Identifying sediment transport mechanisms from grain size-shape distributions

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- 10 **Abstract.** The way in which sediment is transported (creep, saltation, suspension), is traditionally interpreted from grain size distribution characteristics. However, the grain size range associated with transitions from one transport mode to the other is highly variable because it depends on the amount of transport energy available. In this study we present a novel methodology for determination of the sediment transport mode based on grain size and shape data from dynamic image analysis. The data are integrated into grain size-shape distributions and primary components are determined using end-member modelling. In
- 15 real-world datasets, primary components can be interpreted in terms of different transport mechanisms and/or sediment sources. Accuracy of the method is assessed using artificial datasets with known primary components that are mixed in known proportions. The results show that the proposed technique accurately identifies primary components with the exception of those primary components that only form minor contributions to the samples (highly mixed components).
- 20 The new method is also tested on sediment samples from an active aeolian system in the Dutch coastal dunes. Aeolian transport processes and geomorphology of these type of systems are well known and can therefore be linked to the spatial distribution of end members to assess the physical significance of the method's output. The grain size-shape distributions of the dune dataset are unmixed into three primary components. The spatial distribution of these components is constrained by geomorphology and reflects the three dominant aeolian transport processes known to occur along a beach-dune transect:
- 25 bedload on the beach and in notches that were dug by man through the shore-parallel foredune ridge, modified saltation on the windward and leeward slope of the intact foredune, and suspension in the vegetated hinterland. The three transport modes are characterised by distinctly different trends in grain shape with grain size: with increasing size, bedload shows a constant grain regularity, modified saltation a minor decrease in grain regularity and suspension a strong decrease in grain regularity. These trends, or in other words, the shape of the grain size-shape distributions, can be used to determine the transport mode
- 30 responsible for a sediment deposit. Results of the method are therefore less ambiguous than those of traditional grain-size distribution end-member modelling, especially if multiple transport modes occur or if primary components overlap in terms of grain size but differ in grain shape.

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1 Introduction

Clastic sediment records are generally complex mixtures of grains due to variability in provenance, conditions in the source

- 5 and sink areas (climate, tectonics) and sorting during entrainment, transport and deposition. One of the greatest challenges in sedimentology is to reconstruct signals of climate, tectonics and provenance from the sedimentary record (e.g. Garzanti et al., 2007; Métivier et al., 1998; Prins and Weltje, 1999a; Zhang et al., 2016). These reconstructions are improved when the mixed sedimentary record is unmixed into its primary constituent components (Weltje and Prins, 2007), a procedure which is also termed end-member modelling. Various end-member modelling algorithms are used in sedimentology (e.g. Dietze et al., 2012;
- Heslop et al., 2007; Paterson and Heslop, 2015; Weltje, 1997; Yu et al., 2016; Zhang et al., 2018). Although the algorithms are capable of unmixing different types of data, they are commonly used on grain size distribution data (e.g. Dietze et al., 2014; Liu et al., 2016; Stuut et al., 2002) and mineralogical data (Itambi et al., 2009; Weltje, 1995).

There are however at least two issues that complicate inferences based on single-property (size or mineralogy) end-member

- 15 modelling. First, sediment behaviour during uptake, transport and deposition is dictated by three grain properties: size, shape and density (mineralogy) (Winkelmolen, 1971). Therefore, single-property end-member modelling results are prone to noise from variability in the other two grain properties. The second issue is that the characterisation of sediment transport modes by their grain size-distribution alone produces ambiguous results: the grain size range associated with the transitions between transport modes (surface creep, saltation and suspension) depends on the amount of transport energy available and is therefore
- 20 highly variable (Visher, 1969). However, accurate identification of the transport mode is essential to a valid interpretation of sedimentary records since the transport modes sort sediment grains differently during transport and are associated with different transport velocities and distances.

In addition to sorting on grain size, sediment transport modes also sort shape in different ways. Studies on the influence of particle shape on surface creep are sparse. Eisma (1965) inferred that it is likely that surface creep favours spherical grains because these roll more easily. There are contradicting views regarding shape sorting during saltation: spherical grains bounce higher (Eisma, 1965) and further (McCarthy and Huddle, 1938) and thus travel faster than non-spherical grains. However, they are also more difficult to entrain (Winkelmolen, 1971). Likewise, studies on shape sorting in saltating transport under natural conditions obtained contradictive results: some publications observed an increase in sphericity with transport distance

30 (MacCarthy and Huddle, 1938; Mazzullo et al., 1986), others a decrease (Eisma, 1965; Winkelmolen, 1971). This is further complicated by the fact that inter-grain collision during (aeolian) saltation effectively rounds grains over longer distances (Kuenen, 1960). During transport in suspension, settling velocity is the dominant sorting parameter (McCave, 2008; Pye,

1994). Settling velocity is higher for more spherical and regularly-shaped grains (e.g. Dietrich, 1982; Komar and Reimers, 1978; Wadell, 1934). Hence, in a suspended population of grains, larger grains are expected to be more irregularly shaped than smaller ones to remain below the fall velocity threshold for suspended transport. For example, Shang et al. (2018) observed that elongation increases with increasing size in Chinese loess. This decrease in grain regularity with increasing size should

5 lead to a characteristic size-shape trend of suspended sediment that is different from that of sediment transported as bedload; using grain shape in addition to grain size is therefore a promising approach to determine transport modes with less ambiguity.

In this study we outline a new method for determination of sediment transport processes involving 1) the integration of grain size and shape data into size-shape distributions (e.g. Itoh and Wanibe, 1991) and 2) end-member modelling on these distributions. To determine the accuracy of the method, it is first tested on artificial grain size-shape datasets with known end members and known end-member mixing proportions. Subsequently, the method is applied to an active aeolian system in the Dutch coastal dunes (Ruessink et al., 2018). Aeolian transport processes and geomorphology of these type of systems are relatively well constrained (Arens et al., 2002) and can therefore be linked to the spatial distribution of end members to assess the physical significance of the method's output. The real-world dataset is also used to compare results of unmixing of size-shape distributions to results of traditional unmixing based on grain-size distributions.

2 Material and methods

2.1 Dune dataset

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The fieldwork area for our dataset is situated south of the town IJmuiden in a coastal dune region named National Park Zuid-Kennemerland (Appendix-Fig. 1A and 1BA1 and A2). In 2013, five notches were dug through the shore-parallel foredune
ridge to promote aeolian activity and dune migration (Appendix A2Fig. 1B). The notches are roughly orientated along the dominant wind direction: west-southwest to east-northeast. Parabolic dunes have developed at the downwind end of the notches and large volumes of sand have been blown land-inward. From 2013 to 2016, approximately 87*10³ m³ of sand was transported land-inward, 55% of which derived from the beach and 45% from erosion of the notches (Ruessink et al., 2018). Further land inward, vegetation has been removed from fossil parabolic dunes to stimulate reactivation of dunes (Appendix 25 Fig. 1BA2).

In order to assess the physical meaning of results from the new method, we divided the study area into its five main geomorphologic features (Appendix A3Fig 1C): 1) The beach, which acts as a sediment source for aeolian transport when dry. 2) The foredune, on which marram grass (partly) impedes bedload transport. Near the crest, aeolian suspension and modified saltation are stimulated through increased wind velocities and high turbulence (Arens et al., 2002). 3) The notches, which enable bedload transport towards the sand lobes that prograde into the vegetated hinterland (Ruessink et al., 2018). 4) The vegetated hinterland, where lower wind velocities and vegetation prevent bedload transport (Arens et al., 2002). And 5), the

parabolic dunes that were reactivated by removal of the vegetation cover. These dunes may form an additional source for the sediment flux in the hinterland (Arens et al., 2013).



5 Fig. 1. Fieldwork area in the coastal dunes of the National Park Zuid-Kennemerland. Figure 1A shows the general location of

the study area. Figure 1B displays the locations of surface samples and sediment traps. Figure 1C covers the same area and shows subregions based on geomorphologic features. Aerial photograph © PDOK.nl, 2017.

In April 2017, shallow surface samples were obtained from one of the bare notches (n = 12) and from an undisturbed part of
the foredune ridge (n= 18) (Appendix-Fig. 1BA2). Based on available flux data from sediment traps (not shown here),
deposition rates land inward from sediment-trap row A (or perhaps B) are insufficient to sample recently transported material
from the surface (Appendix-Fig. 1BA2). Samples from sediment traps (n = 23) are therefore used to study the land inward
area. The traps are based on a design by Leatherman (1978) and consist of an 80 cm pvc pipe with a mid-height of
approximately 1.5 m above ground level (Appendix BA). Their opening is oriented into the dominant southwestern wind
direction. At the back of the pipe a mesh with openings of 106 μm lets air and smaller particles through while trapping particles
larger than 106 μm. Three_-time intervals characterised by high flux rates ('storm events') were sampled from the sediment
traps (Table 1). Together, the sediment trap samples and surface samples form the dune dataset (Van Hateren et al., 2019).

 Table 1. Wind conditions and sampling periods of the sediment trap samples. Sediment trap names are in reference to Appendix

 A2Fig. 1B.
 Meteorological data were obtained from weather station IJmuiden, 3.5 km north of the fieldwork area.

Sampling	Number	Sediment traps	Mean daily	Maximum	Vector averaged
period	of	that were	wind speed	daily wind	wind direction
	samples	sampled	(m/s)	speed (ms ⁻¹)	(degrees)
27/10/2015 -	4	A1, B1, C3	8.5	15.5	214
17/11/2015		D3			
17-11-2015 -	15	All	11.8	17.1	255
01-12-2015					
01-12-2015 -	4	A1, B1, C3,	10.2	17.5	215
15-12-2015		D2			

2.2 Dynamic image analysis

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Sediment samples of approximately 2 grams are pre-treated with 5 ml H_2O_2 to remove organics, 5 ml HCl (10 ml if shell fragments are abundant) to remove carbonates and 300 mg $Na_4P_2O_7 \cdot 10H_2O$ to disperse charged particles (Konert and Vandenberghe, 1997). Size and shape data are based on images of the grains obtained using a Sympatec Qicpic dynamic image analyser (Fig. <u>1A2A</u>). The image analyser is set-up using a cuvette with 2 mm aperture. Pre-treated samples are sieved through a 1.6 mm mesh to protect the glass walls of this cuvette, thus limiting the maximum measurable grain size to 1600 µm. This is not of concern for the dune sands studied here, which show a maximum grain size of approximately 700 µm. The sediment samples are subsequently suspended in degassed water using a stirrer and pumped repeatedly through the cuvette for 10 minutes while being filmed at 25 frames per second, resulting in 15 thousand frames per sample. The frames measure 1024 by 1024 pixels with a pixel size of approximately 5 µm.

Image processing is carried out using a Matlab script written by the first author, for which Appendix \underline{BC} shows a workflow diagram. The particle size and shape characteristics that form the output of this script are described in Table 2 and an example is given in Fig. <u>1B2B</u>. In the first step of the script some limitations and conditions are set. Subsequently, the script iterates

- 5 over each video, over each frame in the video and over each particle found in the frames. For each particle, the length of its outer edge (perimeter) is computed, as well as its area and the length of its convex hull (a polygon drawn around the particle without taking into account the concave areas). These basic parameters are stored for each particle. Particle size, volume, aspect ratio, convexity and Cox circularity are subsequently computed from these basic parameters. It is important to note that the major and minor grain diameters, which are used to compute the aspect ratio, are based on the diameters of a fitted ellipse.
- 10 These diameters are less sensitive to small scale particle roughness than the traditional Feret diameters (Feret, 1930). <u>"The"</u> grain size of the particle is given in the form of an area equivalent diameter (Table 2), essentially the average particle diameter of the two-dimensional image of the grain. Because the two-dimensional shape of the particle is known, grain size obtained by image analysis is more robust than traditional size measurements (e.g. sieving, laser diffraction and settling) where an assumption has to be made of particle shape before computing size (Konert and Vandenberghe, 1997). For the same reason,
- 15 "the" diameter of the particle is given in the robust form of an area equivalent diameter (Table 2). We use ranges of interest in the graphs of size and shape distributions to focus on those size and shape classes that contain significant amounts of volume for the given dataset (Table 2).

Table 2. Summary of particle characteristics and derived size and shape variables. The table shows lower and upper limits for the variables as well as the size of the respective size or shape classes. The range of interest designates the range over which the sediments studied here contain significant volume for a given variable. The φ unit refers to Krumbein's log base 2 grainsize scale (Krumbein, 1938).

Variable	Name	Description	Equation	Lower	Upper	Size	Number	Range of
				<u>limit</u>	<u>limit</u>		of classes	interest
<u>P</u> _p	Perimeter	Length along	Ξ	Ξ	Ξ	Ξ	Ξ	z.
		particle boundary						
$\underline{\mathbf{P}}_{ch}$	<u>Convex</u>	Length along	Ξ	Ξ	±.	±.	=	± 1
	<u>hull</u>	convex points on						
		<u>boundary</u>						
<u>A</u>	<u>Area</u>	Surface area of the	=	Ξ	=	Ξ	=	± 1
		particle						

$\underline{D}_{\underline{A}}$	<u>Major</u>	Major diameter of	±.	Ξ	±.	Ξ	±.	±.
	<u>diameter</u>	ellipse fitted to						
		particle						
<u>D</u> _B	Minor	Minor diameter of	±.	Ξ	± 1	±.	± 1	±.
	<u>diameter</u>	fitted ellipse						
<u>D2d</u>	<u>Area</u>	Diameter of circle	A	<u>13 µm</u>	<u>2828 µm</u>	$\frac{1}{8} \phi$	<u>62</u>	<u>105-707 μm</u>
	<u>equivalent</u>	with area equal to A	$2\sqrt{\pi}$			0		
	<u>diameter</u>		•					
Con	Convexity	Ratio between	P_{ch}	<u>0</u>	<u>1</u>	<u>0.01</u>	<u>100</u>	<u>0.8-1</u>
		convex hull length	P_p					
		and perimeter						
		length						
<u>Cc</u>	<u>Cox</u>	Ratio that describes	$4\pi \frac{A}{2}$	<u>0</u>	<u>1</u>	<u>0.01</u>	<u>100</u>	<u>0.4-1</u>
	<u>circularity</u>	extent to which the	P_p^2					
	<u>(Cox,</u>	area of a particle						
	<u>1927)</u>	approximates that						
		of a circle with the						
		same perimeter						
Ar	Aspect	Ratio of the major	D_B	<u>0</u>	<u>1</u>	<u>0.01</u>	<u>100</u>	<u>0.3-1</u>
	<u>ratio</u>	and minor diameter	D_A					
$\underline{\mathbf{V}}_{\underline{\mathbf{A}}}$	Ξ	Volume	$\frac{4}{2}\pi^{-0.5}A^{1.5}$	Ξ	±.	Ξ	±.	±.
		approximated from	3					
		A, assuming a						
		spherical particle						
		shape						

2.3 Construction and unmixing of size-shape distributions

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We explore the applicability of three shape parameters that are known to affect particle transport behaviour: convexity, Cox
circularity (Cox, 1927) and aspect ratio (Table 2; Beal and Shepard, 1956; Dietrich, 1982; MacCarthy and Huddle, 1938;
Winkelmolen, 1971; Shang et al., 2018). These parameters relate to different aspects of a particle's shape: aspect ratio describes

the overall shape of a particle. In contrast, convexity is primarily affected by a particle's surface irregularity whereas Cox circularity is affected by both.

Grain size-shape distributions (SSDs) are constructed from grain size (D2d, Table 2) and the three shape variables, resulting
in the distributions named ArD2d, ConD2d and CcD2d. The SSDs are created by assigning individual particles to their respective size-shape classes (Fig. 1C2C; Table 2). Next, the volume of the grains in each size-shape class is summed, and the distribution is normalised to a sum of 100% using the total volume. This procedure gives rise to three-dimensional distributions (X = size, Y = shape, Z = volume) (Fig. 1D2D) that can be visualised as a combination of a grain size (X – Z) and a grain shape (Y-Z) distribution (Fig. 1E2E).



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Fig. <u>42</u>. A: Binary image of sediment grains. B: Computation of particle characteristics (note inversed black-white scale). C: Assignment of grains to size-shape classes. D: Grain size-shape distribution (ConD2d in the example, star marker designates the mode of the distribution). E: grain size (upper panel) and grain shape (lower panel) cross-sections through the SSD along respectively A-A' and B-B'.

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End-member modelling algorithm AnalySize (Paterson and Heslop, 2015) is used to unmix the SSD datasets because it produces the most accurate results of the algorithms currently available (Van Hateren et al., 2017). The computed end members are hereafter referred to as end member EMx_{-y} where x denotes the end member number from coarse to fine and y denotes the

total number of end members in the given end-member modelling solution. For example, the coarsest EM of a dataset with four EMs is referred to as EM1-4.

The fit of end-member modelling solutions to the data is used to infer the most likely number of end members. The fit is

- 5 described by variance squared, also termed the coefficient of determination (R²). We define two types of R²: 1). class-wise R², denoting the fit per grain size class (grain-size distributions) or grain size-shape class (SSDs), and 2) sample-wise R², denoting the fit per sample (Van Hateren et al., 2017). By increasing the number of end members, R² will increase. However, at a certain point the increase in fit is not due to geologically significant end members but due to fitting of noise. We therefore seek the minimum number of end members sufficient to explain most of the variation in the dataset. In grain-size data analysis, this
- 10 minimum number of end members is traditionally estimated by a flattening off of the curve of average R² versus the number of end members, also known as the inflection point (Prins and Weltje, 1999b; Weltje, 1997). However, tests with artificial grain size data have pointed out that this method sometimes yields an incorrect number of end members (Van Hateren et al., 2017). Rather than taking the average, we therefore use the full distribution of class-wise R² to obtain more detailed information on the most likely number of end-members (Prins and Weltje, 1999b; Van Hateren et al., 2017). In addition, we use the
- 15 distribution of sample-wise R².

2.4 Artificial datasets for testing and validation of the method

Artificial datasets with known end members and end-member abundances (Van Hateren et al., 2019) are used to evaluate 1) the accuracy of unmixing of SSDs under different mixing scenarios and 2) the potential of, and difference between, class-wise and sample-wise R^2 for identification of the most likely number of end members in a SSD dataset. The known end members

20 of the artificial datasets are hereafter referred to as input end members IEMx_{-y} similar to the notation for modelled end members.

Following an approach similar to Van Hateren et al. (2017), three datasets are created with increasingly complex mixing scenarios: The least complex dataset, 3EM_nonoise, is created using as IEMs three samples of the dune dataset with markedly
different size-shape distributions (Appendix DC). Two-hundred sets of three random numbers are generated with a uniform distribution between 0 and 1 using a random number generator. Each set of three numbers is subsequently normalised to sum-to-one. The two-hundred sets represent the contributions of the IEMs to each artificial sample (end-member abundances). By multiplying each set of three random numbers with the three IEM SSDs, two-hundred artificial samples are generated.

30 The second dataset, 4EM_noise, is used to test accuracy of the method in the presence of noise and an additional end member. Addition of noise decreases accuracy of unmixing results in grain size distribution datasets (Van Hateren et al., 2017). The IEMS of the 4EM_noise dataset are the same as those of the 3EM_nonoise dataset except for an additional end member that, in terms of its grain size, is between the coarsest and intermediate IEM of the 3EM_nonoise dataset (Appendix ED). Noise is included in the dataset by multiplying the volume in each size-shape class of the artificial samples by a random number with a normal distribution characterised by a mean of 1 and a standard deviation of 0.05.

The third and most complex dataset, 4EM_noise_highmix, is similar to 4EM_noise (Appendix E) but has different end-member abundances. This dataset is used to test the accuracy of the output for highly mixed datasets. In such datasets, one or more of the primary components do not form a dominant contribution to any of the samples. Highly mixed data significantly deteriorate accuracy of unmixing (Heslop, 2015; Van Hateren et al., 2017). We use the following mixing scenario: IEM1₋₄ occurs in only 5 samples at abundances between 0.2 and 1 (20 and 100%). IEM2₋₄, the highly mixed end member, occurs in 100 samples at low abundance between 0.05 and 0.2 (5% and 20%). IEM3₋₄ and IEM4₋₄ occur in all two-hundred samples at randomly varying

10 abundance.

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Because the number of end members, the end-member abundances and the end-member SSDs are known, the precision of the unmixing procedure can be <u>deduced_determined</u> from 1) the correlation between IEM SSDs and modelled end-member SSDs, 2) the correlation between the input and modelled end-member abundances and 3) the correlation between the input and modelled data expressed as class-wise and sample-wise R². Furthermore, the applicability can be assessed of class-wise and

sample-wise R² for identification of the most likely number of end members, which is an unknown in real-world datasets.

3 Results

3.1 End-member-modelling results for the artificial datasets

3.1.1 End-member-modelling results for the 3EM_nonoise dataset

- 20 Due to absence of noise in the 3EM_nonoise dataset, explained variance of the end-member modelling outcome reaches 100 percent at three end members. Because model fit cannot be improved further, the AnalySize algorithm aborts at three end members (the algorithm fits a maximum of 10 end members for real-world datasets that naturally include noise). Figure 2-3 therefore displays class-wise R² distributions for results with one to three end members (1EM to 3EM solutions). The 'average' SSD of the dataset as well as the modelled end-members are shown as contours to indicate the relevant size-shape classes. The 1EM solution fits the input data poorly while the 2EM output increases model fit significantly but lacks explanatory power in the size-shape region that coincides with the missing third end member (Fig. 23, Appendix DC). Using three end members increases goodness of fit of all size-shape classes to an R² of 1. Appendix G1-F1 shows median sample-wise and class-wise R² versus the number of end members. Class-wise R² shows a near linear increase from one to three end members whereas the curve of sample-wise R² inflects at two end members. In other words, the improvement in sample-wise R² is significantly
- 30 higher from 1 to 2 end members than it is from 2 to 3 end members.



Fig. 23. Class-wise R² distributions for end-member modelling results of the ConD2d 3EM_nonoise dataset from a 1EM up to a 3EM solution. Solid black lines denote end-member contours: lines drawn along those size-shape classes where the volume
of the end-member SSD equals 0.5%. The median SSD of the dataset (average SSD) is represented by a dashed line at 0.2% volume. White stars denote the modes of the end-member size-shape distributions.

Since the 3EM_nonoise dataset is noise-free and consists of three IEMs, an accurate 3EM solution should be identical to the input data, which is nearly the case (Fig. 34). The abundances show 100% explained variance; however, linear trends between the original and determined abundances reveal a slope slightly higher than one, meaning that high input abundances are calculated too high and that low input abundances are calculated too low (below input abundances of approximately three percent, determined abundances go to zero) (Appendix H1G1). Thus, the computed end members are to a minor degree still mixtures of the IEMs.





Fig. 34. Input end members (top) and determined end members (bottom) for the ConD2d 3EM_nonoise dataset, with R² values denoting the fit between them (lower right corners). The first R² value indicates the correlation of the determined end member with IEM1-3, the second with IEM2-3 etcetera. White stars mark the modes of the SSDs.

3.1.2 End-member modelling results for the 4EM_noise dataset

Figure 4-5_shows class-wise R^2 distributions of solutions for the 4EM_noise dataset. Similar to results for the 3EM_nonoise dataset, a 1EM solution fits the data poorly and a 2EM solution increases the fit significantly but lacks explanatory power in the intermediate and coarse size-shape regions. A 3EM solution fits the intermediate region significantly better but still lacks explanatory power in the coarse region. Compared to that of the 3EM solution, the class-wise R^2 distribution of the 4EM solution displays an increase in R^2 in the coarse range because EM1.4 more closely resembles IEM1.4 than does EM1.3 (Fig.

45; Appendix ED). The increase in median class-wise R^2 is small because the improvement occurs in relatively few size-shape classes (Appendix G2F2). Median sample-wise R^2 similarly increases by a low amount. The increase in sample-wise R^2 diminishes from four end members onwards (Appendix G2BF2B). Class-wise R^2 even displays a minor decrease of fit. In

contrast to results for the 3EM nonoise dataset, the explained variance does not reach 100%.

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Fig. 45. Class-wise R² distributions for end-member modelling results of the ConD2d 4EM_noise dataset. Solutions up to eight end members are shown. Solid black lines denote end-member contours: lines drawn along those size-shape classes where the volume of the end-member SSD equals 0.5%. The median SSD of the dataset (average SSD) is represented by a dashed line at 0.2% volume. White stars denote the modes of the end-member size-shape distributions.

Figure <u>5-6</u> compares the input and determined end-member SSDs. In spite of the noise added to this dataset, the determined end members are very similar to the IEMs. Calculated abundances fit the input abundances well, although a minor scattering

20 is present (Appendix H2G2). Similar to the results for the noise-free dataset, linear trends have a slope higher than one, indicating that the determined end members are, to a minor extent, mixtures of the IEMs.



Fig. 56. End members determined for the ConD2d 4EM_noise dataset. Input end members (top) are compared to determined end members (bottom) including R^2 values. The first R^2 value indicates the correlation of the end member with IEM1₋₄, the second with IEM2₋₄ etcetera. White stars mark the modes of the SSDs.

5 3.1.3 End-member modelling results for the 4EM_noise_highmix dataset

Similar to the results in sect. 3.1.1 and 3.1.2, the 1EM solution modelled for the 4EM_noise_highmix dataset fits the dataset poorly (Fig. 67). The 2EM class-wise R² distribution is notably different from that of the 4EM_noise dataset: the entire coarse range (>350 μ m) is not well reproduced. The reason for this disparity is that IEM1.4 and IEM2.4 are not represented in this solution and thus the coarse range is underrepresented (Appendix FE; Fig. 7).

10 A 3EM solution covers the coarser range, invoking a strong increase in class-wise R^2 to a level comparable to that of the 4EM solution of the 4EM_noise dataset (Fig. <u>76</u>; Appendix <u>FG2</u> and <u>G3F3</u>). In contrast to the results for the 4EM_noise dataset, addition of a fourth end member does not result in a significant improvement of class-wise and sample-wise R^2 .



Fig. <u>67</u>. Class-wise R² distributions for end-member modelling results of the ConD2d 4EM_noise_highmix dataset. All solutions up to eight end members are shown. Solid black lines denote end-member contours: lines drawn along those size-shape classes where the volume of the end-member SSD equals 0.5%. The median SSD of the dataset (average SSD) is represented by a dashed line at 0.2% volume. White stars denote the modes of the end-member size-shape distributions.

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Size-shape distributions of the end members and IEMs are shown in Fig. 78. The 4EM solution computed for the 4EM_noise_highmix dataset differs in one notable aspect from that calculated for the 4EM_noise dataset: IEM2.4 is not identified as a primary component of the dataset. Rather, the SSD of EM2.4 more closely resembles IEM3.4 leading to overestimated abundances of EM2.4 and underestimated abundances of EM3.4 in the 4EM solution (Appendix H3G3). However, the SSDs and the relative abundances of the 3EM solution show a good fit to the SSDs and abundances of the three non-highly mixed IEMs (Appendix FE; Appendix GH4).



15 Fig. 78. End members determined for the ConD2d 4EM_noise_highmix dataset. Input end members (top) are compared to

determined end members (bottom) including R^2 values. The first R^2 value indicates the correlation of the determined end member with IEM1-4, the second with IEM2-4, etcetera. White stars mark the modes of the SSDs.

3.2 Results for the dune dataset

5 End-member-modelling results for the dune dataset are presented in three subsections: statistics for the ConD2d dataset are shown first to derive the number of end members necessary to explain size-shape variability of the dataset. End-member SSDs and abundances of the robust solution are presented in the second subsection. The third subsection compares results of unmixing based on SSDs to results of unmixing based on grain size distributions (D2d).

3.2.1 Unmixing of the size-shape distributions

10 Appendix <u>LH</u> displays the trend of median class-wise and sample-wise R² against the number of end members. Class-wise R² reaches a plateau at three end members whereas sample-wise R² inflects gradually between two and four end members. This gives a first indication that the likely number of end members is between two and four.

Two methods are employed to visualise the fit of the end-member solutions to the dataset in more detail. Class-wise R² 15 distributions show the fit per size-shape class (fig. <u>89</u>). The spatial distribution of sample-wise R² is shown by plotting it on top of an aerial photograph of the study area (Appendix <u>J411</u>). The goodness of fit of the samples is compared to the subregions based on geomorphology as shown in <u>Appendix A3Fig. 1C</u>, shown in simplified form in appendix <u>J1-11</u> and described in Sect. 2.1. If the unmixing result fits poorly to samples from a specific subregion it is likely that an additional end member is needed to explain the data in that region.

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One end member is insufficient to capture the size shape variability of the dataset: the class-wise R² distribution shows low values across all size-shape classes (Fig.§ 9). The 1EM solution does not fit well to the samples either, as expressed by low sample-wise R² (Appendix III). The spatial distribution of sample-wise R² for the 2EM solution shows a good fit to the sediment trap samples of the hinterland. However, the fit to samples of the notch and foredune ridge is poor. The 3EM solution drastically improves fit in these subregions (Appendix III). Regarding the class-wise R² distribution, the 2EM solution performs poorly in the range where its EM1-2 and EM2-2 overlap, indicating that an additional end member is required to fit these classes (Fig. 89). A 3EM solution represents this intermediate size-shape range much better. Furthermore, comparison of the class-wise R² distribution to the median data contour shows that this unmixing result performs well in the entire size-shape range where significant volume is present in the data (Fig. 89).

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Although the 3EM solution displays high and evenly spread sample-wise R^2 , there are two regions that stand out: first, slightly lower explained variance occurs at those inland samples that are positioned downwind of fossil dunes that had their vegetation

cover removed (Appendix <u>H11</u>; <u>Appendix A2 and A3Fig. 1B and Fig. 1C</u>). A 4EM solution does not improve explained variance of these samples significantly (Appendix <u>H11</u>). Second, the 3EM solution displays low sample-wise R² on the northern foredune sampling transect, in a small region near the crest (Appendix <u>H11</u>). This is improved by component EM2.4 of the 4EM solution which occurs specifically in this region (Appendix <u>LK</u>). The specific geographical location of the component indicates that it has some geological significance. Furthermore, it is also determined in the 5EM and 6EM solutions (Appendix <u>K1</u>) and therefore is a robust component. However, it is of minor importance in terms of geographical extent and in terms of the number of samples it represents. The class-wise R² distribution of the 4EM solution shows amelioration of fit below a convexity of 0.9 and above a size of 250 μm, but volume in this range is insignificant (Fig. <u>89</u>). Further increasing the number of end members does not increase model fit significantly except that the 6EM solution increases sample-wise R² for the inland samples downwind of unvegetated dunes (Appendix <u>H11</u>; <u>Appendix A2 and A3Fig. 1B and Fig. 1C</u>). In conclusion, a 3EM output appears most robust and it reproduces the bulk of spatial variability in grain size and shape, although a four end-member solution locally improves sample-wise R².

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1.00 Convexity 0.90 0.85 Class-wise R² 0.6 0.4 0.85 0.2 2EM 4EM 3EM 1EM 0.80 0 1.00 Convexity 0.90 0.85 0.85 6EM 7EM 8EM 5EM 0.80 125 177 250 354 500 707 125 177 250 354 500 707 125 177 250 354 500 707 125 177 250 354 500 707 Grain size (μm) Grain size (μm) Grain size (μm) Grain size (μm)

15 Fig. 89. Class-wise R² for end-member modelling results of the ConD2d distributions of the dune dataset. All solutions up to eight end members are shown. Solid black lines denote end-member contours: lines drawn along those size-shape classes where the volume of the end-member SSD equals 0.5%. The median SSD of the dataset (average SSD) is represented by a dashed line at 0.2% volume. White stars denote the modes of the end-member size-shape distributions.

3.2.2 End-member composition and abundances of the three-end-member solution

20 The end-member SSDs of the 3EM solution computed for the ConD2d distribution dataset differ markedly from one another (Fig. 910): most volume of coarse-grained EM1.₃ is contained between 250 and 500 μ m. Its mode lies at a grain size of 339 μ m and a convexity of 0.945. This convexity dominates over the entire size range. The intermediate EM2.₃ is finer grained, with most of the volume between 160 and 350 μ m. Its mode is positioned at a size of 201 μ m and a convexity of 0.945. In

contrast to EM1₋₃, it shows a gradual decline in convexity with increasing size. Most volume of fine-grained EM3₋₃ lies between 150 and 250 μ m. Its mode is located at a size of 185 μ m and a convexity of 0.935. It shows a strong decrease in convexity with increasing size.



Fig. 910. SSDs of the ConD2d 3EM solution determined for the dune dataset. White stars mark the modes of the SSDs.

The end-member abundances of the 3EM solution show a strong spatial differentiation that corresponds with morphological features: EM1.3 dominates the unvegetated notch that was dug through the foredune (average abundance 81%). EM2.3
dominates most of the sparsely vegetated foredune (average abundance 46%) as well as the vegetated area directly downwind of the sand lobe that is prograding from the notch (average abundance 80%). EM3.3 dominates the vegetated hinterland (trap rows B to D, average abundance 94%) (Fig. 1011). It is also noteworthy that samples from traps A1, A2 and B2 contain significantly more of EM3.3 than the surface samples taken at the same locations and thus also lower the average abundance of EM2.3 for the foredune (Fig. 1011; Appendix A2Fig. 1B).

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Fig. <u>1011</u>. Pie-charts showing abundances of the 3EM solution computed for the ConD2d distributions of the dune dataset. Pie-charts with a black outline denote surface samples and are plotted at the sampling location. Pie-charts with a white outline denote sediment trap samples and are plotted near the sampling location. The exact locations of sediment traps are marked by black dots. Two of the subregions defined in appendix A3 are shown in simplified form. Aerial photograph © PDOK.nl, 2017.

3.2.3 Comparison of results to traditional end-member modelling on grain-size distributions

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Besides the size-shape variable ConD2d, we also tested CcD2d and ArD2d. These variables make use of the shape variable Cox circularity and aspect ratio, respectively. In this section we intercompare end-member modelling results of the three size-

- 10 shape variables. Furthermore, we compare the results using size-shape variables to results from traditional end-member modelling on grain-size distributions (D2d). To enable direct comparison between grain size distributions and SSDs, the latter are transformed to grain size distributions by summation of the volumes of all shape classes per size class and subsequent renormalisation to 100% (Fig. <u>4412</u>). The 3EM solution is used for the comparison. This number of end members is also robust for traditional grain-size based end-member modelling: median R² values level off at three end members (Appendix <u>M4L1</u>),
- 15 grain size classes with significant volume show high R^2 indicating that class-to-class variability is well resolved (Appendix

<u>M2L2</u>) and sample-wise R^2 is high throughout the fieldwork area indicating that spatial variability is also well resolved (Appendix <u>J2L2</u>).

ConD2d end-member grain-size distributions show significant deviations from those determined for D2d: most notably a finer modal size for EM2.₃, but also a more extended fine tail for EM1.₃ and coarse tail for EM3.₃ and (Fig. <u>11A12A</u>). The grain size distributions of CcD2d show deviations at the same grain-size ranges. However, the deviations are weaker than for ConD2d (Fig. 12+B). In contrast, size distributions of the ArD2d end members equal those of D2d (Fig. 12+C). Furthermore, the SSDs of ArD2d end members lack the trend in grain shape with grain size that was observed for ConD2d and CcD2d (Fig. <u>10</u>; Appendix <u>M</u>N).



Fig. <u>112</u>. ConD2d (A), CcD2d (B) and ArD2d (C) 3EM solutions determined for the dune dataset. The SSDs are displayed as grain size distributions (solid lines) and compared to grain size distributions of the D2d 3EM solution (dashed lines).

- 15 Table 3 and Appendix O-N compare end-member abundances for 3EM solutions of ConD2d, D2d, CcD2d and ArD2d. The main trends of all variables correspond: EM1₋₃ prevails in the notch, EM2₋₃ on the foredune and in the vegetated area within 100 m downwind of the notch, and EM3₋₃ in the hinterland. However, differences exist between the variables: ConD2d and CcD2d show higher proportions of EM1₋₃ in the notch than do ArD2d and D2d (Table 3). The four variables show similar proportions of EM2₋₃ on the foredune, but differences occur in the samples directly downwind of the notch. Here, proportions
- 20 are highest for ConD2d, followed by CcD2d, D2d and ArD2d (Table 3). Similarly, proportions of EM3.₃ in the hinterland are slightly higher for ConD2d, followed by CcD2d, ArD2d and D2d (Table 3). In summary, unmixing outcomes of ConD2d are generally most extreme, followed by CcD2d (they show the highest abundances of the dominant end-member). Results from ArD2d and D2d are generally less extreme. This clustering of results agrees with what was observed for the end-member grain-size distributions in Fig. <u>1112</u>: ArD2d distributions are highly similar to those of D2d, whereas ConD2d and CcD2d
- 25 distributions differ respectively strongly and weakly from the D2d distributions.

Area, prevalent end	ConD2d	CcD2d	ArD2d (%)	D2d (%)
member	(%)	(%)		
Notch, EM1-3	81	75	62	62
Foredune, EM2-3	46	47	52	53
<100m downwind	80	66	57	58
from notch, EM2-3				
Hinterland, EM3-3	94	90	90	89

Table 3. Average end-member abundances of the dominant end-member per subregion as defined in Appendix A3.

4 Discussion

4.1 Accuracy of end-member modelling on size-shape distributions

5 4.1.1 Accuracy of the unmixing methodology under different mixing scenarios

The precise 3EM solution for the 3EM nonoise dataset confirms that the method is highly accurate under the condition that no noise is present in the dataset. Results for the 4EM noise dataset indicate that computed end members remain correct reproductions of the input end members in presence of noise. However, the noise induces minor deviations in the end-member proportions. Two conclusions can be drawn on basis of the results for the 4EM_noise_highmix dataset. First, primary components that occur in a limited number of samples but at high proportions (IEM1.4) can be accurately determined by AnalySize. Second, highly mixed primary components (IEM2.4) cannot be determined accurately by AnalySize. This outcome

is similar to results for highly mixed grain-size distribution data (Van Hateren et al. 2017). The implication for real-world datasets is that highly mixed components will be overlooked during the end-member modelling procedure. However, our results indicate that the remaining end members and their relative proportions are computed accurately.

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4.1.2 Methods for determination of the most likely number of end members

In the current study we use artificial datasets with a known number of end members. This allows us to test three methods for detection of the statistically feasible number of end members: median class-wise R^2 , median sample-wise R^2 and class-wise R^2 versus size and shape (a class-wise R^2 distribution). The latter is similar to a graph of class-wise R^2 versus grain size for grain size data.

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Our results for artificial datasets indicate that interpretation of the number of end members is straightforward in the absence of noise but ambiguous when noise is present: the noise-free dataset (3EM nonoise) displays class and sample-wise R^2 values of one when the number of determined end members equals the number of end members present in the dataset. In contrast, the R^2 values for the noise-containing dataset (4EM_noise) never reach 1, which is more in line with end-member modelling results for real-world datasets. In this case, median R^2 can only be used as a rough indication of the number of end members since an 'inflection point' (Prins and Weltje, 1999b; Weltje, 1997) is ill-defined: median R^2 values for the dataset level off at three end members rather than four. A class-wise R^2 distribution provides a better estimation of the number of end members: the presence of four end members is apparent from an increase in class-wise R^2 in the coarser size range going from a 3EM to

5 a 4EM solution. The presence of the highly mixed end member in the dataset 4EM_noise_highmix is not apparent from the class-wise R² distribution, indicating that such an end member will likely be ignored in the end-member modelling of real-world data.

There are two additional conceivable methods for determination of the geologically feasible number of end members: 1) A graph of sample-wise R² against depth (core/outcrop) or against sample location (spatial data such as the dune dataset) and 2) using samples of known origin to demonstrate the geological meaning of the end members (Weltje and Prins, 2003). These two methods cannot be tested with artificial data and thus will be discussed using the dune dataset.

- Results for the dune dataset indicate that spatially resolved sample-wise R² can be used to determine the number of end members, especially when the spatial distribution of model fit is compared to known geomorphology of the area. For example, the 2EM solution fits poorly to the samples of the notch and foredune area. This indicates that two primary components are insufficient to describe the processes occurring in these subregions. The 3EM solution satisfactorily fits all main subregions, indicating that it captures the main transport processes that are active in the study area. The dune dataset also provides two examples of modern-day samples of known transport processes that can be used as reference material for paleo-studies. Surface
- 20 samples from the notch area can be used as a reference for aeolian bedload sediment because the surface of the notch area was characterised by aeolian current ripples. Furthermore, samples from sediment traps, especially from rows C and D which are furthest land-inward (appendix AFig. 1B), can be used as a reference for aeolian suspension because 1) the distance from the main source areas (beach/ notches) excludes modified saltation from reaching the traps, 2) land-inward from the foredune ridge, denser vegetation rules out new entrainment of sediment (Arens et al., 2002; Lancaster and Baas, 1998) and 3) the height
- 25 of the sediment traps further reduces the chance of contamination by local saltation.

4.2 The value of end-member modelling on size-shape distributions: implications of the dune dataset

4.2.1 Geological significance of the three-end-member ConD2d model

The spatial distribution of end members of the 3EM solution relates strongly to the geomorphology of the area: EM1.₃ occurs mainly on the bare surfaces of the beach and notch, EM2.₃ occurs on the sparsely vegetated foredune and within the vegetated area directly downwind of the notch, and EM3.₃ occurs in the vegetated hinterland. This geographical differentiation suggests that the end members are linked to the three aeolian processes known to operate on a beach to dune transect: 1) bedload, consisting of saltation, reptation and creep, the motions of which are predominantly affected by gravity, 2) modified saltation, which is affected by both gravity and turbulence and 3) suspension, of which the motions are predominantly affected by turbulence (Arens et al., 2002; Hunt and Nalpanis, 1985).

- 5 As mentioned in Sect. 4.1.2, aeolian current ripples on the supratidal beach and in the notch confirm that EM1₋₃ is linked to the bedload population. Component EM2₋₃ specifically occurs on the windward and leeward slope of the foredune. Several processes on the foredune increase the proportion of grains travelling in modified saltation (Arens et al., 2002): 1) On the windward slope of the foredune, relief and marram grass induce turbulence, thereby increasing the proportion of grains that travel in modified saltation and suspension. 2) At the same time, the vegetation partly impedes bedload transport. 3) At the
- 10 foredune crest, flow separation induces even stronger vertical air motion, forcing the grains into short-term suspension. The grains that are less susceptible to turbulence are deposited at the leeward side of the foredune (modified saltation population), whereas the grains that are more susceptible to turbulence (the true suspension population) travel further land inward where EM3.₃ dominates. As stated in Sect. 4.1.2, the interpretation of EM3.₃ as suspension component is further corroborated by the distance from the source (beach/notches), the dense vegetation in the hinterland, and the fact that the sediment traps are at
- 15 approximately 1.5 m above ground level. Sediment traps om the foredune also show a high contribution of EM3₋₃, which is on average higher than that of the surface samples at the same location. This is likely related to the height of the traps, causing them to trap the sediment that is in transport (suspended load and modified saltation) rather than the sediment that is deposited (bedload and modified saltation).
- 20 The three end members were also set apart by a markedly different *shape* of their size-shape distributions: the bedload population was characterised by a constant grain regularity with increasing size, the modified saltation population by a minor decrease in grain regularity and the suspended population by a strong decrease in grain regularity. These differences are likely caused by differences in size-shape sorting between the transport modes. Movements of grains in saltation are driven mainly by gravity (Hunt and Nalpanis, 1985), which is a function of particle mass. Because the beach sediments in our fieldwork area
- 25 are of uniform density with negligible heavy mineral content (Eisma, 1968), particle mass is mainly determined by particle size. Size, not shape, is therefore the predominant sorting agent during saltation. Eisma (1965) furthermore inferred that it is likely that surface creep favours spherical grains because they roll more easily. It therefore follows that the overall bedload population should show relatively regularly shaped grains and no significant trend of grain shape with grain size. This is indeed the case for EM1.3.
- 30

Settling of grains in suspension is driven by gravity and restrained by aerodynamic drag of a particle. The latter factor also depends on grain shape: irregular grains have more drag, and thus settle slower (Komar and Reimers, 1978) and are also more susceptible to turbulence. It therefore makes sense that the SSD of suspension component EM3₋₃ shows a strong decrease in grain regularity with increasing size: the irregularity of the coarser grains compensates for their larger weight. Chinese loess

deposits are on the order of two to ten times finer grained than EM3.₃ and show a similar decrease in grain regularity with increasing size (Shang et al., 2018). This indicates that: 1) a decrease in grain regularity with increasing size is characteristic of sediments transported in aeolian suspension, and 2) for a given transport mode and a similar grain shape range, the grain-size of sediment depends on, and is a reflection of transport conditions (amount of transport energy available and transport

5 distance). SSDs are therefore a good indication of the mode of transport; grain-size distributions are not.

Modified saltation is a process that is intermediate between saltation and suspension: grains are saltating (sorted by susceptibility to gravity) but are also shortly suspended (sorted by susceptibility to gravity and turbulence). The size-shape distribution of EM2.₃ is indeed intermediate between EM1.₃ and EM3.₃, both in terms of its grain size and its minor decline in grain regularity with increasing grain size.

4.2.2 A comparison of traditional grain-size based and novel size-shape based end-member modelling

End member distributions obtained using size-shape variable ArD2d are remarkably similar to those obtained using traditional size-based end-member modelling (D2d). This suggests that during transport, grains are not sorted by their aspect ratio. However, Shang et al. (2018) did observe sorting of aspect ratio. This incongruity may be explained by the difference in how aspect ratio was defined in the two studies: We defined aspect ratio based on the major and minor diameters of ellipses fitted

to the particles. These diameters represent the overall particle shape since their length is not sensitive to small-scale particle roughness: the ellipse fitting procedure 'averages out' small humps. In contrast, the major and minor Feret diameters as used in Shang et al. (2018) are affected by such small humps.

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In contrast to ArD2d, end-member modelling results of CcD2d and especially ConD2d differ from D2d (grain size): the mode of their intermediate end member is significantly finer-grained and it overlaps more substantially with EM3-3. This overlap may actually be the cause of the observed difference: end-member modelling on size-shape distributions would be more suitable for identification of an end member that strongly overlaps with another in terms of grain size but differs in grain shape. Of the three studied size-shape variables, results of ConD2d shows the strongest unmixing (highest abundances of the dominant end-member). This indicates that ConD2d may be the most appropriate variable for the identification of transport processes.

5 Conclusions

We introduce a novel method that can be used to reconstruct sediment transport processes from sedimentary deposits. The 30 method makes use of end-member modelling on grain size-shape distributions, which are constructed from grain size and shape data obtained by dynamic image analysis. Tests with artificial size-shape distribution datasets indicate that the known end-members and end-member mixing proportions are accurately computed by the method, even when noise is present in the data. End-members with limited occurrence are also identified; highly mixed components, however, cannot be determined accurately. The tests also point out that the distribution of the fit of unmixing results per size-shape class (the class-wise R^2 distribution) can be used to indicate the number of end-members present.

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The size-shape distribution unmixing method is also applied to real-world data from an active aeolian system in the Dutch coastal dunes. Results show that a comparison of the spatial distribution of model fit (sample-wise R^2) to local geomorphology further increases insight into the number of end-members present. The geological meaning of end members can be validated by comparing their size-shape distributions to reference samples of different transport processes.

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Three end members are determined for the dune dataset. The spatial distribution of these end members is in accordance with the local geomorphology and reflects the three dominant aeolian transport processes known to occur along a beach to dune transect: bedload, modified saltation and suspension. These processes are characterised by distinctly different end-member size-shape distributions, resulting from differential (size and) shape sorting: with increasing size, bedload shows a constant

15 grain shape, modified saltation a minor decrease in grain regularity, and suspension a strong decrease in grain regularity (when using convexity or Cox circularity as shape parameter).

Compared to traditional end-member modelling on grain-size distributions, unmixing of SSDs gives rise to different endmember grain-size distributions due to shape sorting effects. Results of the new method also show higher proportions of the

20 dominant end members, indicating a better discrimination of the aeolian transport processes (especially when using convexity as shape parameter). The principal advantage of the new method, however, is that the characteristic shapes of the end-member size-shape distributions can be used as a fingerprint of the transport mode. The new method therefore resolves the ambiguity that arises when the transport mode is reconstructed using grain-size distributions.

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Code availability

Not available

Data availability

30 Data are available from the Pangaea database (https://issues.pangaea.de/browse/PDI-21911)

Appendices

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Appendix A. Fieldwork area in the coastal dunes of the National Park Zuid Kennemerland. A1 shows the general location of the study area. A2 displays the locations of surface samples and sediment traps. A3 covers the same area and shows subregions based on geomorphic features. Aerial photograph © PDOK.nl, 2017.



Appendix \underline{BA} . Sediment trap on a vegetated dune



Appendix <u>CB</u>. Flow diagram for the image processing script.



Appendix <u>DC</u>. Input and determined end-member SSDs for the 3EM_nonoise dataset.



Appendix <u>ED</u>. Input and determined end-member SSDs for the 4EM_noise dataset.



Appendix FE. Input and determined end-member SSDs for the 4EM_noise_highmix dataset.



Appendix GF. Median class- and sample-wise R^2 versus the number of end members for the artificial datasets: 3EM_nonoise (1), 4EM_noise (2) and 4EM_noise_highmix (3). Figure 2B and 3B zoom in on Fig. 2A and 3A.



Appendix <u>HG</u>. A comparison of modelled and input end-member abundance for the artificial datasets (1: 3EM solution for 3EM_nonoise, 2: 4EM solution for 4EM_noise, 3: 4EM solution for 4EM_noise_highmix, 4: 4EM solution for 4EM_noise_highmix but without the highly mixed end-member).



5 Appendix III. Median class- and sample-wise R² versus the number of end members for the ConD2d distribution dune dataset.



Appendix JI. Sample-wise R² plotted over the sample locations for variable ConD2d (J1) and variable D2d (J2). The first interval of the colour scale is enlarged to elucidate the changes in R², which mainly occur above a value of 0.9. Points with a black outline denote surface samples and are plotted at the sampling location. Points with a white outline denote sediment trap samples and are plotted near the sampling location. The exact locations of sediment traps are marked by white dots. Two of the subregions defined in appendix A3 are shown in simplified form. Aerial photograph © PDOK.nl, 2017.







Appendix \underline{LK} . End-member abundances for variable ConD2d determined for the dune dataset. Pie-charts with a black outline denote surface samples and are plotted at the sampling location. Pie-charts with a white outline denote sediment trap samples and are plotted near the sampling location. The exact locations of sediment traps are marked by black dots. Two of the subregions defined in appendix A3 are shown in simplified form. Aerial photograph © PDOK.nl, 2017.



Appendix <u>ML</u>. Median class-wise and sample-wise R^2 for D2d end-member modelling results of the dune dataset (1) and size-resolved class-wise R^2 (2).



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Appendix <u>NM</u>. CcD2d (1) and ArD2d (2) 3EM solutions determined for the dune dataset.



Appendix ΘN . Pie-charts showing abundances of the 3EM solution determined for the ConD2d (1), CcD2d (2), ArD2d (3) and D2d (4) distributions of the dune dataset. Pie-charts with a black outline denote surface samples and are plotted at the sampling location. Pie-charts with a white outline denote sediment trap samples and are plotted near the sampling location. The exact location of sediment traps is marked by black dots. Two of the subregions defined in appendix A are shown in simplified form. Aerial photograph © PDOK.nl, 2017.





Author contributions

JAH wrote the initial draft of the paper, devised a way to integrate grain size and shape data, designed the code used for image processing, data processing and data visualisation, and performed laboratory analyses. UVB performed fieldwork in the National Park Zuid-Kennemerland, laying the foundation for the dune dataset. He also performed laboratory analyses,

- 5 performed initial tests on shape sorting during aeolian transportation and helped improve the draft versions of the paper. SMA initiated and continued the sediment monitoring project in the National Park Zuid-Kennemerland using sediment traps. He also helped improve the initial draft of the paper. RTVB helped improve writing and construction of the manuscript and provided feedback on the method. MAP conceived the idea of end-member modelling of integrated size and shape data for a better understanding of sedimentological processes, performed fieldwork in the National Park Zuid-Kennemerland, initiated
- 10 grain size and shape analysis on the dune sediments, helped improve the draft versions of the paper and provided feedback and discussion on how to implement the method.

Competing interests

The authors declare that they have no conflict of interest.

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Response to the Anonymous Referee

Dear anonymous referee,

Thank you for your positive review and valuable comments and suggestions.

Below you will find your comments and our replies in section 1. Section 2 contains a list of the changes that were made to the manuscript.

Section 1. Comments and replies

Below we have made a list of your comments (in quotation marks and Italic) and our replies.

Comment 1) "A more detailed description of the technique is suggested (Some suggested points: Why are these methods better than previous sizing techniques? What are the advantages

10 and drawbacks compared to other imaging approaches? The repeated pumping of the sample causes data redundancy [one particle will appear on more than one captured frames]. Is it a problem, or not?)."

1A) "Why are these methods better than previous sizing techniques?"

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Many methods for measuring grain size have been/are employed, the most prevalent being sieving, settling and laser diffraction.

The first advantage over these methods is obvious: in addition to size analysis, image analysis allows measurement of grain shape, the traditional methods do not.

20 The second advantage is less obvious: the varying shape of natural sediment particles causes deviations in the size measurements obtained by sieving and laser diffraction: A sieve mesh actually measures the intermediate diameter of a particle and relatively large yet elongate particles can pass the mesh. With settling measurements, one has to make an assumption of the particle's shape (and density) to convert settling velocity to grain size.

In laser diffraction, the assumption is made that all particles are spherical. Since natural sediment grains are generally not spherical, this causes errors in the obtained grain size distribution. Grain size obtained by image analysis is more robust in this sense: the (2D) shape of the particle is known, and therefore one can choose any definition of 'particle size'. For example, the largest diameter (2D), smallest diameter (2D) or 'average diameter'. We feel the latter is the most robust. For this reason, we used a diameter based on the surface area of the particle (D2d), as described in the manuscript. The third advantage of image analysis over traditional sizing techniques is that information is obtained on the size of each single grain passing the camera

30 rather than just the grain size distribution of the entire sample. This means 1) that single grains with a certain size can be extracted from the data for specific research questions. For example, one may want to know the largest grain per sample, 2) that single very large grains are detected (in our experience this is not the case with laser granulometry), 3) that grain size distributions can be made by percentage of the total volume of all grains per size class, but also by percentage of total diameter

or percentage of total number of particles, 4) that there are more options for statistical analysis of the sediment samples (which are as of yet not used).

There is however also a major drawback to the new technique: due to the pixel size of approximately 5 µm (or 2 µm with a different set-up which allows measurement of finer-grained particles but limits the maximum measurable grain size to 400 µm due to the 500 µm cuvette width), a reliable measurement of particle shape is not possible for anything finer than medium silt (Shang et al., 2018, Aeolian silt transport processes as fingerprinted by dynamic image analysis of the grain size and shape characteristics of Chinese loess and Red Clay deposits. Sedimentary geology, 375, 36-48). This is a financial, and not a technical limitation: the boundary could be lowered substantially with higher-resolution cameras.

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1B) "What are the advantages and drawbacks compared to other imaging approaches?".

The main advantage of dynamic image analysis (where particles pass a camera suspended in air or water) compared to the more classic static image analysis (where particles are photographed, for example under a microscope) lies in its statistical robustness and low measuring time: many particles can be measured in relatively little time (5 minutes for a typical number of particles of 150 thousand for sand (this manuscript) or 5 minutes for ~ a million particles for silts (Shang et al., 2018)). The large number of particles ensures that the size-shape distributions are statistically robust.

- 20 There are additional differences with the static methods: If the sample consists of unconsolidated sediment spread out on a flat surface, the orientation of the particles is known: particles lying on a surface have their smallest axis oriented vertically, and therefore their largest and intermediate axis show up on the image. This is both an advantage and disadvantage over our method: it is favourable that the orientation is known, but any inferences about the volume of the particles will always be overestimations of the actual volume.
- 25

Non-automated measurements using a microscope enable the computation of shape variables that are difficult to automate, such as surface texture of the grains or Power's roundness. However, such measurements are user-dependent, very time consuming and will comprise only a limited number of measured grains leading to less robust results.

30 1C) "The repeated pumping of the sample causes data redundancy [one particle will appear on more than one captured frames]. Is it a problem, or not?"

The most often used method for measuring grain size is laser diffraction. In most of the laser diffraction set-ups, the sample is repeatedly pumped through the cuvette as well. Therefore, this "problem" is universal in grain size measurements. In our view,

however, it is not a problem but rather something that adds to the strength of the measurement. Because the flow in the large cuvette is quasi-turbulent, the particles will pass the camera at different angles each time. The total measurement therefore becomes to some extent a 3D average of the various 2D shapes that one obtains by looking at a particle at different orientations. A size-shape distribution therefore becomes more robust then had the sediments passed the camera only once.

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Comment 2) "The description and the presented flow diagram ensure the reproducibility of the introduced measurement and data processing approach for experts of the field, but researchers without deeper knowledge on image analysis-based grain size and shape characterization may have trouble to understand the key steps of the method."

10 We assume that this comment deals mainly with chapter 2.2 (dynamic image analysis). We enhanced apprehensibility of the chapter by adding a short description of the flow diagram (see section 2).

In our opinion, chapter 2.3 (construction and unmixing of size-shape distributions) and chapter 2.4 (artificial datasets for testing and validation of the method) go into sufficient detail to explain the method to non-experts.

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Comment 3) "The applied self-written Matlab script (with imfill, regionprops and convhull functions) is using the raw images of the acquired frames not processed data of the Sympatec Qicpic's software, allowing for a more detailed and freely customizable data handling. Are there any differences among the results of your own calculations (by using 'regionprops') and area by the davies of former?"

20 and ones by the device software?"

Besides flexibility and customisability, there are two reasons for applying a self-written script:

3.1) The Qicpic software (our version at least) does not allow filling of blank spaces in particles. These blank spaces occur because some minerals, such as quartz, are transparent, causing them to appear donut-shaped in the images. Due to our quartzrich samples, we were not able to use any of the built-in functions for computing area-based shape parameters. Matlab, on the other hand, has built-in functions to perform the task of filling blank spaces in objects. At the moment, however, we use the perimeter to determine the 2D surface area of the particles and therefore blank spaces are less of a problem.

30 3.2) The Qicpic software (and many of Matlab's built-in functions such as regionprops('ConvexHull')) consider pixels to have an area (a pixel is a little square). In our method, we base computations on the pixel's centre location.

Comment 4) "The presented size-shape distributions are equivalent to volume-weighted scatter plots of size and different shape parameters of individual particles. (It is a relatively well

known approach of image analysis-based granulometric characterization, actually, a default data visualization mode in the software of Malvern Morphologi automated static image analyser device)."

- 5 We were not aware that grain size-shape distributions are a well-known approach. The size-shape distributions or volumeweighted scatter plots of size and different shape parameters can indeed be found in Malvern's documentation: <u>https://www.cif.iastate.edu/sites/default/files/uploads/Other Inst/Particle%20Size/Particle%20Characterization%20Guide.pd</u> <u>f</u>. Furthermore, we found one application in powder metallurgy: Takashi Itoh & Yoshimoto Wanibe, 1991: Particle Shape Distribution and
- 10 Particle Size–Shape Dispersion Diagram, Powder Metallurgy, 34:2, 126-134, DOI: 10.1179/ pom.1991.34.2.126. However, we found no applications of a similar method in sedimentology. Thus, grain size-shape distributions are not new, but their application to the study of sediments is new. More importantly, the combination with endmember modelling is also new. We added the reference of Itoh & Wanibe to the manuscript (see section 2).
- 15 Comment 5) "Last columns of Table 2 are not visible in the manuscript."

Thank you for noting this error. Part of the last column is indeed not visible in the manuscript. This is changed in the revision.

Comment 6) "The overall structure of the paper is good, however, figure from the Appendix A could be moved into the main text."

Appendix A is moved into the main text of the revision.

References

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Shang, Y., Kaakinen, A., Beets, C. J., & Prins, M. A. (2018). Aeolian silt transport processes as fingerprinted by dynamic image analysis of the grain size and shape characteristics of Chinese loess and Red Clay deposits. Sedimentary geology, 375, 36-48

Section 2. Changes made to the manuscript.

In this section we describe the changes we made to the manuscript based on your comments. Changes are in quotation marks and in italic.

- 5 Comment 1) "A more detailed description of the technique is suggested (Some suggested points: Why are these methods better than previous sizing techniques? What are the advantages and drawbacks compared to other imaging approaches? The repeated pumping of the sample causes data redundancy [one particle will appear on more than one captured frames]. Is it a problem, or not?)."
- 10 1A) "Why are these methods better than previous sizing techniques?"

A comparison of dynamic image analysis to other sizing techniques is outside the scope of this manuscript. The full reply in section 1 was therefore not taken up into the manuscript.

However, we have included a brief explanation of the advantage of knowing the two-dimensional shape of a particle when
determining its size (page 6, line 10 to 14). We deleted: "For the same reason, "the" diameter of the particle is given in the robust form of an area equivalent diameter (Table 2)." And we added: ""The" grain size of the particle is given in the form of an area equivalent diameter (Table 2), essentially the average particle diameter of the two-dimensional image of the grain. Because the two-dimensional shape of the particle is known, grain size obtained by image analysis is more robust than traditional size measurements (e.g. sieving, laser diffraction and settling) where an assumption has to be made of particle shape before computing size (Konert and Vandenberghe, 1997)."

1B "What are the advantages and drawbacks compared to other imaging approaches?".

A detailed comparison of dynamic image analysis to other imaging approaches is also outside the scope of this manuscript. 25 We therefore did not include our answer into the revised manuscript.

1C) "The repeated pumping of the sample causes data redundancy [one particle will appear on more than one captured frames]. Is it a problem, or not?"

30 The answer to 1C) was not included in the manuscript because repeated pumping of a sample is very common in grain size measurements and therefore not new to our method.

Comment 2) "The description and the presented flow diagram ensure the reproducibility of the introduced measurement and data processing approach for experts of the field, but researchers without deeper knowledge on image analysis-based grain size and shape characterization may have trouble to understand the key steps of the method."

We enhanced apprehensibility of the chapter by adding a short description of the flow diagram (page 6, line 4 to 8):

"In the first step of the script some limitations and conditions are set. Subsequently, the script iterates over each video, over each frame in the video and over each particle found in the frames. For each particle, the length of its outer edge (perimeter) is computed, as well as its area and the length of its convex hull (a polygon drawn around the particle without taking into

5 account the concave areas). These basic parameters are stored for each particle. Particle size, volume, aspect ratio, convexity and Cox circularity are subsequently computed from these basic parameters. "

Comment 3) "The applied self-written Matlab script (with imfill, regionprops and convhull functions) is using the raw images of the acquired frames not processed data of the Sympatec Qicpic's software, allowing for a more detailed and freely customizable data handling. Are there any differences among the results of your own calculations (by using 'regionprops') and ones by the device software?"

A discussion on the differences between the Sympatec software, the built-in Matlab functionality and our functions is outside the scope of the manuscript. However, the fact that we fill blank spaces in the particles and that we compute size and shape by the pixel's centre locations are important for reproducibility of this work. This information was already present in the workflow

diagram of the script (Appendix B, which was appendix C in the previous version of the manuscript)

Comment 4) "The presented size-shape distributions are equivalent to volume-weighted scatter plots of size and different shape parameters of individual particles. (It is a relatively well known approach of image analysis-based granulometric

20 characterization, actually, a default data visualization mode in the software of Malvern Morphologi automated static image analyser device)."

We changed: "In this study we outline a new method for determination of sediment transport processes involving 1) the integration of grain size and shape data into size-shape distributions and 2) end-member modelling on these distributions."

25 (Introduction, page 3, lines 8-10) to: "In this study we outline a new method for determination of sediment transport processes involving 1) the integration of grain size and shape data into size-shape distributions (e.g. Itoh and Wanibe, 1991) and 2) endmember modelling on these distributions".

Comment 5) "Last columns of Table 2 are not visible in the manuscript."

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Table 2 was changed in the revised manuscript to include the last column.

Comment 6) "The overall structure of the paper is good, however, figure from the Appendix A could be moved into the main text."

Appendix A has been moved into the main text as Fig. 1.

Response to Simon Blott

Dear Simon Blott,

Thank you for your positive comments and your suggestions.

5 Section 1 contains our replies to your comments. Section 2 describes the changes made to the manuscript based on your comments.

Section 1

Below we have made a list of your comments (in italic and quotation marks) and our replies.

- Comment 1) "It is lengthy, but it is difficult to see how it could be substantially shortened without removing relevant material".
 We also feel that, although the manuscript is long, there is not much opportunity for shortening it.
 Comment 2) "One small point is that Table 2 appears truncated and missing the right hand side".
 Thank you for noting this error. Part of the last column is indeed not visible in the manuscript. This is changed in the revision.
 Comment 3) "And it is also unfortunate that important material is in the Appendices at the back I found myself referring to
- 15 these throughout, which is a little tiresome moving back and forth to the end of the manuscript. I would recommend moving at least the first two appendices into the main text".

Do you suggest to move appendix A1 and A2 into the main text, or A and B? We moved A1, A2 and A3 into the main text, but appendix B is not moved as it is of less importance.

Section 2

Below we have made a list of your comments and the accompanying changes we made to the manuscript.
 Comment 1) *"It is lengthy, but it is difficult to see how it could be substantially shortened without removing relevant material"*.
 We did not shorten the manuscript.

Comment 2) "One small point is that Table 2 appears truncated and missing the right hand side".

Table 2 was updated to include the last column.

25 Comment 3) "And it is also unfortunate that important material is in the Appendices at the back - I found myself referring to these throughout, which is a little tiresome moving back and forth to the end of the manuscript. I would recommend moving at least the first two appendices into the main text".

We moved appendix A1, A2 and A3 into the main text as figure 1.