to be constant along x. Accordingly, there would be a modest reduction in u(zabs) at all x positions rather than a larger reduction local to the sand and dust grains that would be required to achieve u(zabs) ≈ u(zrel).

Further, the authors reduce the randomized velocity fluctuations within the viscous sublayer following the absolute height above the bed, but no correction is made to fluctuations along protruding grains following zrel. Based on my understanding of the simulations, this treatment of the mean and fluctuations will lead to unrealistic velocities and overestimated forces on the windward side of the grains. The original and revised manuscripts have not addressed this limitation in the model, and it remains uncertain to what extent the overestimate from this limitation is balanced by the conservative choices above noted by the authors. My overall opinion of the manuscript, in particular the second paragraph in the original review, therefore remains unchanged following the revision.

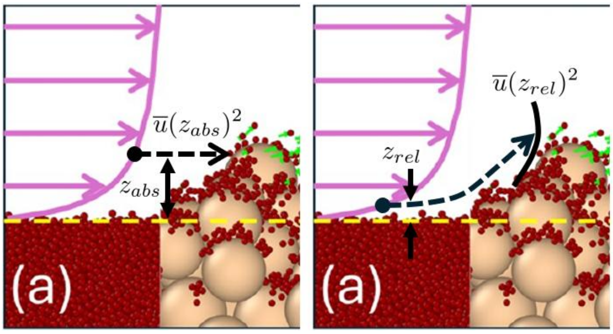

Figure 1: Average flow field exerting drag and lift on the dust: model assumption (left) and topography-induced flow (right). From on manuscript Fig. 2(a).

Reply: Thank you for the helpful and clear schematic diagram and for the effort in explaining your point regarding the wind velocity reduction. We fully agree that further work along the lines specified above is needed before definite quantitative predictions on the entrainment threshold over complex topographies can be made.

We understand that you agree with our main conclusion that the grain-scale topographic effect discussed in part II of the manuscript (bidisperse beds) should indeed lead to an overall reduction in the wind threshold (as you stressed in report #1), and that *your main criticism refers to our quantitative conclusion of a 1-order-of magnitude reduction in the entrainment threshold as obtained from simulations in this part II*. As we understand from your reports, your main criticism is that the overall reduction in the transport threshold predicted by our model may have been overestimated due to neglecting a more sophisticated treatment of the grain boundary layer – more specifically along the windward side of protruding sand grains.

Moreover, as we now better understand from your second report, you acknowledge that this overestimate may have been compensated, to some extent, by our conservative model for the grain boundary layer in the lee side of the protruding grain (through fully turning off the wind in the lee), but that this compensation was, probably, partial only, not in full. We agree that this aspect should be better emphasized in our manuscript, to make clear to the reader what the significance of our results is for future studies.

Summary of the changes made in the manuscript: Building on the discussion conducted through this referral process and **following the editorial recommendations after this second round of review**, we have now revised our manuscript by incorporating discussions accounting for your observations, criticisms and directions for improvement of the flow model.

Specifically:

Change #1: We have thoroughly revised the paragraph starting at line 228, on page 8, containing the discussion on the flow model, along the lines above. This paragraph contains now the following text:

"(…) However, it should be emphasized that the hydrodynamic description adopted in our model should be improved in future work to incorporate several features of turbulent wind flow that are essential for improving the quantitative assessment of dust emission rates. In particular, our simulations neglect the displacement of the flow streamlines around protruding sand grains, the internal boundary layer that forms around these large particles, and the concatenated occurrence of local wind velocity fluctuations that are highly coupled with the sand grain topography. These ingredients, absent from our simulations, should attenuate the wind velocities around the sand grains in bidisperse beds (Fig. 2), compared to the values predicted from boundary layer theory as a function of the elevation relative to the bed height, h_0 (Fig. 2a, right). We thus expect that, in real soils, the grain topographic effect should lead to a gentler attenuation of the dust $u_{*\mathrm{ft}}$ than the one-order-of-magnitude factor predicted in the example of Fig. 2. Therefore, building on the spatially averaged description of the turbulent wind field employed in our model and in previous DEM simulations [12–15, 37, 38], the next step would be the development of highly accurate computational fluid dynamic simulations that resolve local turbulent wind velocity fluctuations and particle boundary-layer, with the aim at elucidating the effect of particle size distribution quantitatively. Following the detailed technical description of the particle-based representation, in Section Methods we thus also provide explicit discussions on the caveats and uncertainties due to limitations of the stochastic flow model, and discuss future directions on how to improve the model."

Change #2: In addition to elaborating on your remarks within the main text (see above), we have now added to Section Methods, pages 15-17, lines 471-558, a new subsection entitled "Caveats and uncertainties due to limitations of the model, and a discussion of future directions for model improvement". This new subsection contains a more detailed discussion on the issues raised in your report as well as suggested routes for future work on highly accurate computational fluid dynamic simulations, with the aim at improving the flow model applied to bidisperse cases and, more generally, polydisperse simulations that include very large differences in particle size, as noted in your report.

Furthermore, in consistence with the aforementioned (major) changes, we have also made the following (minor to moderate) changes:

Change #3: In the abstract, we now emphasize our observations for the bidisperse scenario from a more qualitative perspective, while more strongly highlighting the groundbreaking results we obtained in both reproducing quantitatively the threshold curve for monodisperse simulations and in elucidating the physics of this threshold. Specifically, we have now revised the two sentences of the abstract referring to the threshold values obtained for the monodisperse and bidisperse simulations:

"Our model reproduces measurements of the minimal threshold wind shear velocity for direct aerodynamic entrainment in monodisperse beds as a function of particle size, thereby elucidating the influence of interparticle forces and turbulent wind velocity fluctuations. However, we find that a wind-speedup effect induced by grain-scale topography in bidisperse beds of sand and dust grains yields lower-than-predicted thresholds for direct aerodynamic dust entrainment."

Change #4: In consistence with these changes and in consideration of your pertinent criticisms, we have now rephrased the discussion sentences on the significance of our results for the bidisperse beds, to align these sentences with the discussion highlighted above. Specifically, we have now:

a) removed "much" from "dust grains can be much more easily" in the sentence starting at line 145, thereby starting this sentence with emphasis on the quantitative nature of the predictions from the monodisperse simulations: "In addition to the quantitative prediction of the threshold for dust entrainment from monodisperse beds, here we report numerical results indicating that dust grains can be more easily entrained (…)"; furthermore removed "substantial" from "The reason for this substantial decrease" in the subsequent sentence.

b) removed "well" from "wind shear velocities well below the predicted direct entrainment threshold", line 174

c) removed "strongly" from "numerical simulations strongly suggest", line 228, and removed "by a substantial amount (one order of magnitude in the mixed-dust bed scenario discussed in Fig. 2)" from the subsequent sentence, adding to the very same sentence the phrase: "although the significance of this effect for predicting dust emission in natural soils should be further elucidated in future work."

d) replaced "well below" by "below" in the sentence "The occurrence of dust emission at wind speeds well below the (…)" at line 252

e) removed "by a considerable amount" from the first sentence of the second to last paragraph of the main text, line 313.

Reviewer 2

The author has addressed and resolved most of the issues I raised, and the quality of the manuscript has been substantially improved. I recommend publication after the following minor revision: (1) The unit formats are inconsistent. In the title of Figure 1, both "kg s^{-2}" and "kg/s^{-2}" are used, while slashes (e.g., m/s) are predominantly adopted elsewhere in the text. It is recommended that the entire manuscript be revised to a uniform unit format.

Reply: Thank you for the recommendation of publication after minor revision and for noting this issue with the format of the units. We have now passed all units – in Figs. 1 and 2 of the main document, in Fig. S7 of the Supplemental Material and throughout the text in the main document – to the format using slashes.

Reviewer 3

I thank the authors for considering and addressing my comments. However, I would like to clarify one important point: What I consider a consolidated soil is by no means "perfectly non-erodible", contrary to what the authors specify in their rebuttal letter. There are many hard surfaces, for example, crusted and paved sediments, which are very erodible (e.g. Gonzalez-Romero et al., 2023). Perhaps there are different interpretations of what is a "consolidated" surface. In this context, it would be good to clarify what the authors consider "consolidated, shallow erodible soils" as in their revised manuscript (l. 292).

Reply: We fully agree, thank you for the note. We have now rephrased the referred sentence by clearly distinguishing between “perfectly non-erodible” surfaces (e.g., bare ground or bedrock) and “consolidated” surfaces, the latter including crusted and paved sediments, as well noted by the reviewer. Specifically, we have replaced this sentence by the following text, building on your pertinent remarks (provided in both your referee reports) and on the explanations provided in Gonzalez-Romero et al. (2023) (our new Ref. [39]), more precisely in their excellent introduction section:

[line 298] “Also, as noted for instance in Ref. [39], consolidated soils, such as crusts and paved sediments, can act as significant dust sources. This occurs when sandblasting by loose sand-sized particles from adjacent dunes [40] breaks down sediment aggregates, thereby exposing fine dust grains to entrainment [41]. Of course, in scenarios of shallow erodible soils atop perfectly non-erodible surfaces, such as bare ground or bedrock, dust sources are intrinsically limited, (…)“

Furthermore, at the end of the same paragraph, we have now replaced reference to “consolidation degree” with the following phrase, which emphasizes, once more in the manuscript, that the effect investigated in Fig. 2 is due solely to aerodynamic entrainment of dust (thereby not involving sand transport at all), so that it is relevant for loose soils, for consolidated soils, and for shallow erodible surfaces:

[line 308] “(…) the mechanism elucidated in Fig. 2 should be considered for developing dust schemes not only for loose soils, but also for consolidated and shallow erodible surfaces (since the effect refers purely to direct aerodynamic dust entrainment and does not involve transport of sand-sized particles).”

Review of the revised manuscript "Threshold for entrainment of mineral aerosols from grain-scale simulations" by S. Kamath, Y. Shao & E. J. R. Parteli

The authors have adequately addressed the minor comments. They also emphasized the conservative assumptions employed in the model:

1. Velocity on the leeward side of the protruding sand is set to zero, thus neglecting any possible initiated motion in this region.

2. The acceleration of the flow over the protruding sand (corresponding to compression of the streamlines) is neglected, such that the enhanced drag and lift on the protruding sand is not reflected in the results.

I acknowledge #1, and I understood this point in the original review comments. My concern is the windward side of the sand grains. I agree with the #2 point that the flow speed is enhanced over the top of the sand, but crucially this is with respect to two points *along the streamline*, which approximately follows a relative height z_{rel} as shown in the right of the figure below.

My understanding of the simulation is that the force on the dust is based on the *absolute* coordinates shown in the left of the figure, where I expect the force from $\overline{u}(z_{abs})$ is a multi-fold increase above $\overline{u}(z_{rel})$. The model reduces $\overline{u}(z_{abs})$ according to drag feedback from the particles (equation 13), but this correction appears to be constant along x. Accordingly, there would be a modest reduction in $\overline{u}(z_{abs})$ at all x positions rather than a larger reduction local to the sand and dust grains that would be required to achieve $\overline{u}(z_{abs}) \approx \overline{u}(z_{rel})$.

Further, the authors reduce the randomized velocity fluctuations within the viscous sublayer following the absolute height above the bed, but no correction is made to fluctuations along protruding grains following z_{rel}. Based on my understanding of the simulations, this treatment of the mean and fluctuations will lead to unrealistic velocities and overestimated forces on the windward side of the grains. The original and revised manuscripts have not addressed this limitation in the model, and it remains uncertain to what extent the overestimate from this limitation is balanced by the conservative choices above noted by the authors. My overall opinion of the manuscript, in particular the second paragraph in the original review, therefore remains unchanged following the revision.

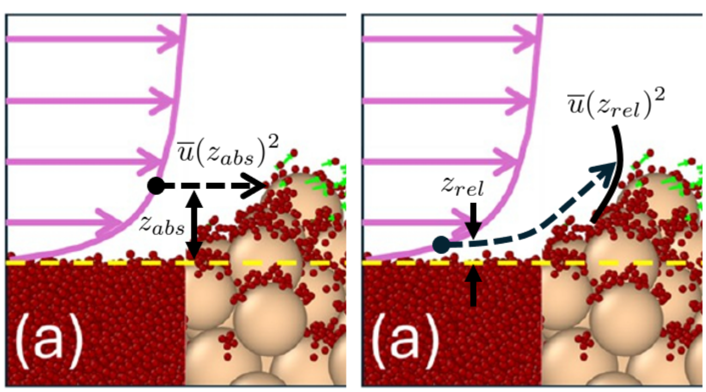

Figure 1: Average flow field exerting drag and lift on the dust: model assumption (left) and topography-induced flow (right). From on manuscript Fig. 2(a).

Review of "Grain-scale topography boosts emission of mineral aerosols" by S. Kamath, Y. Shao & E. J. R. Parteli

The authors use simulations of particles exposed to a boundary layer flow to study dust emission. The monodisperse particle bed simulations align well with previous observations for a range of particle sizes and cohesion. Simulations with a bidisperse particle mixture reveal that small dust particles can be exposed to higher positions within the flow when "stuck" to the tops of larger sand particles through inter-particle interactions. The exposed dust particles are subjected to higher wind speeds owing to their higher position, leading to enhanced emissions of dust in the bidisperse mixture.

The interpretation makes sense, and I suspect there is a real enhancement of dust emissions due to grain-scale topography in mixtures with larger particles. However, the result is also in part due to limitations of the stochastic model for representing the flow. It cannot be discerned from the present results how much of the outcome should be attributed to a real mechanism versus limitations in the methodology. I therefore recommend the article not be published, and encourage the authors to either validate the simplified two-way coupling in the bidisperse mixture or employ a more sophisticated flow model.

Further details on my main criticism are discussed below, followed by minor line-by-line comments. As an aside, if the results can be properly validated, it would be interesting to compare the findings with fluvial sediment transport in mixed-size beds. In that case the smaller particles mostly "hide" in the interstitial space between larger particles, leading to a reduction in transport of the small particles (Wilcock & Crowe, *J. Hydraulic Eng.* 2003). The opposite finding in this study appears to be due to inter-particle attractions which allow the smaller particles to remain at the top of the bed exposed to the flow.

Flow simulations

The flow model imposes a mean velocity profile that varies with height above the bed according the fundamental theory for boundary layer flows. The velocity fluctuations around the mean are also imposed using stochastic generation based on an assumed Gaussian distribution of the fluctuations. The only impact of the particles on the flow is to modify the mean velocity profile based on the total drag and volume on the particles (Eq. 13).

Accordingly, for a larger particle extending farther into the flow as seen in Fig. 2(a), the modelled flow velocity through the particle will correspond to the mean $\overline{u}_x$ at that height and a random fluctuation. In this case, the local smaller particles will almost certainly be exposed to a high velocity as noted in line 167.

In reality, the flow will be displaced around the protruding particle, introducing local fluctuations highly coupled with the particle location and an internal boundary layer forming around the particle. Due to this, the velocities around the protruding particles will be reduced compared to the mean. This reduction, due the coupling between the particle and the local fluctuations, is missing from the model.

The flow model is therefore missing crucial dynamics occurring locally around the particles that will be very consequential to the quantitative emission outcomes. The simplified flow model thus makes it difficult to trust the conclusions of the study. The validation of the flow model is unfortunately limited to the monodisperse case (Fig. 1). The simplified model is acceptable for the monodisperse case when the topography effects are the same size as the dust (Fig. 2a left side), but in the bidisperse case the topography induces much larger fluctuations and flow deformation around the large particles (Fig. 2a right side) that needs to be incorporated into the model to accurately predict the dust emissions.

Minor comments

1. *Line 18.* It is misleading to use the phrase direct numerical simulation here, given that this term is usually reserved for fully-resolved simulations of the Navier-Stokes equations in fluids literature.
2. *Line 71.* “Stable” boundary layer may be confused with a stably-stratified atmospheric boundary layer. Would “stationary” be a suitable descriptor?
3. *Line 87.* The assumption of isotropic turbulence is inconsistent with the fluctuation amplitude varying across directions (line 376).