

TDK

The size evolution of pebbles in a particle-fluid system.

Author:

Jaca Gregorio

Physicist Engineering BSc, II.
year.

Supervisor:

Dr. Török János

Associate professor
BME Elméleti Fizika Tanszék



BME
2024

Abstract

There are many theories on the evolution of the shape and size of gravels (Sternberg 1875, Bloore 1977, Domokos 2012, Sipos 2021). These models provide general equations for changes in pebble size and shape due to abrasion, however, each model requires a collision kernel, which describes the probability of collisions between pebbles of different sizes. Smoluchowski described the size-dependent average cross-section of impact of grains colliding with each other as early as 1917 (Smoluchowski 1917), but this only works under certain conditions, mostly in two-dimensions and in a vacuum with a narrow size distribution. However, most pebble abrasion occurs in water under various flow conditions. Up to now, little experimental or simulation work has been done in such environments.

Our aim in this work is to measure these collision kernels in fluid flow environments and apply them to abrasion models to recover experimentally available particle size distributions. In order to achieve this, we used a CFDEM (Goniva 2012) simulation system in which we built up a shear flow in which floating particles can collide. We wrote an algorithm which detects the particle collisions and recovers the collision matrices. We used these matrices to predict the possible scenarios with respect to particle size distributions.

Contents

1	Introduction and Motivation	4
2	Methods	5
2.1	CFD	5
2.2	DEM	6
2.3	Coupling	8
2.4	Energy and Courant number considerations	8
2.5	Meshing schemes	9
2.6	Simulations	10
3	Results	11
3.1	Mutual Collisions	11
3.2	Distributions of collision variables	12
3.3	Size dependency of collision statistics	14
3.4	Collision Kernels	16
3.5	Kernel Models	16
3.6	Collective abrasion	18
4	Conclusions and Discussion	20
	Appendix	20
5	Abrasion Model	21
5.1	Abrasion dependency on size	22
5.2	Effect on size distribution	22
6	Simulation Parameters	23
7	Acknowledgements	23
8	Own Results	24

1 Introduction and Motivation

The study of pebble size and shape evolution in fluvial ecosystems provides useful insights into the geological and hydrodynamic processes and flows of different environments. The distribution dynamics in fluid flow environments result from billions of collisions over long time periods, combined with transport [1]. Field observations indicate that different environmental conditions tend to display distinct pebble distributions. By analyzing their effects on the collision statistics and the size evolution of pebbles, we can discover their causes in the flow properties. Then, by measuring pebbles' shape and size we can obtain evidence for the type of particle collisions and fluid flow that must have been present in order to generate the pebbles we find. This could have important implication for Martian observations, where the flowing liquid is long gone [2].

Since the early observations by Sternberg in 1875 [3], researchers have proposed models to explain particle interactions and their effects [4]. In particular, much emphasis has been placed on understanding the role of abrasion in the size and shape evolution of these rocks at both the individual and collective level. Each of these models contributes to our knowledge of pebble evolution, yet there is a need for empirical and simulation data that help validate and improve them.

There is limited empirical data available for researchers in this field due to the challenges of accurately measuring particle collisions in fluid environments, which severely hinders its development and progress. There is a considerable lack of comprehensive experimental studies, both in terms of the range of cases studied empirically and in the data they can measure [5]. Some detailed studies, for example, recreate the hydrodynamic conditions of river flows and use high speed cameras to track particle trajectories capturing the interactions between pebbles confined in the experimental setup [6]. While very useful, these type of laboratory studies are limited by practical considerations, measurable quantities and the time scales at which these phenomena can be observed.

Simulations, on the other hand, are less constrained by physical limitations and, with their flexibility and versatility, allow us to simulate diverse environments which can be specially tricky to study experimentally. For example, extending simulations to microgravity environments is trivial, while a laboratory study of this kind presents many difficulties. For this reason, they have become an invaluable tool for data collection, which provides detailed information about each contact. It is possible to record many variables for each collision event, such as the size of the particles colliding, the collision force, overlap, and velocity [7] which is generally impossible or extremely hard in experiments. This provides us with the necessary data to study both how individual collisions and mutual abrasion operate, and how collective abrasion works. At the same time, experimental data is necessary to validate the methods and results obtained in simulations in order to ensure accuracy and realism. Both approaches complement each other, as experimental data is needed to validate and test the accuracy of the simulations, and simulations can provide more detailed information and extend the applicability of empirical finding to a broader range of conditions, which may be out of current empirical reach. On the other hand, in this study we make several observations which can be verified in experiments especially since the BME has now a flume experimental setup specifically built to study particle collisions and abrasion.

Our objective is to simulate a wide range of setups, including some that are harder to study empirically. In this work we will exclusively focus on shear flows in the laminar regime. We are unaware of any studies of this kind, and we wish to contribute to the field by providing a more comprehensive dataset of particle collisions. Although there are many environmental causes for the abrasion of pebbles, we will focus on collision driven abrasion.

2 Methods

We will use numerical simulations to study the collision statistics of different sized pebbles in a shear flow. This necessitates the usage of a complex multi component simulation code. These are relatively recent open source variants that appeared only in the last decades. Our choice of LIGGGHTS-CFDEM[7] was based upon previous knowledge of the code, since we needed to modify it in order to get access to properties generally not printed by these programs, like collision force and overlap. In the following section we will describe the components of the simulations.

In the following on all cases we will report dimensionless numbers but all the simulations were done using *SI* units, that is[8]:

- mass = kilograms
- distance = meters
- time = seconds
- energy = Joules
- velocity = meters/second
- force = Newtons
- torque = Newton-meters
- pressure = Pascals
- dynamic viscosity = Pascal*second
- density = kilograms/meter³

The simulation units are better defined by the material parameters. The most important ones: Young modulus: $E = 5 \cdot 10^7$ and viscosity $\nu = 0.01$. The Reynolds number experienced in our simulations varies between $Re = 500 - 5000$.

2.1 CFD

The incompressible Navier-Stokes equations, which express mass and momentum conservation, together with the boundary and initial conditions determine the dynamics of the fluid domain. The equations read as

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) &= -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}, \end{aligned} \tag{1}$$

where the variables denote the following physical properties:

- $\mathbf{u}$: Velocity vector field.
- ρ : Fluid density.
- p : Pressure field of the fluid

- μ : Dynamic viscosity of the fluid.
- $\mathbf{f}$: External force per unit volume acting on the fluid, like gravity, electromagnetic forces, or interactions with other bodies.

It is impossible to solve these equations analytically in most cases, so they are in general solved numerically using Computational Fluid Dynamics (CFD). These equations are discretized in time introducing time steps (Δt) across which they are numerically integrated. The equations of fluid dynamics used in CFD consider the fluids to be continuous, and, in order to solve these equations numerically the fluid domain also needs to be discretized. There are many discretization schemes available; we use the finite volume method (FVM). The FVM subdivides the flow domain into a finite number of finite volumes, which allows us to define each flow quantity once in each grid point. These quantities are solved only at the grid points and values elsewhere can be obtained using interpolation methods. This reduces our problem to solving a set of coupled algebraic equations¹.

To do this, we use OPENFOAM, an open source CFD software, which offers many solvers, which are specialized for different flows. Considering the requirements for our cases, an immersed boundary method (IBM) solver, `cfdemSolverIB`, was chosen. This is a transient solver for incompressible flows and is used for cases with bodies immersed in a fluid. The algorithm used for this solver calculates the motion of the particles using the fluid velocity and pressure fields from the previous time step. The Navier-Stokes equations are solved in the fluid domain ignoring the particles. Then the velocity and pressure fields calculated are corrected considering the particles present and their velocity. The IBM provides an accurate representation of the interaction between the fluid and solids without the need of a body-fitted mesh around each particle. This method should be used in cases where the particle diameter is larger than the fluid cell mesh. A ratio between 2.2 and 3.4 is recommended for fluids like water [9]. In our case, the diameter was between 1 and 4 times larger than the largest side of the cell mesh. The IBM is advantageous in cases with irregular shaped particles that may experience large displacements and convenient when the computational cost of a dynamic mesh is prohibitive, which is why decided to use it. Several analyses were conducted to corroborate the convergence and validity of our cases.

2.2 DEM

In order to model the particle phase, a discrete approach called Discrete Element Method (DEM) is used [7]. It resolves the motion of each particle individually and handles the collisions between them. The trajectories of each particle are explicitly solved. The equations of motion are the following

$$\begin{aligned} m \frac{d^2 \mathbf{r}}{dt^2} &= \mathbf{F}_c + \mathbf{F}_b + \mathbf{F}_f \\ I \frac{d\boldsymbol{\omega}}{dt} &= \mathbf{T}_r + \mathbf{r} \times \mathbf{F}_c + \mathbf{r} \times \mathbf{F}_f, \end{aligned} \quad (2)$$

where

- m : Mass of particle i .

¹It is worth noting that we obtain an approximate solution, and much care must be invested in validating the results obtained and their convergence

- $\mathbf{r}$: Position vector of particle i .
- $\mathbf{F}_c$: Contact force acting on particle i (due to collisions with other particles).
- $\mathbf{F}_b$: External forces like gravity, electromagnetism.
- $\mathbf{F}_f$: Force from the interaction with the fluid.
- I : Moment of inertia.
- ω : Angular velocity.
- $\mathbf{T}_r$: Additional torque to model non spherical particles.

The Hertz contact model is used to resolve the collisions between two particles. The contact force is calculated as follows: [10, 4]

$$\mathbf{F}_c = \left(k_n \delta^{3/2} \mathbf{n}_{ij} - \gamma_n \mathbf{v} \mathbf{n}_{ij} \right) + \left(k_t \delta_t^{3/2} \mathbf{t}_{ij} - \gamma_t \mathbf{v} \mathbf{t}_{ij} \right) \quad (3)$$

where

- δ : overlap between the two particles
- k : elastic constant
- γ : viscoelastic damping constant
- $\mathbf{v}$: relative velocity of the two particles
- μ_r : coefficient of rolling friction

and the n and t sub-indexes refer to the normal and tangential components respectively. Please note that contrary to linear spring models the overlap is raised to the power $3/2$ for both the tangential and the normal spring. It is worth clarifying that δ_t is the tangential displacement between the two particles that occurs during the contact and it is truncated to fulfill

$$F_t \leq \mu_r F_n \quad (4)$$

The contact can be represented with a nonlinear spring-dashpot model (Fig. 1), where both the tangential and normal components contain a nonlinear spring that stores energy from the relative displacement and a viscous damper that dissipates energy from the contact.

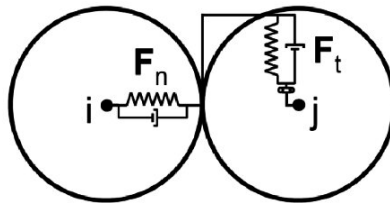


Figure 1: Graphical representation of the spring-dashpot model [11]. There are two nonlinear springs; one in the normal and another in the tangential direction. The tangential direction is determined by the relative displacement of the surfaces of the particles. There are viscous dampers attached to each spring.

The DEM part of the software was modified to report the contacts made by interacting particles. Writing out snapshots at every time-step is impossible due to insufficient disk storage therefore we have implemented a new printout at the contact force calculation. In this way at each time-step we have a list of interacting particles, with their overlap and the total force they exert on each other.

2.3 Coupling

The coupling of the CFD and DEM components allow us to simulate particles-fluid systems. There are two distinct methods available for the coupling depending on the relative size of the particles and the mesh grid. An unresolved approach can be used in cases where the particle size is smaller than the grid, and a resolved approach is applicable otherwise. We use the latter, which is implemented in the IBM. There is flexibility in the coupling where both the CFD and DEM time-steps can be different, and the coupling occurs at a regular interval. This is useful when more accuracy is required in one than in the other. In our case, we use a smaller DEM time-step as we require a higher resolution due to the short collisions of hard spheres; 10 DEM time-steps are coupled for each CFD time-step.

2.4 Energy and Courant number considerations

There are other metrics that aid us in finding the appropriate simulation parameters. The Courant number is the ratio of the fluid step size and the mesh cells' size. The Courant–Friedrichs–Lewy (CFL) condition

$$\text{CFL} = \frac{u\Delta t}{\Delta x} \leq C_{\max}$$

is a condition for the convergence of the solution of the differential equations that describe the fluid flow[12]. It is important to chose a $C_{\max}$ consistent with the CFD solver used. In our case, while the solver allows for $C_{\max}$ values higher than 1, we aimed for a value close to 1.

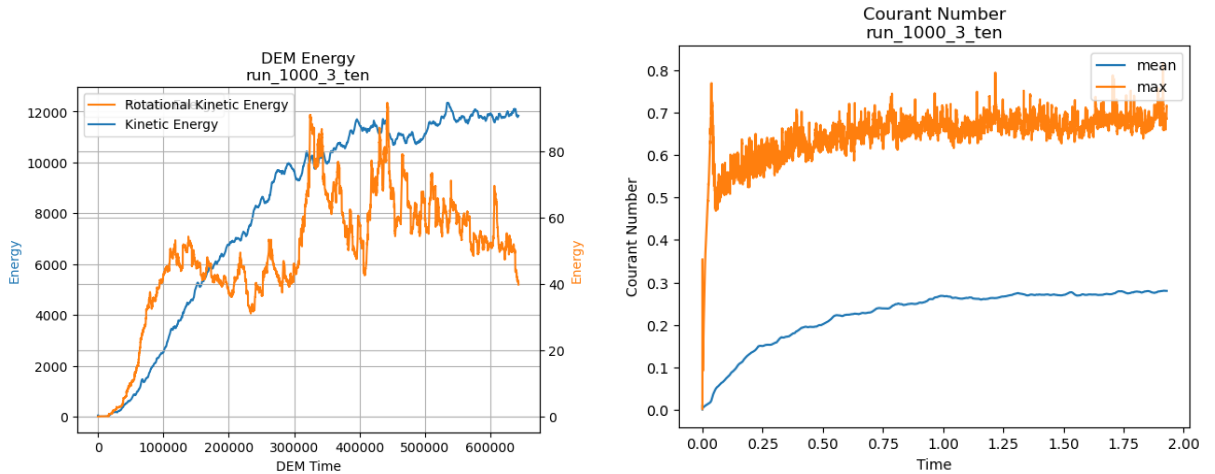


Figure 2: Left: Energy of particles, Right: Courant number

In order to be confident that the solutions obtained converge, we ran simulations with a much smaller Courant number, by reducing the Δt , and observed very similar results. We iterated over this process to find the highest value of the Δt that ensured a convergence across all the cases, even those with higher velocities. After the simulations were finished, we analyzed the Courant

number and found reasonable values for every case (Fig. 2). The fact that we were using an uniform mesh also simplified this process as Δx is fixed.

Another important consideration is that initially, both the flow and the particles are static, and it takes some time for the shear flow to develop. This is of critical importance, as the data obtained from the first time interval of the simulation, before the flow properly develops and stabilizes, is not representative of the physical system we aim to model; rather, it contains transient components. To identify this time, we measure the kinetic energy of the particles, which after an initial increase reached a plateau with obvious fluctuations. In our analysis we disregarded collisions in the transient regime.

2.5 Meshing schemes

Finding the appropriate simulation parameters is of crucial importance when the objective is to obtain a large amount of relevant data, taking into account the characteristics of our simulations and the constraints we have. For this, a lot of different approaches were tried and many values for each parameter were tested. For the CFD component, we tried many different meshing approaches to discretize the flow domain, finding appropriate ones for different cases. In the example of two particles moving in a stationary fluid, as seen in Fig. 3, a dynamic mesh was chosen. In a dynamic mesh, the size and distribution of the cells is periodically updated to better locally capture a changing fluid domain. In our case, the change is caused by the movement of the particles, and the refinements are done in the vicinity of them. If these approach is chosen, great attention must be given to the frequency of the refinement, which depends on the relative motion of the particles. If the particles' displacement is very large between two refinement events, the refined region of the mesh may not coincide with the position of the particles at that time. Another matter to take into account is the computational resources employed in this refinement, which scales rapidly with the number of particles. Lastly, since the value of the Δt is limited by the smallest cell size, their usage implies longer calculation times.

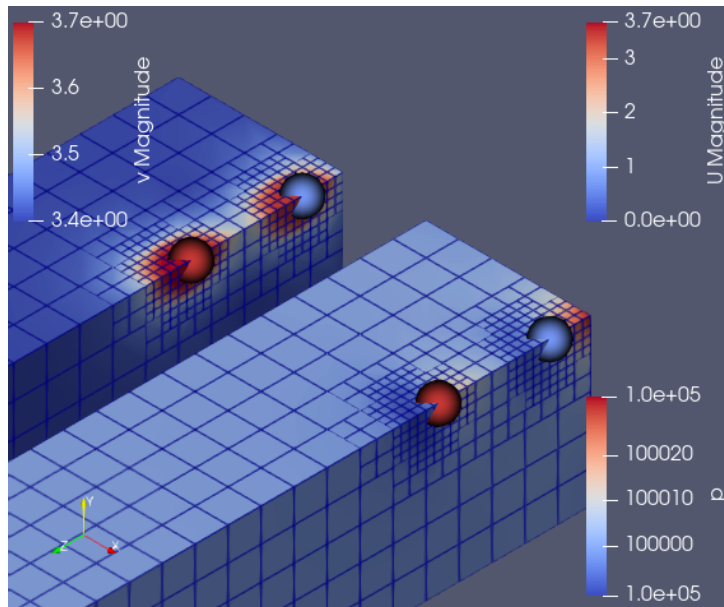


Figure 3: DKT and dynamic mesh. A slice of the domain is shown. Front: fluid pressure. Back: fluid velocity

Many steps were taken to validate the accuracy of our simulations. We began by creating sim-

ple cases and trying to replicate widely observed phenomena, such as drifting–kissing–tumbling (DKT) [13]. As the particles move, they disrupt the flow around them and they create a wake, a region of fluid with higher velocity and reduced pressure behind them. This will cause the two to experience an asymmetric drag as they interact with the fluid, where the leading particle encounters a higher resistance while the one behind experiences significant drag reduction [14]. This causes the trailing particle to move faster and the distance between them to decrease. This is exactly what the data from the simulation shows, and this phenomenon plays an important role in pebble collisions.

In order to simulate a shear fluid flow, a rectangular fluid domain was used, with the longest side of the parallelepiped coinciding with the flow direction. This was done considering the CFL condition; as U is larger in that direction, a larger Δx or a smaller Δt is needed, and we opted for the former. The domain is periodic except in the direction of the shear gradient, where we apply a non-periodic boundary condition to account for the velocity variation due to the shear. The periodicity of the domain means that both particles and fluid do not exit the domain if they cross the boundary, but rather that they re-appear in the other side of that boundary. For domain sizes that are sufficiently larger than the particle size, this is a very useful technique. Another meshing approach considered is the “boundary layer meshing” or “wall refinement” in order to better capture the boundary conditions for the velocity of the fluid at the top and bottom walls of our shear fluid domain. Finally, we decided not to use this, but rather to use a homogeneous grid mesh because of performance issues.

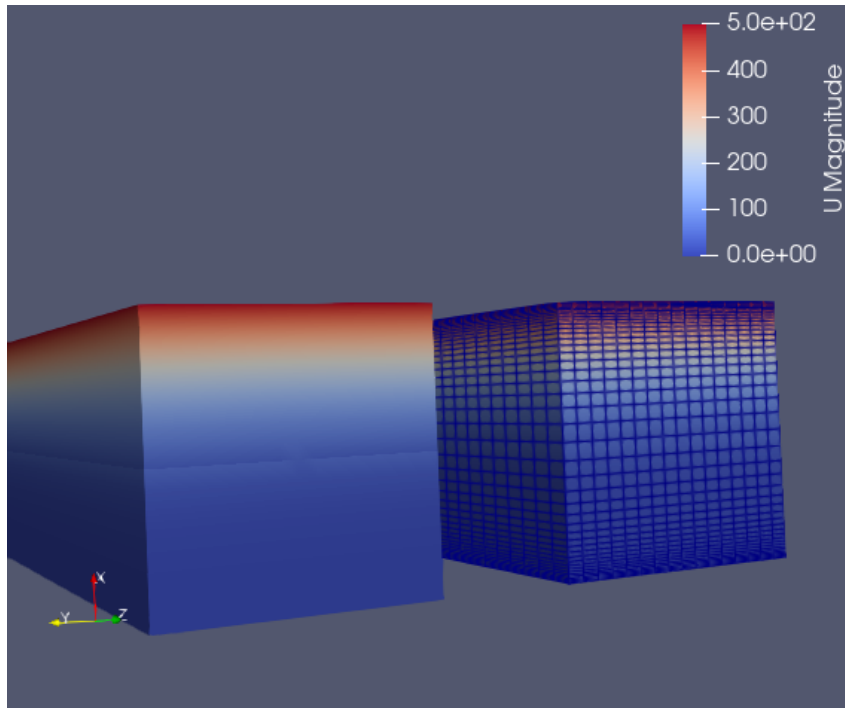


Figure 4: Developing shear flow using a wall mesh

2.6 Simulations

To investigate the influence of particle size distribution and fluid flow conditions on collision dynamics, we simulated 32 distinct cases. Each case was characterized by three primary parameters:

1. Top Fluid Velocity (U): 100, 200, 500, or 1000.
2. Number of Particle Size Groups: 5 or 10.
3. Size Ratio: 1.2, 1.5, 2, or 3, the ratio of the largest to smallest particle diameter.

Using random sequential deposition[15], we created a random placement for the initial position of particles. Spherical particles of a homogeneous material were used. We included no external forces like gravity.

3 Results

First we will point to some general results observed. The total number of collisions increases with the fluid and particle velocity, while it slightly decreases for wider size distributions. By measuring their kinetic energy for different flow velocities (Fig. 2), we found that it increases significantly with fluid velocity. The total number of collisions, force or overlap for all particles in a case, all significantly increase with velocity.

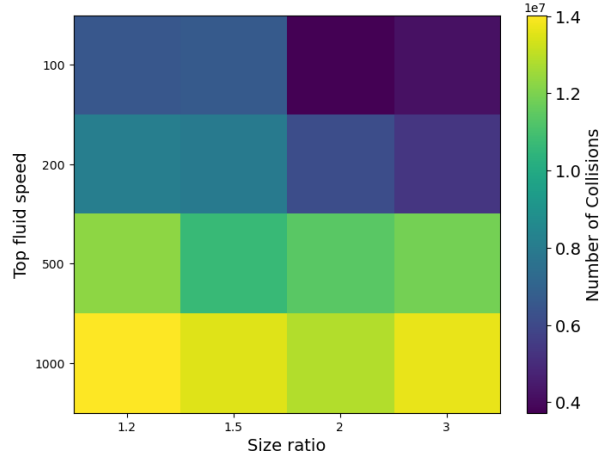


Figure 5: Number of collisions vs Simulation Parameters

3.1 Mutual Collisions

We will first investigate binary mutual collisions between particles which will precede our study of collective collisions. A similar process will be used to present our findings on abrasion. We will show some examples and a short description of the main collision patterns. While these are not very systematic, they provide key insights that will guide our analysis further on.

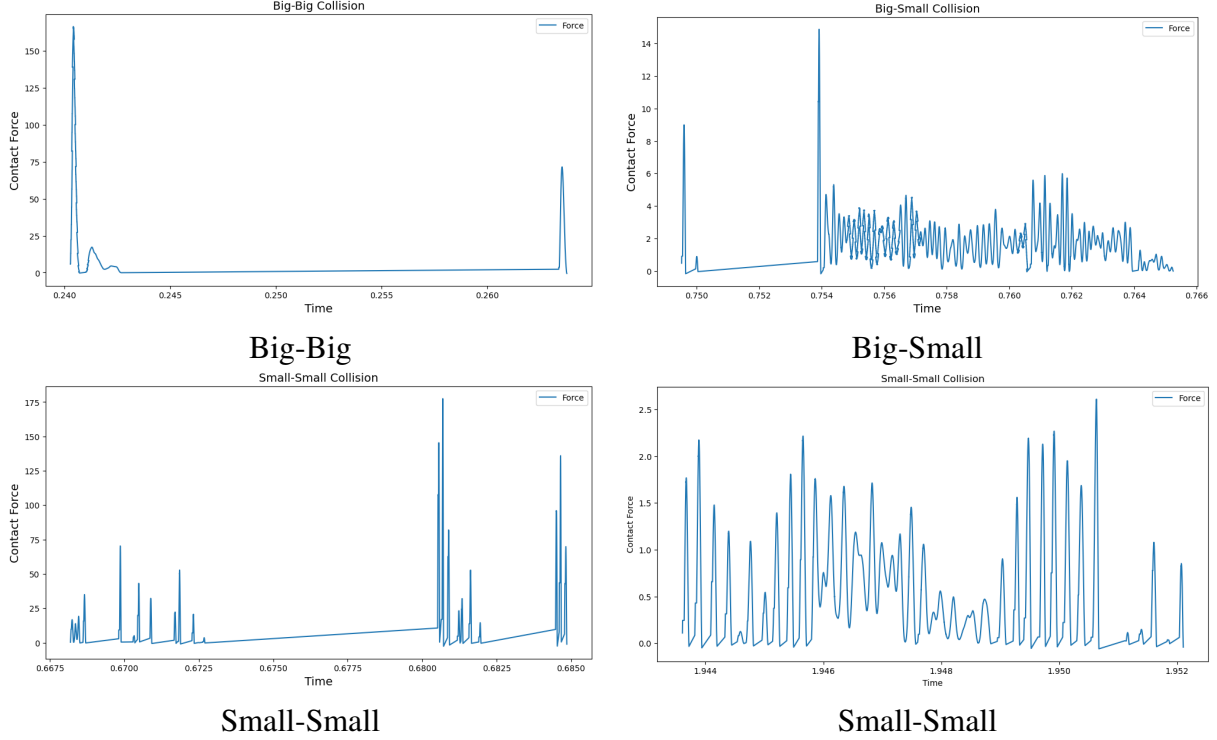


Figure 6: Example Time vs Collision Force plots for pairs of particles.

In Fig. 6 the contacts between some particle pairs are shown. The most remarkable observation is the difference in magnitude for different mutual collisions. Pairs of big particles experiment the strongest collisions, due to higher mass and momentum, and they tend to apply a large impulse over a small time period. This suggest that they play an important role in enhancing mass loss rates, which is supported by empirical studies [6]. On the other hand, collisions between big and small particles are characterized by smaller force and intersection and a longer contact time. As the forces are very small, they remain close together and touch multiple times. Collisions between pairs of small particles are quite varied. Many of them are considerably stronger and shorter than Big-Small collisions, but generally softer than Big-Big collisions, while some of them are extremely weak and are long.

Collision force and intersection is a increasing function of size for same sized particles. This is not the case for unlike particles, where a bigger size difference results in softer collisions. This has important implications for abrasion and subsequently in the particle distribution's dynamics. At lower flow speeds, the collision force tends to be smaller and there is a higher prevalence of soft contacts, specially for pairs of small particles but not so much for pairs of large particles. These individual descriptions are not sufficient to understand the collective collisions between the whole group, for that we need a quantitative statistical analysis.

3.2 Distributions of collision variables

We created distributions of the force and intersection, or normal overlap δ_n , during the collisions for all cases. They illustrate interesting features of the different cases explored. We show two representative cases:

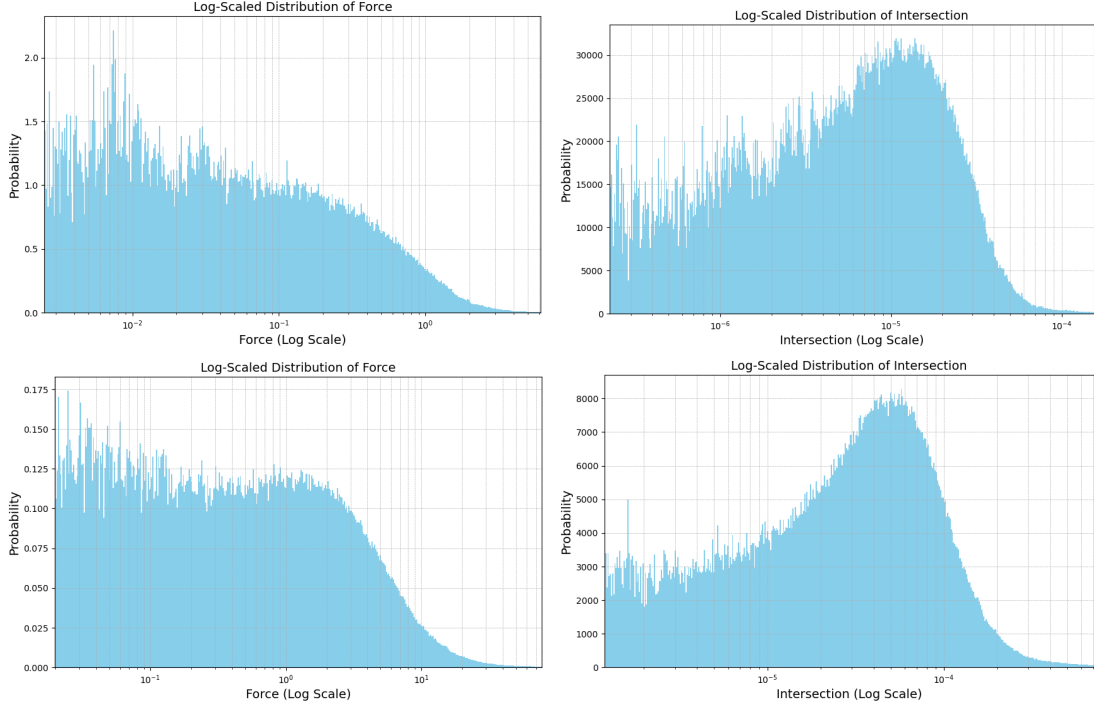


Figure 7: Force and Intersection distributions. Top: $U = 200$, bottom: $U = 1000$, The size ratio was 2 in all cases.

It is remarkable that the distribution of the intersection has a very clear mode, while the same is not true for the force. It is worth noting that this is replicated in practically all cases, with few exceptions, which we will analyze later. In order to understand this, we must refer back to the model used to calculate the forces between two colliding particles. In the Hertzian contact model [3](#), the force depends on the δ_n , but also on the δ_t and the normal and tangential velocities. These terms have a dispersive effect on the force distributions.

As the particles are in a shear flow, their velocities will tend to be aligned to the direction of the flow but will be different depending on their position. Particles will tend to follow stream lines before colliding. Any difference in velocity tangential to the collision will contribute to the force independently of δ_n . This may be more relevant for collisions with a smaller overlap, where the particles' relative velocities may not align with the normal collision direction (which is a sensible assumption for small-overlap collisions) while they may align more with the tangential direction. Overall, we can expect that for the same collision overlap, the force can be different, which can explain the difference in the distributions.

We also observe that at higher velocities the distributions shift to the right, meaning to higher values for both the force and intersection, which is consistent with what is expected for higher velocity regimes and with what we discussed in previous sections. The distributions for the cases with higher velocity appear smoother, which likely results from a larger number of collisions ([Fig. 5](#)). The law of large numbers suggests that as the number of data point increases, the distribution converges to the underlying distribution.

There are some few (3 cases out of 32) interesting exceptions worth analyzing:

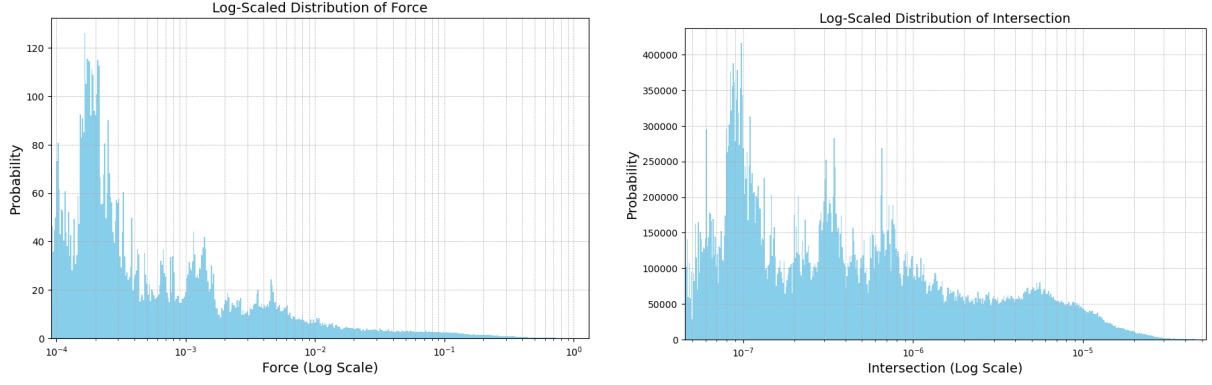


Figure 8: Force and Intersection distributions. $U = 100$, size ratio = 3,

It is interesting to investigate the conditions under which these distribution patterns do not arise and to relate it to the previous analysis we made. The few examples where this does not occur are those with low fluid velocities and big a size ratio distributions. In Fig. 8 we observe distributions that are shifted to the left, meaning that most of the collisions are soft, and that do not exhibit the same characteristics as the others. In these cases we have very large and very small particles interacting with each other. As we previously discussed, the collisions between big and small particles tend to be weak, with a small force and intersection, and repetitive. On top of that, the low velocity increases the probability of soft contacts. This explains the difference in the distribution.

3.3 Size dependency of collision statistics

We want to understand how the amount of wear that a pebble of a given size experiences depends on environmental parameters. To do this, we sum up the collisions a given particle group suffers in a simulation (obviously normalized by the number of particles in the given size group). We recorded the number of collisions, force and overlap.

We first analyze the size dependency of the number of collisions experienced by particles during a given time period. In cases with narrow particle size distribution, there is obviously very limited dependence on particle size which is unfortunately hidden by the statistical noise. Therefore we focus on wider particle size ratios. In Fig. 9 we show the mean number of collisions for different flow parameters and for particle size ratio of 3.

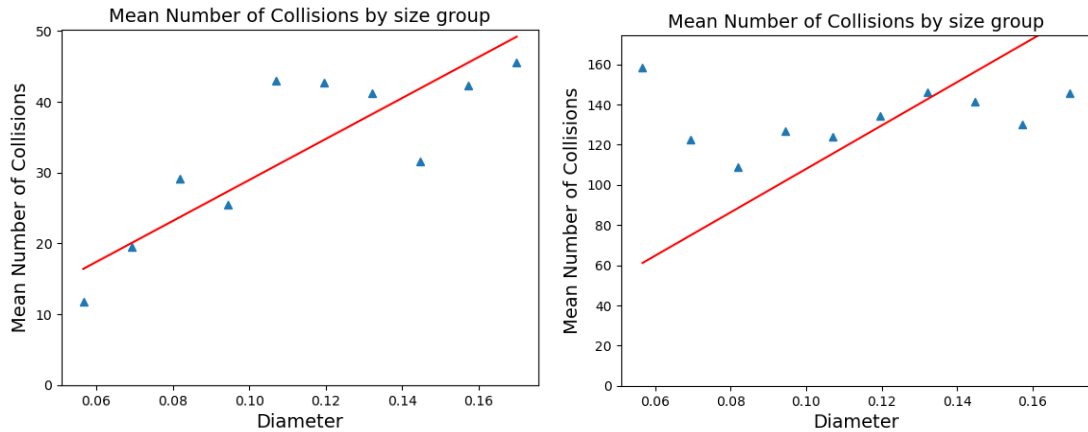


Figure 9: Size dependence on number of collisions for different flow velocities. Left: $U = 100$, right $U = 1000$. For both figures we used 10 diameter groups and a size ratio of 3.

The number of collisions and the overlap increase with flow and particle velocity. Specially at higher velocities, number of collisions depends weakly on particle size. Both results are consistent with empirical observation [6]. However abrasion does not necessarily depend on the number, but mainly on the strength of the collisions. The expected force and overlap for a pair of particles depends on their sizes. If instead of the number of collisions, we show the mean intersection or force experienced by particles of each size, we get similar plots, but the values lie closer to the linear fit with the diameter of the particles.

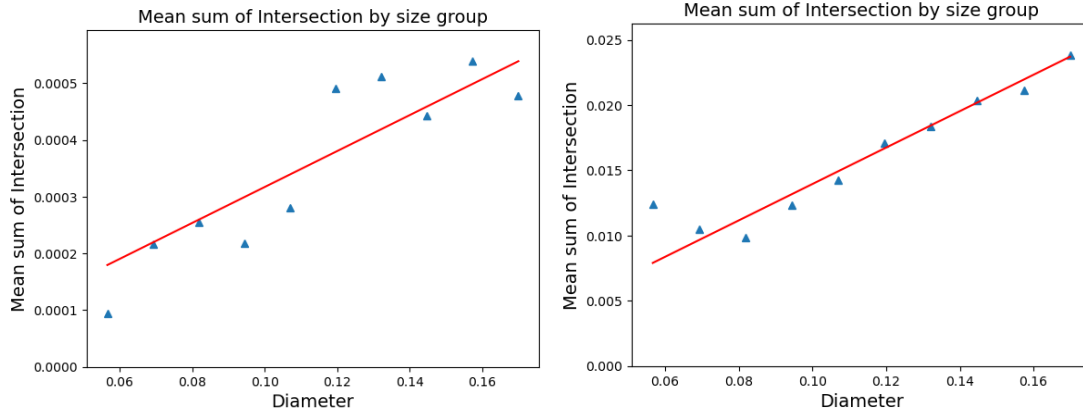


Figure 10: Expected collision normal overlap experienced by each size group. Left: $U = 100$, right $U = 1000$. For both figures we used 10 diameter groups and a size ratio of 3.

We find that across all velocities, that the sum of the intersection that a particle will experience in a given time follows a linear relationship with its diameter, with the exception of the smallest particles. Increasing flow speed affects particles of different sizes differently: small particles collide more frequently and with greater force, while larger particles are less affected by the increase in fluid speed (see Fig. 10). This was also observed when looking at mutual collisions, but it is more clearly seen here. This has important implications for the evolution of the size distribution across different flow regimes. Assuming mass loss is a monotonically increasing function of collision overlap, larger particles will always abrade more than smaller ones, but as fluid velocity increases, the abrasion rate of smaller particles increases disproportionately. Abrasion becomes more significant for smaller particles. This implies that as the flow energy increases, abrasion may produce a more dispersing or widening effect on the particle size distribution. This is consistent with the results obtained by [5] and we will come back to this assumption more in detail later.

Another interesting result found across many cases, specially at higher velocity flows, is that if we only look at the smallest particles in the distribution, the number of collisions or intersection decreases with size, but if we look at the whole size range, it tends to increase (Fig. 10) so the number of collisions has a minima at intermediate particle sizes. This indicates that at larger flow rates small particles predominantly collide with large particles (this can be better observed in Fig. 11, where at higher velocities, small particles tend to collide with larger ones). This means that either the small or the big particles cannot follow the stream lines and thus collide with each other. This might be due to the particles' inertia being too large for them to follow the stream lines. We will later investigate the effect of this on the theoretical kernel models that can be used for different flow regimes. The large velocity difference with the big particles ensures large collision forces also for the small particles.

3.4 Collision Kernels

One of the main results obtained from the simulations are the collisions kernels for different flow conditions and particle size distributions. Two examples are shown in Fig. 11. A collision kernel quantifies the rate at which two particles collide as a function of their size, fluid properties and environmental factors. They are useful for modeling processes involving the interaction between particles, such as abrasion and coagulation, and serve as a basis for understanding abrasion in fluid environments. With the data we obtained, we created the collision kernels for every case.

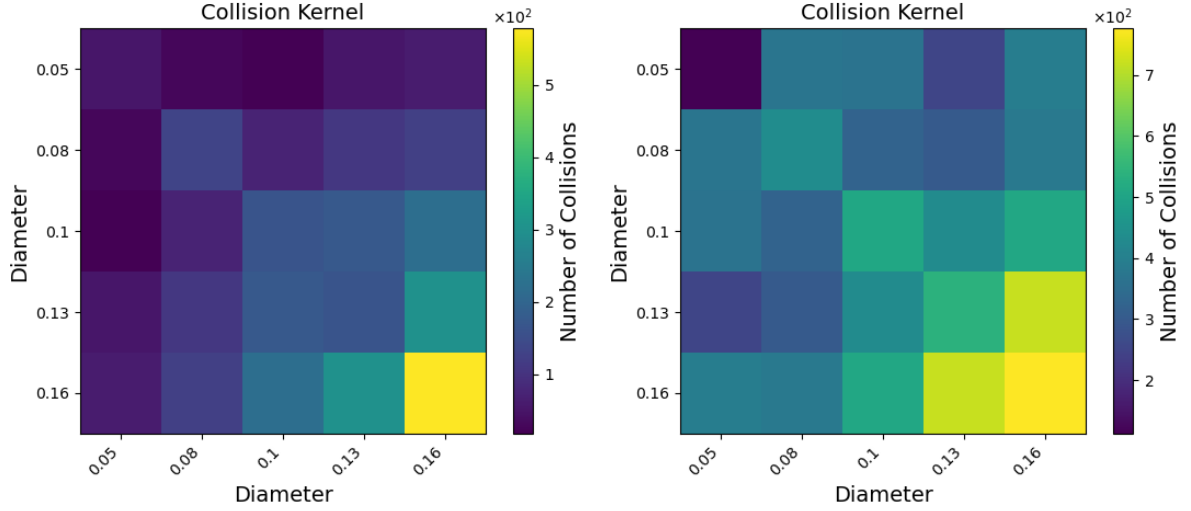


Figure 11: Collision kernel. Left: $U = 100$, Right $U = 500$ for five different particle sizes and size ratio of 3.

We find very similar results as in the previous sections. The total number of collisions increase with flow velocity and this effect is more pronounced for smaller and medium sized particles. In the following section we will analyze how these measured kernels relate to theoretical kernels.

3.5 Kernel Models

There are many theoretical particle collision models developed during the last century[4]. In particular they describe the frequency of interactions for two particles as a function of their sizes. We assess the validity of some of the models presented in [4] for a shear flow by fitting these functions to our collision kernels and calculating the coefficient of determination, r^2 , value for each fit. The r^2 indicates how well the model fits the data, with a value of 1 representing a perfect fit and values closer to 0 indicating an inadequate fit.

Orthokinetic collisions are those determined by a velocity gradient in the flow. Particles are considered to be following streamlines and their collisions are due to being in different positions with respect to the shear direction. Perikinetic collisions are due to the random motion of particles. We define the following kernel functions:

- **Product Kernel:**

$$K_{\text{prod}}(r_i, r_j) = a \cdot r_i \cdot r_j$$

- **Compound Kernel:**

$$K_{\text{compound}}(r_i, r_j) = a \cdot \frac{r_i \cdot r_j}{r_i + r_j}$$

- **Smoluchowski Orthokinetic Kernel:**

$$K_{\text{Smoluchowski ortho}}(r_i, r_j, \dot{\gamma}) = a \cdot \dot{\gamma} \cdot (r_i + r_j)^3$$

- **Smoluchowski Perikinetic Kernel:**

$$K_{\text{Smoluchowski peri}}(r_i, r_j) = a \cdot (r_i + r_j) \cdot \left(\frac{1}{r_i} + \frac{1}{r_j} \right)$$

- **Orthokinetic plus Perikinetic Kernel:**

$$K_{\text{peri plus ortho}}(r_i, r_j) = a \cdot (r_i + r_j) \cdot \left(\frac{1}{r_i} + \frac{1}{r_j} \right) + b \cdot \dot{\gamma} \cdot (r_i + r_j)^3$$

Smoluchowski Orthokinetic Kernel:

$$K_{\text{ortho}}(r_i, r_j, \dot{\gamma}) = a \cdot \dot{\gamma} \cdot (r_i + r_j)^3$$

Smoluchowski Perikinetic Kernel:

$$K_{\text{peri}}(r_i, r_j) = a \cdot (r_i + r_j) \cdot \left(\frac{1}{r_i} + \frac{1}{r_j} \right)$$

Orthokinetic plus Perikinetic Kernel:

$$K_{\text{ortho + peri}}(r_i, r_j) = a \cdot (r_i + r_j) \cdot \left(\frac{1}{r_i} + \frac{1}{r_j} \right) + b \cdot \dot{\gamma} \cdot (r_i + r_j)^3$$

where

- r_i, r_j : Radius of particles i and j , respectively
- a, b : Fitting parameters
- $\dot{\gamma}$: Shear rate, controlling the velocity gradient that drives orthokinetic collisions.

We obtained the great results using the Smoluchowski orthokinetic kernel, where the fits had a mean r^2 of 0.7 and a maximum of 0.92, with the best fits corresponding to a diameter ratio between the biggest and smallest particle of 2 and a medium fluid speed (500). The product and compound kernel were worse than the orthokinetic kernel, with a mean value of r^2 of approximately 0.6 and 0.45 respectively. The perikinetic kernel yielded the worst results, with mostly negative r^2 values that represent a completely inaccurate fit, which was expected as it is meant to be used for cases where particles follow a brownian motion. It was useful as a comparison and to corroborate the consistency our work so far.

Finally, we fitted using a sum of the orthokinetic and perikinetic (Fig. 12) kernel and obtained the best results, where the fits had a mean r^2 of 0.8 and a maximum of 0.92. In this case, the goodness of fit did not strongly depend on the size ratio between the particles but increases a little with the fluid speed as shown in Fig. 12. At higher velocities, the perikinetic component of the kernel improves the modeling of the system. This strengthens our conclusion that at low fluid speeds collisions are due to the velocity gradient but at higher speeds particles can leave the stream lines and their motion becomes more random.

In the following section we will analyze the effect of some of these kernels on the evolution of particle size distributions, in a more general setting. We will model collective abrasion, considering that for a large number of particles, the collision kernel determines the evolution of the size distribution.

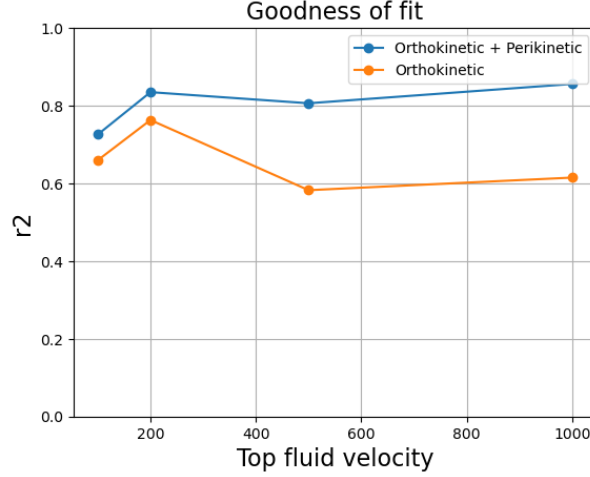


Figure 12: r^2 scores of the kernel fits for different flow speeds and averaging over the size ratios.

3.6 Collective abrasion

We study two main collision regimes representative of different flows, the orthokinetic and the perikinetic. This will provide us with valuable insights on the effect of abrasion in different environments. For simplicity we do not simulate the sum kernel with the fitted parameters as we were interested in basic effect of the changing particle behavior.

If the mass loss is small we can write the time evolution of the radii in the following form [5]:

$$\begin{aligned}\frac{dr_i}{dt} &= -K(r_i, r_j) \\ \frac{dr_j}{dt} &= -K(r_i, r_j)\end{aligned}\tag{5}$$

where

- r_i, r_j : radius of particles i and j , respectively
- K : collision kernel

We solve the equations in a discretized way by creating 200 particles with an initial uniform distribution $r \in [0.9, 1.1]$ and numerically integrating Eq. (5) to obtain the time evolution of the distribution. An ensemble average was done by repeating this process (always using the same initial conditions) and averaging over the resulting distribution. It is worth noting that integrating over time is, in this case, equivalent to doing it over the collisions that these particles experience. The results, illustrated in Fig. 13, demonstrate the contrasting effects of these two regimes.

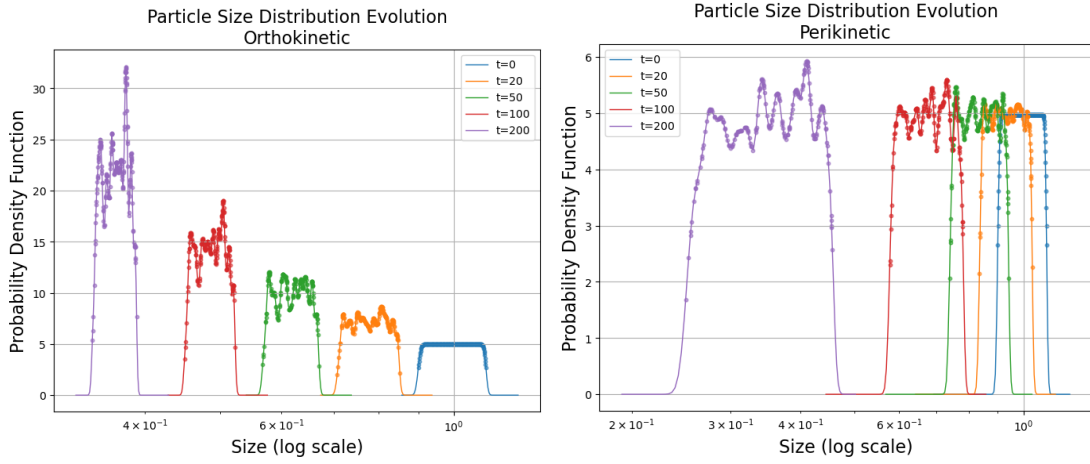


Figure 13: Particle size distribution evolution. Left: Orthokinetic, Right: Perikinetic. Both have the same initial size distribution.

These two kernels have opposite effects of the dispersion of the distribution. It is clear that the two collision regimes give rise to different dynamics and distinct particle size distributions. Orthokinetic kernels, have a focusing effect on the size distribution, while perikinetic kernels have a dispersing effect. Quantitatively, this can be measured by the relative variance evolution, which is a standardized measure of dispersion, as shown in Fig. 14.

As we can see the orthokinetic kernel produces a decreasing relative variance as expected in case of slow flows. It is worth restating that slow flows are better modelled by the orthokinetic kernels as seen in Section 3.5. The perikinetic kernel produces the opposite effect. Our conjecture is that places with turbulent flows (e.g. see shores with heavy wave activity) should exhibit wider particle size distributions than places with relatively steady flows (e.g. streams and rivers). This assumption may be tested by field experiments.

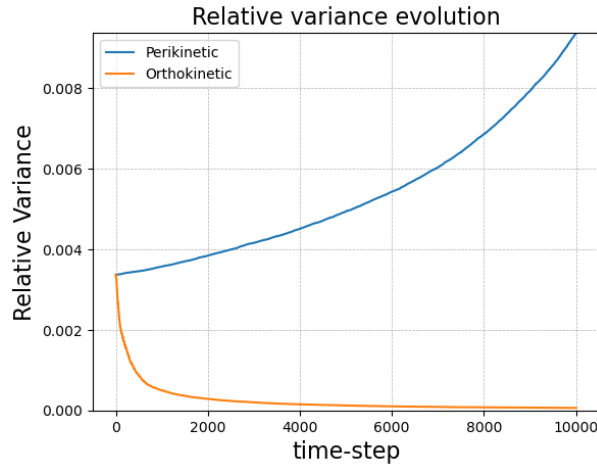


Figure 14: Relative variance evolution under Orthokinetic and Perikinetic regimes.

One limitation of these models is that the perikinetic kernel predicts a finite lifetime for particles (Fig. 15), while field observations, represented in Sternberg's law predict an exponential decay. Particle size evolution under the orthokinetic kernel predicts an infinite lifetime (Fig. 15), however, not an exponential decay. It resembles a power law decay, and if we fit it to our data, the obtained r^2 is 0.87. This is true for the uniform initial distribution as well as the normal initial distribution.

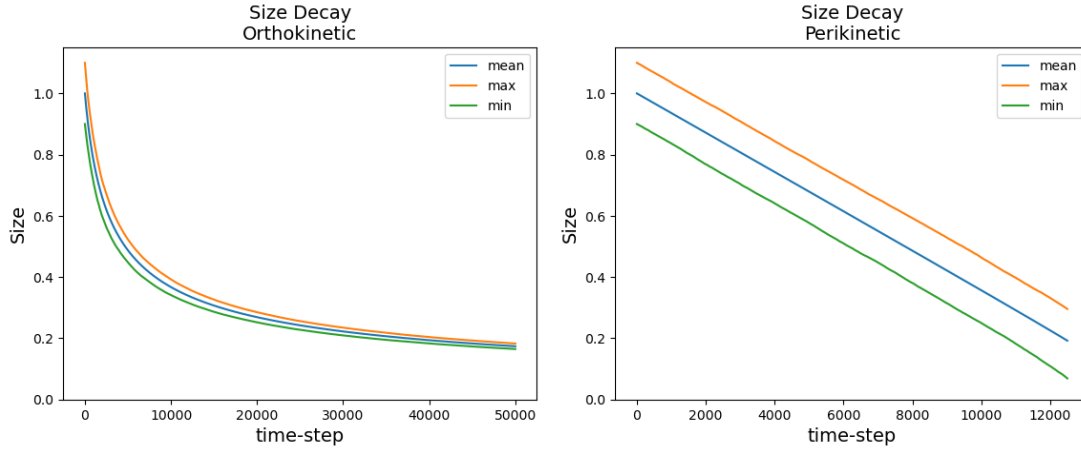


Figure 15: Particle size evolution for different collision kernels.

4 Conclusions and Discussion

In this study, we explored the dynamics of particle-fluid systems in a shear flow environment using CFD-DEM techniques. We calibrated the simulations against a dataset of empirical data and were able to reproduce phenomena like drifting–kissing–tumbling. We expressed particle interactions in terms collisions kernels and used some of the existing theoretical kernels available to fit the data collected. The strong r^2 values for the orthokinetic model support that particles predominantly collide due to the shear flow in orthokinetic interactions. We also found that at larger fluid velocities, the combination of the perikinetic and orthokinetic kernels provides a good model.

We have studied mutual collisions between particles using the discrete collision model introduced in [5]. We showed that orthokinetic collisions have a focusing effect, while the perikinetic collisions have a dispersing effect on the distribution. These simulations led us to our most important conclusions from our simulations, namely that slow flow rates seem to have focusing while larger ones have a dispersing effect on the particle size distributions.

Despite its strengths this study has many limitations. Many simplifications were done, like using only homogeneous spherical particles, which neglects important factors like shape, which are known to influence these processes. We only focused on laminar shear flows, while other flow patters would yield different interactions and dynamics. Furthermore, this study would have benefited from more computational resources. Future studies should combat these shortcomings by considering more complex particle geometries, flow types and size distributions. The influence of other parameters, such as pebble packing density, turbulence, external forces like gravity or contacts with the streambed should be considered, as they are known to have important effects.

To conclude, this work provides a solid simulation-based approach to the study of pebble collisions and size evolution. The data and insights obtained will hopefully contribute to the understanding of these processes and the validation of theoretical models that describe them.

Appendix

5 Abrasion Model

In this section, we will study the abrasion generated by the collisions measured in our simulations. First, we will consider the mutual abrasion of a binary collisions, and then, using the statistical data obtained from the simulations, analyze the effect on each size group. Finally we will investigate the dynamics of the size distribution.

An important remark is that we do not consider the shape of the pebbles. Pebbles start their lives as rock fragments and initially the abrasion and fragmentation is focused on the edges of pebble, without a significant change in axis size until a convex shape is achieved [16]. Only then, abrasion diminishes the axis dimensions. In the simulations and the abrasion model used, we consider the second stage only. The mass loss experimented by a particle depends on many intrinsic factors, such as its material composition and size. Given the enormous diversity of material properties of different rocks, many different abrasion effects will be observed depending on these properties. It is clear that the different mass loss functions may yield a different collective size dynamics.

We consider the set of functions that describe the mass loss as a function of the normal intersection during the collision and the size of the particle. These functions must be monotone increasing with respect to the intersection. In particular, we will investigate functions of the following form:

$$\text{Mass loss}(\delta, r) = \begin{cases} k_c(\delta - \delta_0)^\alpha r^\beta, & \text{if } \delta > \delta_0, \\ 0, & \text{if } \delta \leq \delta_0. \end{cases}$$

where:

- k_c is a constant related to material properties.
- δ is the overlap between the two particles.
- δ_0 is the threshold intersection value, below which no mass loss occurs.
- r is the size of the particle.
- α, β are two constant parameters.
- k_c is a constant related to material properties.

The parameter α determines how the abrasion depends on the collision overlap and β introduces asymmetry in the abrasion based on particle size. Considering the great diversity of materials found in nature, different mass loss functions can be created, and there probably will be a material that is well described by it. In this study, we assume that all pebbles are made of the same material, meaning that k_c is the same for all pebbles.

In order to continue with our analysis, we must pick some physically sound values for α and β , and to do that, we will take field observations into account. Sternberg's law[3] predicts exponential decay of particle mass, which implies that mass loss must be proportional to the particle's mass². Previously, we showed that there seems to be a linear relationship between

²Sternberg's law holds for the evolution of the volume as function of distance along the stream, but if we assume constant transport speed, they are equivalent.

the sum of the overlap experienced by a particle and their diameter (Fig. 10). Now, a heuristic approximation leads us to consider the mass loss to be proportional to the cube of the collision overlap, which makes it proportional to the particle volume and mass.

This approximation has some objections. To find the linear relationship between particle diameter and overlap, we averaged over all the particles in each size group, while the mass loss function is applied to every collision individually. Because the function is not necessarily linear, it is not the same to consider the each collision separately and then take the average compared to taking the average and then looking at the erosion. Regardless, this is still a useful consideration and we will analyze how sensible it was. Based on this we will use values of α of 2 and 3 and β of 0 and 1 and values of δ_0 of either 0 or 8×10^{-5} , which is a reasonable value that excludes very soft contacts. We apply these functions to each collision recorded and obtain the mass loss for each particle, and subsequently for each size group.

We find that total abraded mass increases with fluid velocity, which is due to there being more total collisions at higher velocities as seen in Sections 3 and 3.3, which is consistent with experimental results [6].

5.1 Abrasion dependency on size

We plotted the erosion as a function of their size for different functions and for all simulated cases. For the sake of simplicity in the visuals, we normalize all to 1. Here we display a representative case:

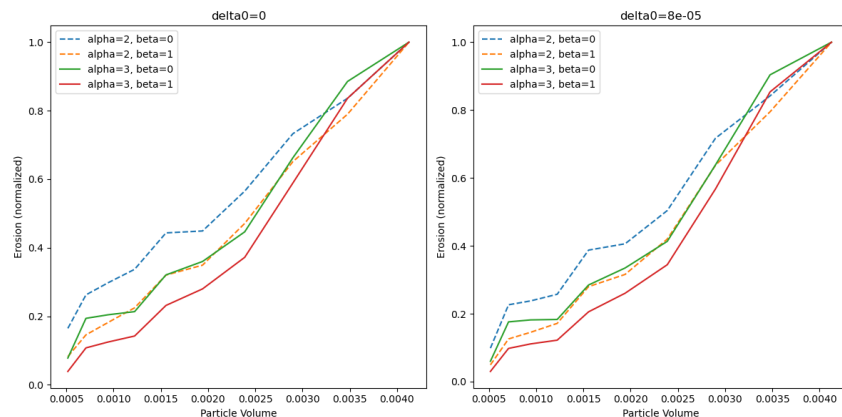


Figure 16: Mass loss as a function of particle volume

There seems to be an approximately linear relationship between particle volume and mass loss, consistent with Sternberg’s law. A surprising feature is the similarity between the shapes of the erosion curves considering the difference in parameters used. The only few exceptions are found in some low velocity cases, where smaller particles experience a much lower erosion. We previously showed that at low velocities, smaller particles collide much less (Fig. 9), which probably explains this difference.

5.2 Effect on size distribution

Following our analysis of the abrasion models, we simulated the effect of abrasion on the particle size distribution. To do this, we applied the mean mass loss per size group, calculated in the

previous section, to each group for a infinitesimally small time interval³. We measured the width of the size distribution, using the relative variance, before and after the abrasion and determined whether abrasion had a focusing or widening effect on the distribution.

We conducted this analysis for various values of α , β and δ_0 , and in practically all of them (98%) that erosion had a narrowing effect in the particle size distribution. This result is consistent with the findings in [5], where the authors show that laminar flows, such as the ones created in this study, and smooth steady conditions cause a focusing of the distribution. It is also consistent with results shown section 3.6, where we found that under orthokinetic interactions, abrasion has a arrowing effect on the distribution. The simulations are well modeled by orthokinetic interactions as shown in section 3.5.

6 Simulation Parameters

DEM

- Gravity, g : 0
- Young's Modulus, E : 5×10^7 Pa
- Poisson's Ratio, ν : 0.45
- Coefficient of Restitution, e : 1
- Coefficient of Friction, μ : 1
- Density, ρ : 1

CFD

- Gravity, g : 0
- Top Velocity, U : variable between 100 and 1000
- Density, ρ : 1
- Kinematic Viscosity, ν : 0.01
- Characteristic Length, L : 0.05 (Based on the diameter of the particles)
- Shear, $\dot{\gamma}$: variable between 100 and 1000
- Reynolds Number, Re : variable between 500 and 5000

$$Re = \frac{UL}{\nu} = U \times 5$$

- Turbulence Properties: Laminar

7 Acknowledgements

I would like to thank my supervisor, Dr. János Török, for his help and support during this work.

³We can only apply it for a small time interval because, after some time, the particle distribution will change due to the abrasion. This will make the interactions between particles different from what it previously, and thus, the our measured data will be less representative of it.

8 Own Results

All of the results presented in this work are mine, except when referring to results obtained by other authors, in which case they are properly referenced. My supervisor helped me to define the research questions and directions as well as suggesting methods or approaches to solve the problems related to this research, while I implemented these solutions myself.

I solved or attempted to solve the following list of scientific questions:

- How pebble collisions in fluid flows can be accurately simulated numerically
- How different existing theoretical models for the collision kernels relate to the simulated systems in a shear flow
- How the system's evolution differs qualitatively and quantitatively in different types of flows as described by different kernels
- How to model the individual mass loss of the simulated particles from the collision data

I applied the following methods:

- CFD and DEM coupled simulations
- Mesh sensitivity analysis
- Discrete simulations and ensemble averaging to solve the differential equations in section 3.6 and model the evolution of the system
- Data analysis and visualization

I obtained the following main results:

- Well-documented phenomena is replicated in CFD-DEM simulations.
- Collisions in shear flows are well described by orthokinetic models.
- At higher fluid velocities, a perikinetic component, in addition to the orthokinetic one, improves the model.
- Orthokinetic regimes have a focusing effect, while the perikinetic regimes have a dispersing effect on the particle size distribution.
- Slow flows have focusing while larger ones have a dispersing effect on the particle size distributions.

References

- [1] Chris Paola, Gary Parker, Rebecca Seal, Sanjiv K Sinha, John B Southard, and Peter R Wilcock. Downstream fining by selective deposition in a laboratory flume. *Science*, 258(5089):1757–1760, 1992.
- [2] Duccio Bertoni, Gabriele Di Renzone, Gabor Domokos, Chiara Favaretto, Alessandro Pozzebon, and Giovanni Sarti. A technique for the measurement of the morphological evolution of marine pebbles. In *2023 IEEE International Workshop on Metrology for the Sea; Learning to Measure Sea Health Parameters (MetroSea)*, pages 433–438. IEEE, 2023.
- [3] Herman Sternberg. Untersuchungen uber langen-und querprofil geschiebefuhrender flusse. *Zeitschrift fur Bauwesen*, 25:483–506, 1875.
- [4] CJ Meyer and DA Deglon. Particle collision modeling—a review. *Minerals Engineering*, 24(8):719–730, 2011.
- [5] András A Sipos, Gábor Domokos, and János Török. Particle size dynamics in abrading pebble populations. *Earth Surface Dynamics*, 9(2):235–251, 2021.
- [6] Mikaël Attal and Jérôme Lavé. Pebble abrasion during fluvial transport: Experimental results and implications for the evolution of the sediment load along rivers. *Journal of Geophysical Research: Earth Surface*, 114(F4), 2009.
- [7] Christoph Kloss, Christoph Goniva, Alice Hager, Stefan Amberger, and Stefan Pirker. Models, algorithms and validation for opensource dem and cfd-dem. *Progress in Computational Fluid Dynamics, an International Journal*, 12(2-3):140–152, 2012.
- [8] units command - LIGGGHTS v3.X documentation — cfdem.com. <https://www.cfdem.com/media/DEM/docu/units.html>. [Accessed 31-10-2024].
- [9] Zekun Wang and Moubin Liu. On the determination of grid size/smoothing distance in un-/semi-resolved cfd-dem simulation of particulate flows. *Powder Technology*, 394:73–82, 2021.
- [10] Heinrich Hertz. Ueber die berührung fester elastischer körper. 1882.
- [11] S Enayatpour, R Khaledialidusti, and TW Patzek. Assessment of thermal fracturing in tight hydrocarbon formation using dem. In *ARMA US Rock Mechanics/Geomechanics Symposium*, pages ARMA–2014. ARMA, 2014.
- [12] Francesco Balduzzi, Alessandro Bianchini, Giovanni Ferrara, and Lorenzo Ferrari. Dimensionless numbers for the assessment of mesh and timestep requirements in cfd simulations of darrieus wind turbines. *Energy*, 97:246–261, 2016.
- [13] Luca Brandt and Filippo Coletti. Particle-laden turbulence: progress and perspectives. *Annual Review of Fluid Mechanics*, 54(1):159–189, 2022.
- [14] Lisa Prahl, A Hölzer, Dragana Arlov, Johan Revstedt, M Sommerfeld, and Laszlo Fuchs. On the interaction between two fixed spherical particles. *International journal of multiphase flow*, 33(7):707–725, 2007.

- [15] James W Evans. Random and cooperative sequential adsorption. *Reviews of modern physics*, 65(4):1281, 1993.
- [16] Gabor Domokos, Douglas J Jerolmack, Andras Á Sipos, and Ákos Török. How river rocks round: resolving the shape-size paradox. *PloS one*, 9(2):e88657, 2014.